



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:17 PM EDT

PDB ID : 2D2C / pdb_00002d2c
Title : Crystal Structure Of Cytochrome B6F Complex with DBMIB From M. Laminosus
Authors : Yan, J.; Kurisu, G.; Cramer, W.A.
Deposited on : 2005-09-07
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

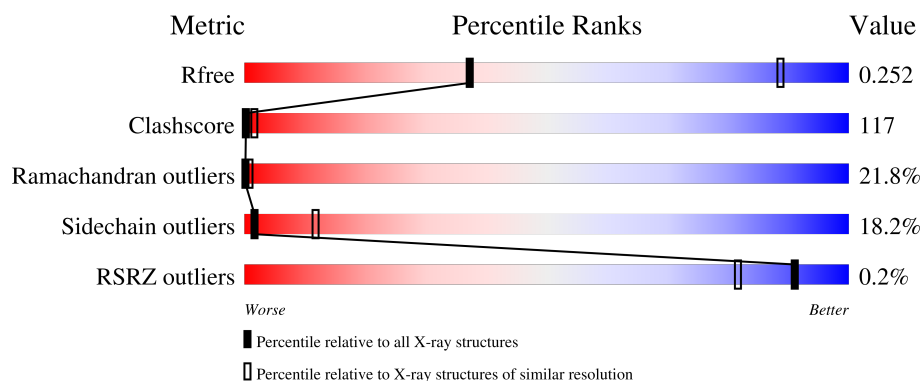
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



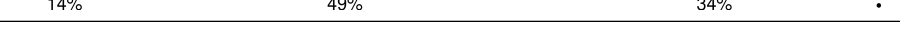
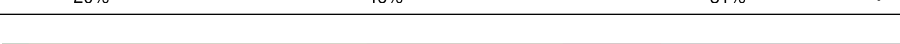
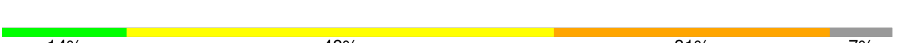
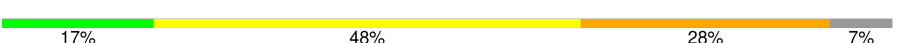
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	6% 53% 30% 5% 6%
1	N	215	9% 49% 28% 7% 6%
2	B	160	9% 41% 26% 9% 14%
2	O	160	• 39% 34% 9% 14%
3	C	289	13% 55% 24% 6% •

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Mol	Chain	Length	Quality of chain
3	P	289	
4	D	179	
4	Q	179	
5	E	32	
5	R	32	
6	F	35	
6	S	35	
7	G	37	
7	T	37	
8	H	29	
8	U	29	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	OPC	B	305	-	-	X	-
11	BNT	B	309	-	-	X	-
11	BNT	O	1309	-	-	X	-
12	CLA	B	201	X	-	-	-
12	CLA	O	1201	X	-	-	-
13	FES	D	201	-	-	X	-
13	FES	Q	201	-	-	X	-
9	HEC	A	301	X	-	-	-
9	HEC	A	302	X	-	-	-
9	HEC	A	303	X	-	-	-
9	HEC	C	301	X	-	-	-
9	HEC	N	301	X	-	-	-
9	HEC	N	302	X	-	-	-
9	HEC	N	303	X	-	-	-
9	HEC	P	301	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 14984 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1593	1062	253	268	10			
1	N	202	Total	C	N	O	S	0	0	0
			1593	1062	253	268	10			

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	137	Total	C	N	O	S	0	0	0
			1067	721	164	177	5			
2	O	137	Total	C	N	O	S	0	0	0
			1067	721	164	177	5			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	286	Total	C	N	O	S	0	0	0
			2200	1406	366	421	7			
3	P	286	Total	C	N	O	S	0	0	0
			2200	1406	366	421	7			

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	168	Total	C	N	O	S	0	0	0
			1280	815	223	235	7			
4	Q	168	Total	C	N	O	S	0	0	0
			1280	815	223	235	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	138	ARG	LYS	conflict	UNP P83794
Q	138	ARG	LYS	conflict	UNP P83794

- Molecule 5 is a protein called Cytochrome b6-f complex subunit VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	32	Total	C	N	O	S	0	0	0
			248	179	34	34	1			
5	R	32	Total	C	N	O	S	0	0	0
			248	179	34	34	1			

- Molecule 6 is a protein called Cytochrome b6-f complex subunit VII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			270	181	39	48	2			
6	S	35	Total	C	N	O	S	0	0	0
			270	181	39	48	2			

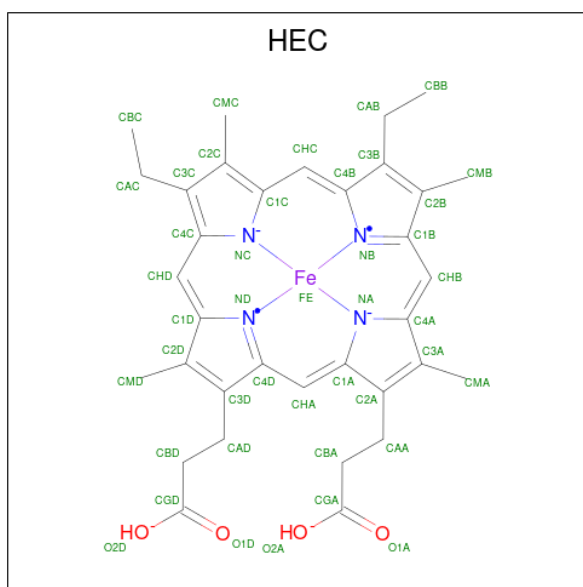
- Molecule 7 is a protein called Cytochrome b6-f complex subunit V.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	27	Total	C	N	O	0	0	0
			216	146	34	36			
7	T	27	Total	C	N	O	0	0	0
			216	146	34	36			

- Molecule 8 is a protein called Cytochrome b6-f complex subunit VIII.

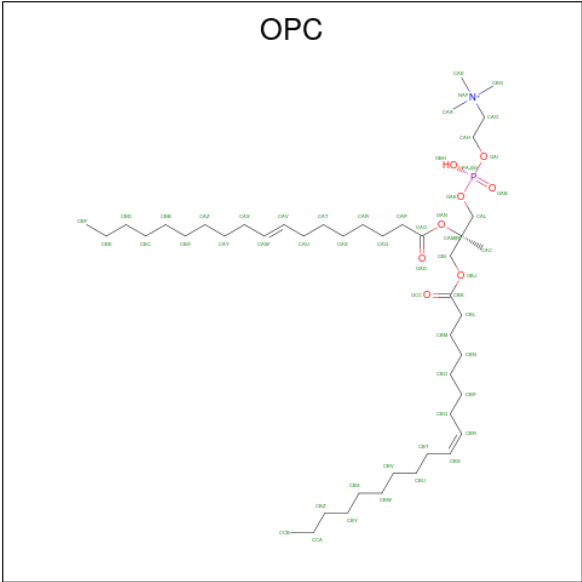
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			
8	U	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			

- Molecule 9 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



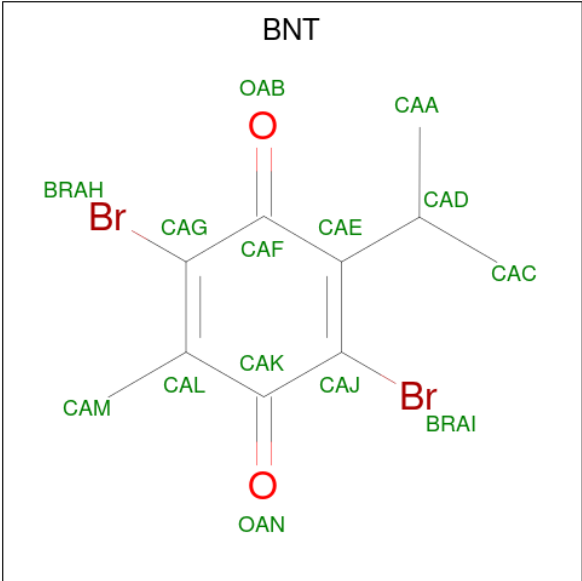
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 10 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (CCD ID: OPC) (formula: C₄₅H₈₇NO₈P).



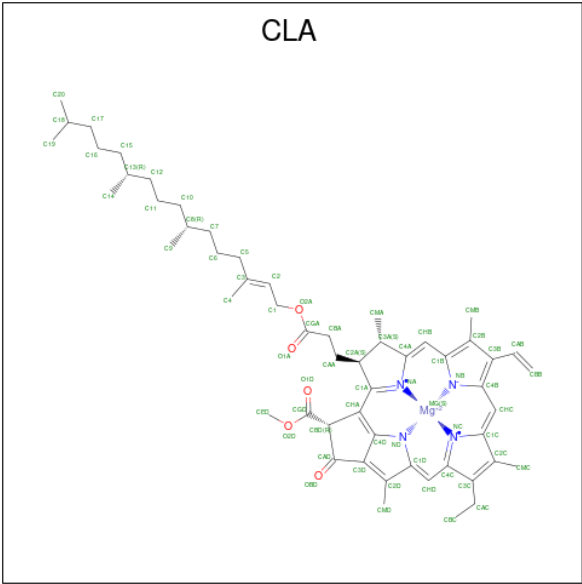
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
10	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
10	N	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
10	O	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 11 is 2,5-DIBROMO-3-ISOPROPYL-6-METHYLBENZO-1,4-QUINONE (CCD ID: BNT) (formula: C₁₀H₁₀Br₂O₂).



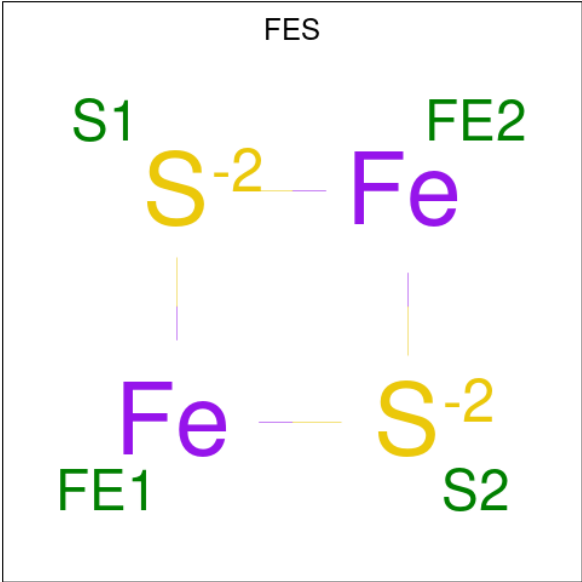
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	Br	C	O	0	0
			14	2	10	2		
11	O	1	Total	Br	C	O	0	0
			14	2	10	2		

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



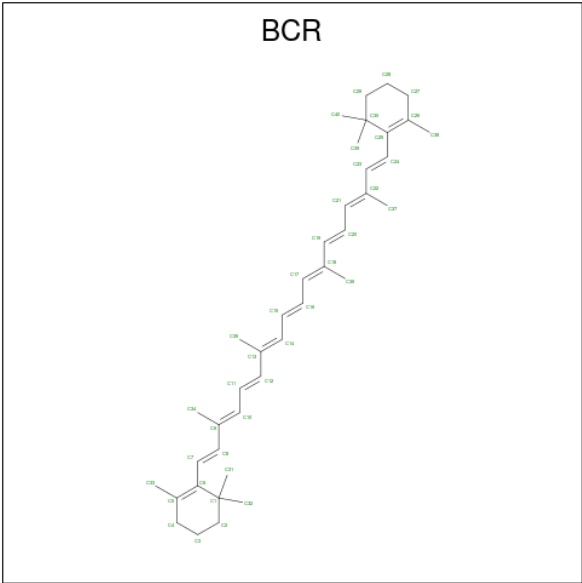
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	D	1	Total	Fe	S	0	0
			4	2	2		
13	Q	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 14 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	E	1	Total	C	0	0
			40	40		
14	R	1	Total	C	0	0
			40	40		

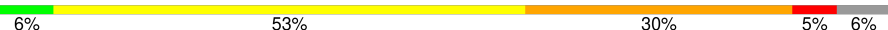
- Molecule 15 is water.

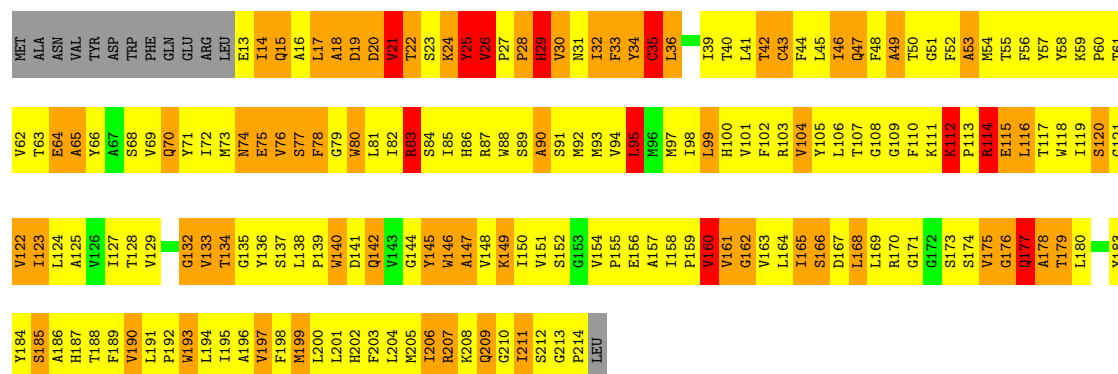
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	O	0	0
			1	1		
15	N	1	Total	O	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

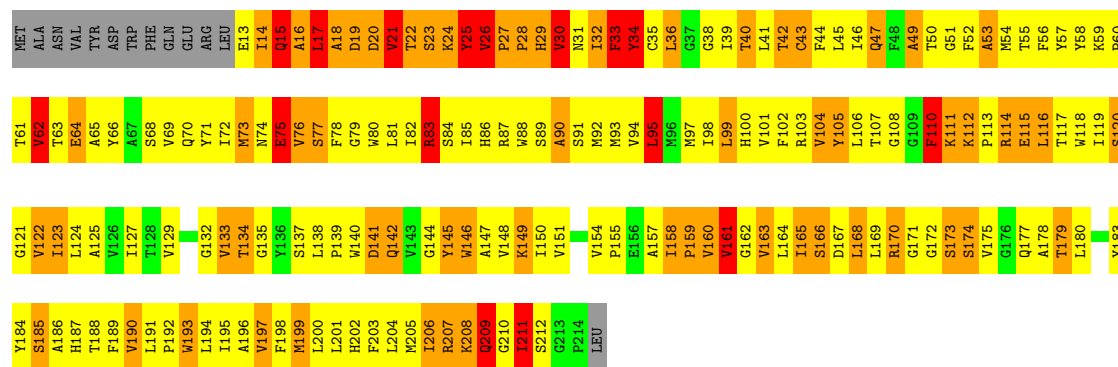
• Molecule 1: Cytochrome b6

Chain A: 



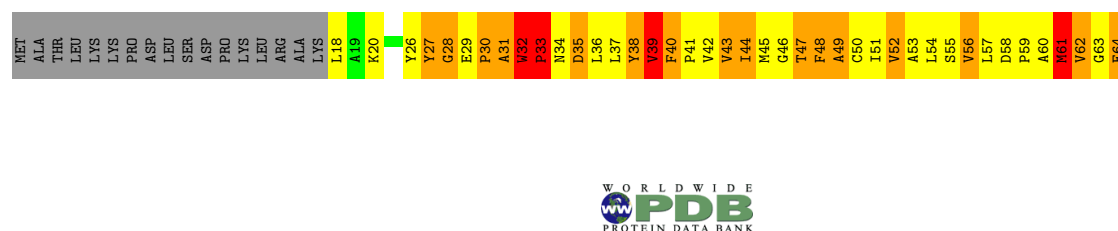
• Molecule 1: Cytochrome b6

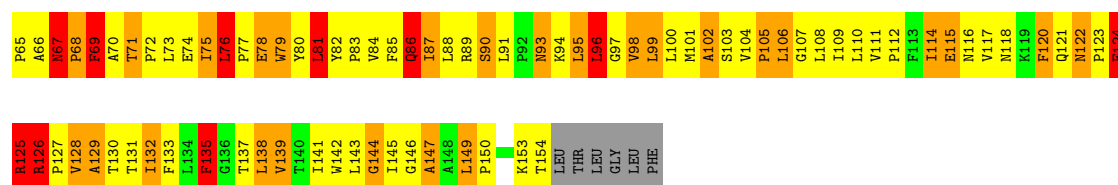
Chain N: 



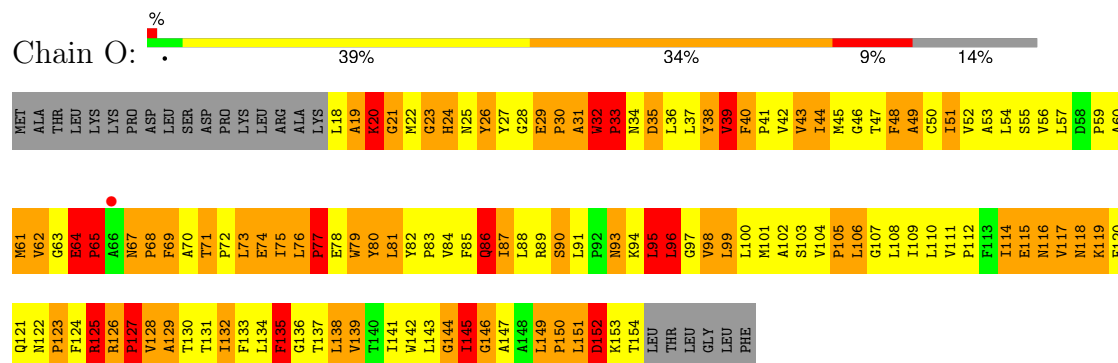
• Molecule 2: Cytochrome b6-f complex subunit 4

Chain B: 

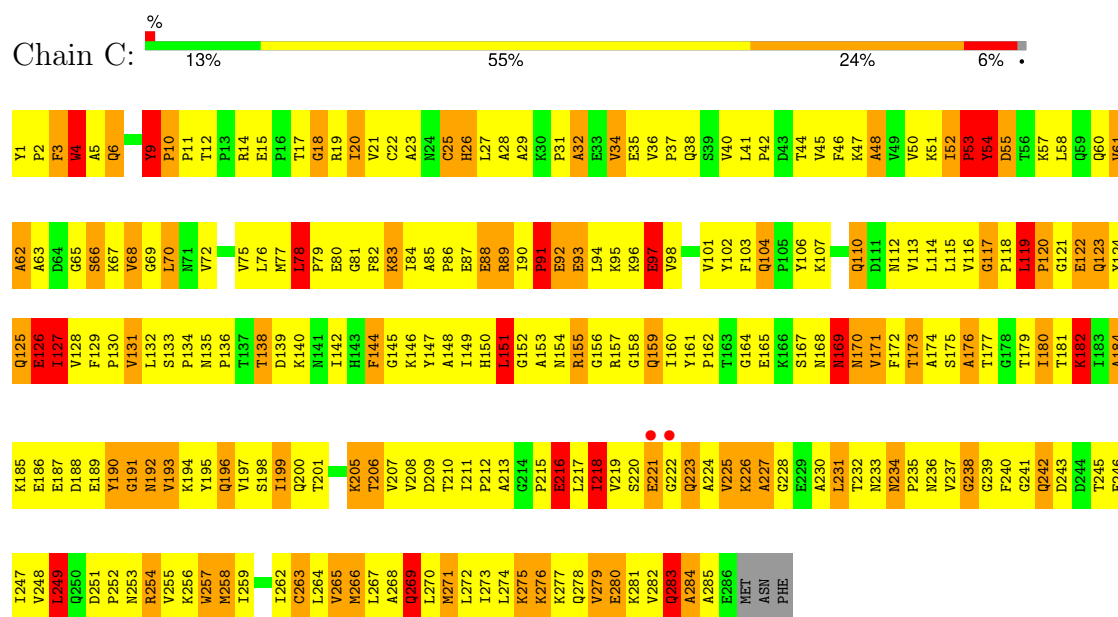




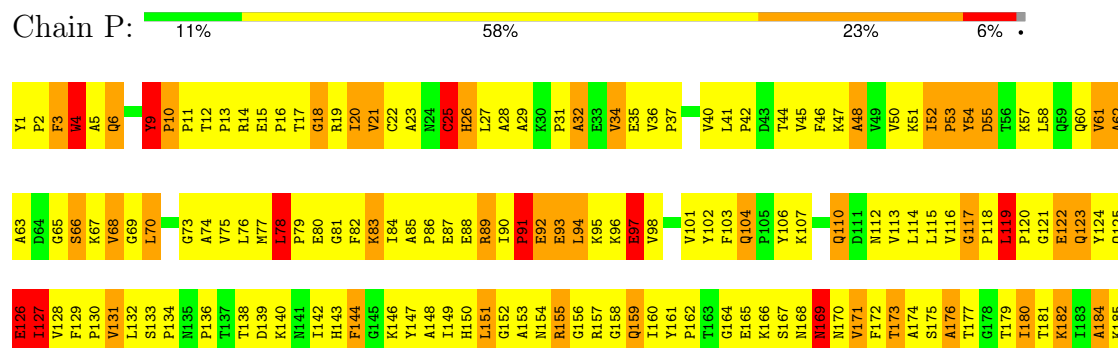
• Molecule 2: Cytochrome b6-f complex subunit 4

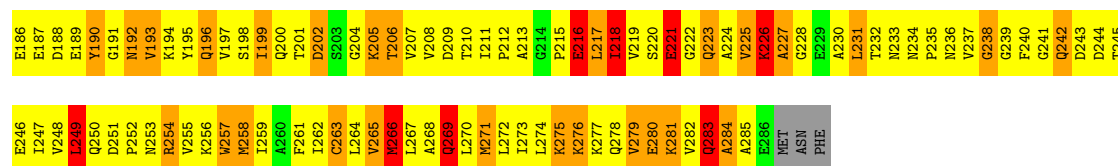


• Molecule 3: Apocytochrome f

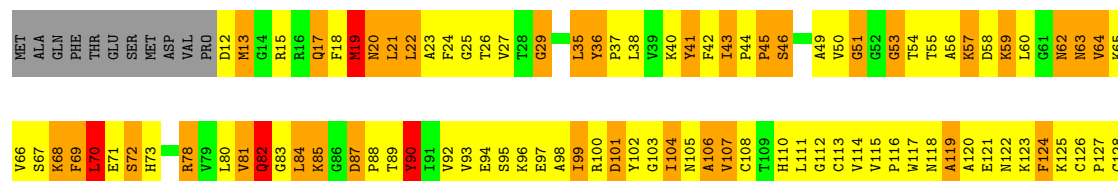
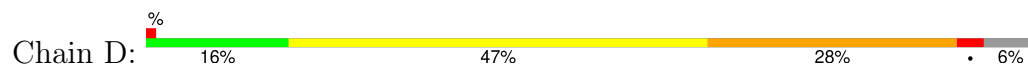


• Molecule 3: Apocytochrome f

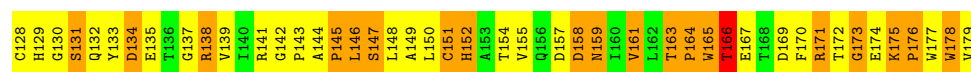
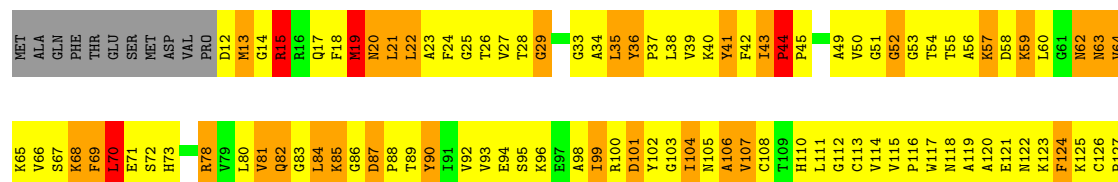
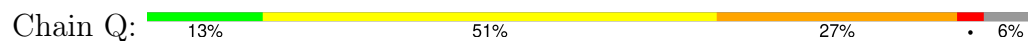




• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



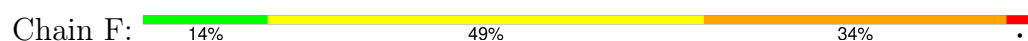
• Molecule 5: Cytochrome b6-f complex subunit VI



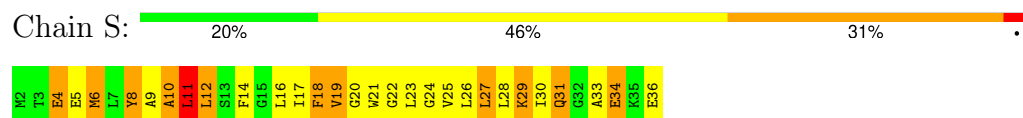
• Molecule 5: Cytochrome b6-f complex subunit VI



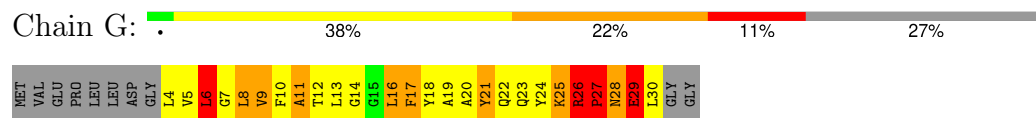
• Molecule 6: Cytochrome b6-f complex subunit VII



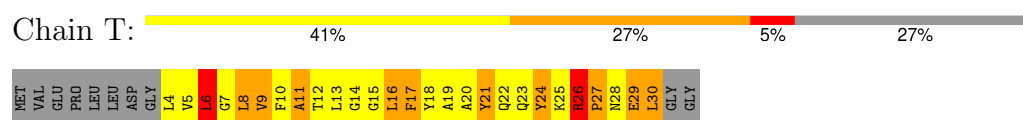
- Molecule 6: Cytochrome b6-f complex subunit VII



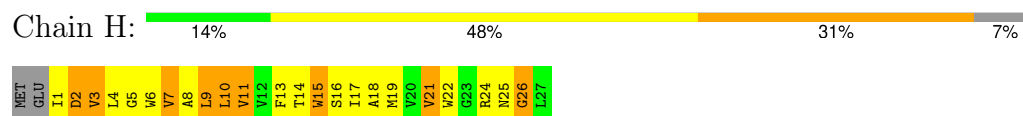
- Molecule 7: Cytochrome b6-f complex subunit V



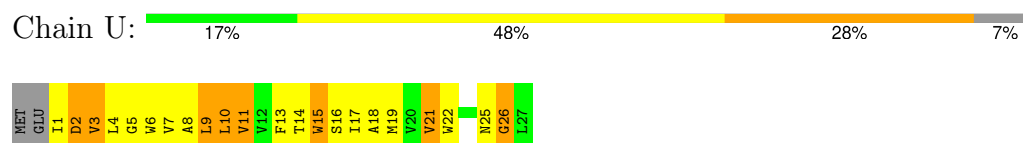
- Molecule 7: Cytochrome b6-f complex subunit V



- Molecule 8: Cytochrome b6-f complex subunit VIII



- Molecule 8: Cytochrome b6-f complex subunit VIII



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	156.59Å 156.59Å 361.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.76 – 3.80 24.76 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.76-3.80) 93.2 (24.76-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.04 (at 3.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.276 , 0.378 0.263 , 0.252	Depositor DCC
R_{free} test set	1490 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	103.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 188.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14984	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, BNT, BCR, OPC, FES, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.76	0/1641	1.23	18/2239 (0.8%)
1	N	0.77	1/1641 (0.1%)	1.18	20/2239 (0.9%)
2	B	0.75	0/1102	1.51	24/1515 (1.6%)
2	O	0.82	0/1102	1.62	27/1515 (1.8%)
3	C	0.67	0/2248	1.22	30/3061 (1.0%)
3	P	0.69	0/2248	1.22	29/3061 (0.9%)
4	D	0.81	0/1312	1.29	19/1786 (1.1%)
4	Q	0.78	0/1312	1.29	21/1786 (1.2%)
5	E	0.83	0/253	1.51	9/340 (2.6%)
5	R	0.83	0/253	1.47	11/340 (3.2%)
6	F	0.74	0/274	1.09	3/366 (0.8%)
6	S	0.78	0/274	1.09	3/366 (0.8%)
7	G	0.80	0/221	1.56	8/299 (2.7%)
7	T	0.88	0/221	1.38	5/299 (1.7%)
8	H	0.71	0/220	1.29	5/301 (1.7%)
8	U	0.72	0/220	1.25	4/301 (1.3%)
All	All	0.75	1/14542 (0.0%)	1.30	236/19814 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	O	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	27	PRO	CA-C	5.85	1.57	1.52

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	126	ARG	CA-C-N	-16.80	98.84	119.84
2	O	126	ARG	C-N-CA	-16.80	98.84	119.84
2	O	40	PHE	N-CA-C	-11.98	96.46	112.75
2	B	40	PHE	N-CA-C	-11.61	96.96	112.75
5	E	16	PHE	N-CA-C	-11.20	99.87	113.19
1	A	25	TYR	N-CA-C	11.13	123.80	110.44
1	A	32	ILE	N-CA-C	11.01	120.32	111.62
2	B	67	ASN	CA-C-N	11.01	133.60	119.84
2	B	67	ASN	C-N-CA	11.01	133.60	119.84
5	R	16	PHE	N-CA-C	-10.65	100.51	113.19
1	A	207	ARG	N-CA-C	-10.62	97.33	110.61
1	A	149	LYS	N-CA-C	-10.48	100.09	113.72
2	O	95	LEU	N-CA-C	-10.28	100.96	113.19
1	N	149	LYS	N-CA-C	-10.08	100.62	113.72
2	B	95	LEU	N-CA-C	-9.99	101.30	113.19
2	B	125	ARG	N-CA-C	-9.97	99.96	111.03
1	A	114	ARG	N-CA-C	-9.72	102.04	112.93
4	D	43	ILE	CA-C-N	9.45	130.11	120.38
4	D	43	ILE	C-N-CA	9.45	130.11	120.38
2	O	119	LYS	N-CA-C	9.39	117.77	108.75
1	N	161	VAL	N-CA-C	-9.35	100.84	113.00
3	C	78	LEU	N-CA-C	-9.32	99.41	110.13
2	B	126	ARG	CA-C-N	9.28	130.24	119.47
2	B	126	ARG	C-N-CA	9.28	130.24	119.47
4	Q	163	THR	CA-C-N	9.13	131.25	119.84
4	Q	163	THR	C-N-CA	9.13	131.25	119.84
2	O	38	TYR	N-CA-C	-9.12	99.50	110.44
2	B	38	TYR	N-CA-C	-9.08	99.55	110.44
4	Q	22	LEU	N-CA-C	-9.04	102.76	113.88
2	B	138	LEU	N-CA-C	-9.03	102.40	113.50
3	P	78	LEU	N-CA-C	-8.99	99.79	110.13
4	D	163	THR	CA-C-N	8.96	131.04	119.84
4	D	163	THR	C-N-CA	8.96	131.04	119.84
1	A	162	GLY	N-CA-C	-8.81	100.65	113.86
1	N	27	PRO	N-CA-C	8.76	121.38	110.70
4	D	22	LEU	N-CA-C	-8.64	103.25	113.88
2	B	31	ALA	N-CA-C	8.64	120.04	108.38
2	O	138	LEU	N-CA-C	-8.62	102.89	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	95	SER	N-CA-C	-8.54	102.78	113.02
3	P	265	VAL	N-CA-C	-8.53	102.02	110.30
5	E	8	TYR	N-CA-C	-8.48	102.83	113.01
3	P	52	ILE	CA-C-N	8.46	130.41	119.84
3	P	52	ILE	C-N-CA	8.46	130.41	119.84
3	P	159	GLN	N-CA-C	-8.44	103.16	113.97
3	C	159	GLN	N-CA-C	-8.33	103.56	114.31
8	H	7	VAL	N-CA-C	-8.30	101.60	110.23
7	G	26	ARG	CA-C-N	8.30	130.21	119.84
7	G	26	ARG	C-N-CA	8.30	130.21	119.84
4	Q	36	TYR	N-CA-C	-8.28	101.94	113.45
3	C	138	THR	N-CA-C	-8.21	102.72	112.89
1	A	18	ALA	N-CA-C	-8.19	100.33	110.65
5	R	8	TYR	N-CA-C	-8.17	103.20	113.01
4	Q	44	PRO	N-CA-C	8.16	120.65	110.70
5	E	12	ILE	N-CA-C	-8.11	102.46	113.00
3	P	138	THR	N-CA-C	-8.01	102.96	112.89
1	A	14	ILE	N-CA-C	-8.00	105.69	113.53
2	O	29	GLU	CA-C-N	7.92	129.74	119.84
2	O	29	GLU	C-N-CA	7.92	129.74	119.84
2	B	144	GLY	N-CA-C	-7.86	94.56	113.18
3	C	52	ILE	CA-C-N	7.86	129.66	119.84
3	C	52	ILE	C-N-CA	7.86	129.66	119.84
4	D	36	TYR	N-CA-C	-7.76	102.67	113.45
5	R	12	ILE	N-CA-C	-7.75	102.92	113.00
4	Q	95	SER	N-CA-C	-7.74	103.73	113.02
7	T	26	ARG	CA-C-N	7.66	129.42	119.84
7	T	26	ARG	C-N-CA	7.66	129.42	119.84
5	E	29	ILE	N-CA-C	-7.54	103.19	112.76
2	B	124	PHE	N-CA-C	-7.51	103.07	112.90
3	P	10	PRO	N-CA-C	7.51	119.86	110.70
2	B	129	ALA	N-CA-C	-7.49	102.97	112.93
3	P	283	GLN	N-CA-C	-7.47	102.82	112.23
3	C	10	PRO	N-CA-C	7.42	119.76	110.70
4	Q	104	ILE	N-CA-C	7.42	119.67	109.80
8	H	26	GLY	N-CA-C	-7.34	103.92	112.73
1	A	142	GLN	N-CA-C	-7.30	103.34	112.90
3	C	265	VAL	N-CA-C	-7.27	103.25	110.30
3	C	174	ALA	N-CA-C	7.23	116.81	108.49
4	D	104	ILE	N-CA-C	7.20	119.38	109.80
2	B	69	PHE	N-CA-C	7.20	126.13	110.80
8	U	15	TRP	N-CA-C	-7.17	103.46	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	26	GLY	N-CA-C	-7.16	104.14	112.73
4	Q	43	ILE	CA-C-N	7.14	127.73	120.38
4	Q	43	ILE	C-N-CA	7.14	127.73	120.38
3	C	117	GLY	CA-C-N	7.12	128.74	119.84
3	C	117	GLY	C-N-CA	7.12	128.74	119.84
1	N	120	SER	N-CA-C	-7.12	102.57	111.11
3	P	182	LYS	N-CA-C	7.09	117.34	108.19
2	O	64	GLU	CA-C-N	7.09	128.70	119.84
2	O	64	GLU	C-N-CA	7.09	128.70	119.84
5	R	29	ILE	N-CA-C	-6.99	103.91	113.00
3	C	283	GLN	N-CA-C	-6.98	103.44	112.23
2	O	116	ASN	N-CA-C	6.97	121.49	107.41
2	O	145	ILE	N-CA-C	6.97	117.68	107.37
3	P	117	GLY	CA-C-N	6.94	128.52	119.84
3	P	117	GLY	C-N-CA	6.94	128.52	119.84
7	T	8	LEU	N-CA-C	-6.93	105.24	113.21
2	B	32	TRP	CA-C-N	6.91	128.48	119.84
2	B	32	TRP	C-N-CA	6.91	128.48	119.84
1	N	110	PHE	N-CA-C	-6.87	103.80	111.28
6	S	31	GLN	N-CA-C	6.86	121.63	112.30
2	B	28	GLY	N-CA-C	6.84	122.39	112.55
2	O	96	LEU	N-CA-C	-6.84	103.75	111.07
3	P	174	ALA	N-CA-C	6.83	116.34	108.49
2	O	144	GLY	N-CA-C	-6.81	97.05	113.18
7	G	8	LEU	N-CA-C	-6.77	105.42	113.21
7	G	25	LYS	N-CA-C	-6.77	98.63	109.39
8	H	15	TRP	N-CA-C	-6.76	103.91	111.28
1	N	209	GLN	N-CA-C	6.75	125.18	110.80
1	A	32	ILE	CB-CA-C	-6.70	105.08	111.05
1	A	209	GLN	N-CA-C	6.70	116.83	108.19
3	P	284	ALA	N-CA-C	-6.70	104.09	113.20
4	D	53	GLY	N-CA-C	-6.68	100.80	114.16
4	Q	101	ASP	N-CA-C	6.68	121.42	111.81
8	H	14	THR	N-CA-C	-6.67	104.16	112.90
2	O	32	TRP	CA-C-N	6.67	128.18	119.84
2	O	32	TRP	C-N-CA	6.67	128.18	119.84
4	Q	21	LEU	N-CA-C	-6.66	105.12	113.18
3	C	119	LEU	CA-C-N	6.61	128.11	119.84
3	C	119	LEU	C-N-CA	6.61	128.11	119.84
3	P	209	ASP	N-CA-C	6.59	116.75	108.45
6	F	31	GLN	N-CA-C	6.53	121.18	112.30
8	U	14	THR	N-CA-C	-6.53	104.35	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	LEU	N-CA-C	-6.51	104.10	111.07
1	N	142	GLN	N-CA-C	-6.46	104.28	111.71
2	O	129	ALA	N-CA-C	-6.44	103.31	112.13
4	D	21	LEU	N-CA-C	-6.42	105.43	113.20
4	D	68	LYS	N-CA-C	-6.41	105.29	113.23
1	N	199	MET	N-CA-C	-6.40	104.38	111.36
3	C	182	LYS	N-CA-C	6.39	116.43	108.19
1	N	76	VAL	N-CA-C	6.37	117.94	108.46
1	A	70	GLN	N-CA-C	-6.35	104.41	111.71
8	U	21	VAL	N-CA-C	6.34	117.84	110.62
7	T	6	LEU	N-CA-C	-6.33	104.25	112.23
6	S	34	GLU	N-CA-C	6.32	118.38	108.96
7	G	27	PRO	N-CA-C	6.31	125.47	112.47
7	G	29	GLU	N-CA-C	6.30	117.95	111.14
4	Q	13	MET	N-CA-C	6.30	118.69	110.43
3	C	12	THR	CA-C-N	6.29	126.00	119.64
3	C	12	THR	C-N-CA	6.29	126.00	119.64
1	A	199	MET	N-CA-C	-6.29	104.51	111.36
1	N	30	VAL	N-CA-C	6.23	122.31	109.34
2	O	74	GLU	N-CA-C	6.21	120.85	113.28
4	Q	68	LYS	N-CA-C	-6.19	105.55	113.23
4	D	62	ASN	N-CA-C	6.18	119.72	109.46
3	C	209	ASP	N-CA-C	6.18	116.23	108.45
3	C	284	ALA	N-CA-C	-6.17	104.81	113.20
3	P	47	LYS	N-CA-C	6.16	117.98	110.41
2	O	31	ALA	N-CA-C	6.10	120.44	108.18
7	T	24	TYR	N-CA-C	-6.09	105.97	113.41
1	N	115	GLU	N-CA-C	-6.08	105.16	113.30
4	Q	169	ASP	N-CA-C	6.02	118.36	109.69
2	B	70	ALA	N-CA-C	6.00	119.25	109.59
3	P	119	LEU	CA-C-N	6.00	127.34	119.84
3	P	119	LEU	C-N-CA	6.00	127.34	119.84
2	O	21	GLY	N-CA-C	5.98	127.35	113.18
4	D	101	ASP	N-CA-C	5.96	120.39	111.81
1	N	70	GLN	N-CA-C	-5.94	104.88	111.71
5	R	26	ILE	N-CA-C	-5.93	108.07	113.71
7	G	6	LEU	N-CA-C	-5.93	104.76	112.23
1	N	26	VAL	N-CA-C	5.91	121.64	108.88
3	C	47	LYS	N-CA-C	5.91	117.67	110.41
2	B	139	VAL	N-CA-C	-5.90	105.09	110.82
4	Q	78	ARG	N-CA-C	5.90	119.56	107.69
2	O	150	PRO	N-CA-C	-5.89	100.33	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	21	VAL	N-CA-C	5.86	117.30	110.62
6	S	18	PHE	N-CA-C	-5.86	104.25	111.40
4	D	13	MET	N-CA-C	5.86	118.27	110.53
5	R	27	LYS	N-CA-C	-5.86	105.72	112.92
1	A	21	VAL	N-CA-C	5.82	121.44	109.34
3	P	126	GLU	N-CA-C	-5.78	106.77	113.88
3	C	249	LEU	N-CA-C	-5.76	100.31	109.76
3	C	126	GLU	N-CA-C	-5.76	106.80	113.88
2	O	139	VAL	N-CA-C	-5.75	105.24	110.82
3	P	166	LYS	N-CA-C	5.70	118.33	110.35
4	D	78	ARG	N-CA-C	5.68	119.11	107.69
4	D	169	ASP	N-CA-C	5.68	117.86	109.69
2	O	119	LYS	CB-CA-C	-5.65	108.23	116.53
5	R	22	ILE	N-CA-C	5.65	121.08	109.34
1	N	19	ASP	N-CA-C	-5.60	106.30	113.02
5	R	14	LEU	N-CA-C	5.57	117.03	111.07
3	P	222	GLY	N-CA-C	-5.57	108.05	115.40
3	P	250	GLN	N-CA-C	5.56	117.46	108.34
3	C	234	ASN	CA-C-N	5.56	126.78	119.84
3	C	234	ASN	C-N-CA	5.56	126.78	119.84
4	Q	49	ALA	N-CA-C	-5.55	106.35	113.01
4	Q	62	ASN	N-CA-C	5.52	118.63	109.46
3	P	249	LEU	N-CA-C	-5.50	100.73	109.59
7	G	26	ARG	N-CA-C	5.49	121.95	109.81
3	P	9	TYR	CA-C-N	5.48	126.03	120.38
3	P	9	TYR	C-N-CA	5.48	126.03	120.38
5	E	26	ILE	N-CA-C	-5.47	108.51	113.71
5	E	27	LYS	N-CA-C	-5.46	106.20	112.92
3	P	12	THR	CA-C-N	5.46	126.66	119.84
3	P	12	THR	C-N-CA	5.46	126.66	119.84
5	R	13	ALA	N-CA-C	-5.42	105.93	112.54
3	P	281	LYS	N-CA-C	-5.41	105.90	113.37
3	C	72	VAL	N-CA-C	5.39	115.66	108.11
1	N	33	PHE	N-CA-C	5.36	122.22	110.80
5	E	22	ILE	N-CA-C	5.36	120.48	109.34
3	C	222	GLY	N-CA-C	-5.35	108.34	115.40
4	Q	19	MET	N-CA-C	5.32	122.12	110.80
2	B	102	ALA	N-CA-C	-5.30	106.89	113.19
1	N	146	TRP	N-CA-C	5.29	120.09	111.37
5	E	11	PHE	N-CA-C	-5.27	99.57	110.80
2	O	67	ASN	N-CA-C	5.26	118.26	110.32
1	N	95	LEU	N-CA-C	-5.25	103.52	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	19	MET	N-CA-C	5.24	121.97	110.80
5	E	30	LYS	N-CA-C	5.23	116.43	107.28
6	F	18	PHE	N-CA-C	-5.22	104.52	112.04
3	C	9	TYR	CA-C-N	5.22	125.75	120.38
3	C	9	TYR	C-N-CA	5.22	125.75	120.38
2	O	33	PRO	N-CA-C	5.17	123.13	112.47
3	P	217	LEU	N-CA-C	5.17	114.86	108.19
4	Q	151	CYS	N-CA-C	5.16	114.84	108.19
5	R	30	LYS	N-CA-C	5.16	116.30	107.28
1	N	40	THR	N-CA-C	-5.15	104.74	111.02
1	A	146	TRP	N-CA-C	5.14	119.85	111.37
6	F	33	ALA	CB-CA-C	-5.14	108.97	116.53
1	A	46	ILE	N-CA-C	-5.14	105.40	111.00
4	Q	175	LYS	CA-C-N	5.14	126.26	119.84
4	Q	175	LYS	C-N-CA	5.14	126.26	119.84
3	C	53	PRO	N-CA-C	5.12	123.01	112.47
4	D	90	TYR	N-CA-C	5.11	118.28	110.20
2	B	61	MET	N-CA-C	5.09	115.76	108.74
3	C	151	LEU	N-CA-C	5.08	117.43	108.75
1	A	120	SER	N-CA-C	-5.07	103.06	111.37
4	D	82	GLN	N-CA-C	-5.07	102.19	110.20
5	R	11	PHE	N-CA-C	-5.05	100.03	110.80
1	N	207	ARG	N-CA-C	-5.05	100.05	110.80
2	B	33	PRO	N-CA-C	5.04	122.86	112.47
3	C	125	GLN	N-CA-C	-5.04	106.82	113.17
2	O	81	LEU	N-CA-C	-5.04	105.86	112.41
3	P	221	GLU	N-CA-C	5.04	118.36	109.80
1	N	22	THR	N-CA-C	5.03	116.72	108.52
1	A	95	LEU	N-CA-C	-5.02	103.88	111.56
2	B	79	TRP	N-CA-C	5.01	121.47	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	TYR	Sidechain
2	O	80	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1593	0	1623	473	0
1	N	1593	0	1623	486	0
2	B	1067	0	1106	369	0
2	O	1067	0	1106	399	0
3	C	2200	0	2216	445	0
3	P	2200	0	2216	496	0
4	D	1280	0	1265	234	0
4	Q	1280	0	1265	230	0
5	E	248	0	284	140	0
5	R	248	0	284	124	0
6	F	270	0	282	96	0
6	S	270	0	282	82	0
7	G	216	0	220	90	0
7	T	216	0	220	103	0
8	H	214	0	224	39	0
8	U	214	0	224	37	0
9	A	129	0	97	17	0
9	C	43	0	31	3	0
9	N	129	0	97	18	0
9	P	43	0	31	4	0
10	B	54	0	83	34	0
10	C	54	0	83	20	0
10	N	54	0	83	14	0
10	O	54	0	83	17	0
11	B	14	0	10	10	0
11	O	14	0	10	12	0
12	B	65	0	70	8	0
12	O	65	0	70	9	0
13	D	4	0	0	3	0
13	Q	4	0	0	2	0
14	E	40	0	56	11	0
14	R	40	0	56	8	0
15	A	1	0	0	1	0
15	N	1	0	0	2	0
All	All	14984	0	15300	3534	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 117.

All (3534) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:TYR:HA	1:A:103:ARG:HH11	1.06	1.18
1:N:162:GLY:O	1:N:165:ILE:HG22	1.45	1.16
1:A:106:LEU:HG	5:E:18:ILE:HD12	1.22	1.16
3:C:171:VAL:HG13	3:C:234:ASN:HB2	1.22	1.14
3:P:271:MET:HB3	4:Q:23:ALA:HA	1.15	1.14
5:E:18:ILE:HA	5:E:22:ILE:HG22	1.31	1.13
1:A:34:TYR:HA	1:A:103:ARG:NH1	1.62	1.12
1:N:112:LYS:H	1:N:113:PRO:HD2	1.09	1.11
2:B:149:LEU:HD13	6:F:3:THR:HG23	1.22	1.11
3:C:173:THR:HG22	3:C:230:ALA:HA	1.34	1.10
2:O:89:ARG:HG3	2:O:90:SER:H	1.16	1.10
2:B:150:PRO:HB3	2:B:153:LYS:HB2	1.28	1.09
5:R:14:LEU:O	5:R:18:ILE:HG12	1.53	1.09
1:N:167:ASP:HA	1:N:170:ARG:HE	1.08	1.08
1:N:32:ILE:HG22	1:N:33:PHE:H	1.20	1.07
10:O:1306:OPC:HAL2	10:O:1306:OPC:HAP2	1.36	1.07
2:B:125:ARG:HA	2:B:125:ARG:HH11	1.15	1.06
2:B:149:LEU:HD21	6:F:2:MET:N	1.71	1.05
7:G:26:ARG:HD3	7:G:27:PRO:HD3	1.36	1.05
5:R:18:ILE:HA	5:R:22:ILE:HG22	1.35	1.05
3:P:171:VAL:HG13	3:P:234:ASN:HB2	1.31	1.04
4:Q:53:GLY:HA2	4:Q:57:LYS:HD3	1.35	1.04
1:A:148:VAL:HA	1:A:151:VAL:HG22	1.36	1.04
2:B:122:ASN:ND2	2:B:124:PHE:HB3	1.71	1.04
1:N:142:GLN:N	2:O:64:GLU:HG2	1.71	1.04
3:P:173:THR:HG22	3:P:230:ALA:HA	1.36	1.03
1:A:66:TYR:CE2	2:B:66:ALA:HA	1.93	1.03
1:A:161:VAL:HG12	1:A:164:LEU:HD12	1.39	1.03
1:N:87:ARG:HD2	2:O:61:MET:HE1	1.38	1.03
1:A:62:VAL:HG13	1:A:177:GLN:HG2	1.36	1.02
5:E:14:LEU:O	5:E:18:ILE:HG12	1.59	1.02
2:B:89:ARG:HG3	2:B:90:SER:H	1.23	1.02
3:P:36:VAL:HG12	3:P:48:ALA:HA	1.39	1.02
1:N:142:GLN:H	2:O:64:GLU:HG2	1.18	1.02
1:N:148:VAL:HA	1:N:151:VAL:HG22	1.41	1.02
2:O:117:VAL:HG13	2:O:118:ASN:H	1.20	1.02
1:A:26:VAL:HB	2:B:29:GLU:HG3	1.38	1.02
2:B:79:TRP:CZ3	5:E:1:MET:HA	1.95	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:53:GLY:HA2	4:D:57:LYS:HD3	1.41	1.01
1:N:28:PRO:HG2	2:O:32:TRP:HB3	1.43	1.01
3:P:271:MET:CB	4:Q:23:ALA:HA	1.90	1.01
4:D:154:THR:HG22	4:D:155:VAL:H	1.24	1.00
1:N:74:ASN:O	1:N:75:GLU:HB2	1.58	1.00
4:D:124:PHE:HB2	4:D:133:TYR:HB2	1.42	0.99
4:Q:124:PHE:HB2	4:Q:133:TYR:HB2	1.41	0.99
4:D:51:GLY:N	4:D:84:LEU:HD21	1.78	0.99
1:A:28:PRO:HD2	2:B:33:PRO:HD3	1.43	0.99
2:B:42:VAL:HG22	3:C:272:LEU:HB3	1.46	0.98
1:N:209:GLN:HE22	2:O:28:GLY:N	1.60	0.98
2:O:125:ARG:NH1	2:O:125:ARG:HB3	1.79	0.98
1:N:105:TYR:OH	2:O:129:ALA:HB1	1.62	0.98
2:O:34:ASN:ND2	2:O:35:ASP:H	1.62	0.98
4:Q:154:THR:HG22	4:Q:155:VAL:H	1.25	0.98
3:P:171:VAL:HG12	3:P:231:LEU:HD11	1.45	0.98
1:A:113:PRO:HA	1:N:16:ALA:HB2	1.45	0.97
3:C:36:VAL:HG12	3:C:48:ALA:HA	1.45	0.97
3:C:102:TYR:N	3:C:118:PRO:HG3	1.78	0.97
2:O:64:GLU:HG3	2:O:65:PRO:HD3	1.46	0.97
5:E:5:ALA:HB1	6:F:10:ALA:HB2	1.46	0.97
3:C:171:VAL:HG12	3:C:231:LEU:HD11	1.45	0.97
3:C:172:PHE:O	3:C:231:LEU:HB3	1.64	0.96
1:N:191:LEU:H	1:N:191:LEU:HD12	1.30	0.96
4:Q:60:LEU:HB2	4:Q:62:ASN:ND2	1.81	0.96
5:E:2:ILE:HA	6:F:6:MET:HB3	1.44	0.95
1:N:23:SER:HA	1:N:25:TYR:CZ	2.01	0.95
3:P:102:TYR:H	3:P:118:PRO:HG3	1.30	0.95
5:R:5:ALA:HB1	6:S:10:ALA:HB2	1.47	0.95
2:B:34:ASN:ND2	2:B:35:ASP:H	1.64	0.95
3:P:101:VAL:HB	3:P:118:PRO:CG	1.95	0.95
2:O:32:TRP:N	2:O:33:PRO:HD2	1.80	0.95
3:P:172:PHE:O	3:P:231:LEU:HB3	1.66	0.95
2:O:51:ILE:H	2:O:51:ILE:HD12	1.32	0.95
1:A:33:PHE:CE1	5:E:18:ILE:HD13	2.01	0.94
3:C:171:VAL:CG1	3:C:234:ASN:HB2	1.97	0.94
3:P:102:TYR:N	3:P:118:PRO:HG3	1.81	0.94
3:C:102:TYR:H	3:C:118:PRO:HG3	1.26	0.94
1:A:36:LEU:H	1:A:36:LEU:HD22	1.30	0.94
3:P:273:ILE:HG21	7:T:22:GLN:HB3	1.48	0.94
1:A:114:ARG:H	1:A:114:ARG:NH1	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:123:ILE:H	1:N:123:ILE:HD12	1.30	0.94
2:B:32:TRP:N	2:B:33:PRO:HD2	1.81	0.94
2:O:38:TYR:HB2	3:P:276:LYS:HD3	1.47	0.94
6:F:27:LEU:HD11	8:H:15:TRP:HE1	1.30	0.94
4:Q:67:SER:HA	4:Q:70:LEU:HD21	1.50	0.94
6:S:28:LEU:HA	6:S:31:GLN:HE21	1.32	0.94
6:S:8:TYR:O	6:S:12:LEU:HB2	1.67	0.94
3:C:101:VAL:HB	3:C:118:PRO:CG	1.97	0.93
1:A:213:GLY:HA2	5:E:30:LYS:HZ1	1.32	0.93
1:A:114:ARG:HH11	1:A:114:ARG:N	1.66	0.93
5:R:2:ILE:HA	6:S:6:MET:HB3	1.51	0.93
7:T:21:TYR:HA	7:T:24:TYR:CD1	2.04	0.93
1:A:123:ILE:H	1:A:123:ILE:HD12	1.31	0.93
4:D:110:HIS:HB2	4:D:144:ALA:HA	1.49	0.93
2:O:125:ARG:HH11	2:O:126:ARG:H	1.02	0.93
3:C:146:LYS:HG2	3:C:248:VAL:HG22	1.51	0.92
1:N:211:ILE:HD13	1:N:212:SER:H	1.35	0.92
10:O:1306:OPC:HAL2	10:O:1306:OPC:HAT2	1.48	0.92
3:C:31:PRO:HB2	3:C:53:PRO:HG3	1.50	0.92
1:A:47:GLN:OE1	1:A:86:HIS:HA	1.69	0.92
1:A:191:LEU:HD12	1:A:191:LEU:H	1.31	0.92
1:A:142:GLN:HE21	2:B:68:PRO:HB2	1.34	0.92
2:B:150:PRO:CB	2:B:153:LYS:HB2	1.98	0.92
2:O:43:VAL:HG22	7:T:23:GLN:OE1	1.70	0.92
7:G:6:LEU:HD22	7:G:6:LEU:H	1.35	0.92
4:Q:110:HIS:HB2	4:Q:144:ALA:HA	1.51	0.92
10:N:1305:OPC:HAT1	10:N:1305:OPC:HAX1	1.51	0.92
1:A:39:ILE:HD12	2:B:47:THR:HG21	1.51	0.91
1:A:158:ILE:HG23	1:A:159:PRO:HD2	1.52	0.91
1:N:158:ILE:HG22	1:N:161:VAL:HG23	1.50	0.91
6:S:27:LEU:HD11	8:U:15:TRP:HE1	1.35	0.91
1:A:33:PHE:HE1	5:E:18:ILE:HD13	1.32	0.91
2:O:42:VAL:HG13	3:P:269:GLN:HB2	1.51	0.91
3:P:146:LYS:HG2	3:P:248:VAL:HG22	1.53	0.91
1:N:77:SER:OG	4:Q:41:TYR:HA	1.69	0.90
4:D:81:VAL:HG12	4:D:82:GLN:H	1.36	0.90
2:B:50:CYS:O	2:B:54:LEU:HG	1.71	0.90
6:F:8:TYR:O	6:F:12:LEU:HB2	1.70	0.90
1:N:47:GLN:OE1	1:N:86:HIS:HA	1.70	0.90
1:A:140:TRP:CZ3	2:B:67:ASN:HA	2.06	0.90
3:P:40:VAL:HG13	3:P:247:ILE:HD11	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:4:LEU:C	8:U:6:TRP:H	1.78	0.90
1:A:113:PRO:HA	1:N:16:ALA:CB	2.00	0.89
4:D:38:LEU:O	4:D:41:TYR:HB3	1.72	0.89
7:G:21:TYR:HA	7:G:24:TYR:CD1	2.07	0.89
1:N:140:TRP:HE1	1:N:180:LEU:HD13	1.37	0.89
8:H:4:LEU:C	8:H:6:TRP:H	1.78	0.89
2:O:122:ASN:C	2:O:124:PHE:H	1.78	0.89
1:A:14:ILE:HD12	1:A:15:GLN:N	1.88	0.89
1:A:214:PRO:HG3	5:E:29:ILE:HD13	1.53	0.89
7:T:21:TYR:HA	7:T:24:TYR:CE1	2.06	0.89
2:B:65:PRO:HB3	2:B:68:PRO:HB3	1.54	0.88
4:D:51:GLY:HA2	4:D:54:THR:HB	1.55	0.88
4:Q:81:VAL:HG12	4:Q:82:GLN:H	1.37	0.88
1:A:62:VAL:HG23	1:A:63:THR:H	1.37	0.88
3:C:188:ASP:H	3:C:193:VAL:HG22	1.36	0.88
1:N:119:ILE:HG23	2:O:109:ILE:HD11	1.55	0.88
10:O:1306:OPC:HAP2	10:O:1306:OPC:HAT2	1.56	0.88
5:R:7:PHE:HA	5:R:10:VAL:HG12	1.56	0.88
2:B:42:VAL:CG2	3:C:272:LEU:HB3	2.03	0.88
3:C:40:VAL:HG13	3:C:247:ILE:HD11	1.54	0.88
3:P:31:PRO:HB2	3:P:53:PRO:HG3	1.54	0.88
3:P:274:LEU:O	3:P:278:GLN:HB2	1.74	0.88
1:A:47:GLN:HE22	1:A:89:SER:HB3	1.38	0.88
2:O:89:ARG:HG3	2:O:90:SER:N	1.87	0.88
5:R:11:PHE:HA	5:R:14:LEU:HD23	1.56	0.88
3:P:101:VAL:HG23	3:P:103:PHE:CE2	2.08	0.88
3:C:149:ILE:HB	3:C:245:THR:HG23	1.57	0.87
1:N:167:ASP:HA	1:N:170:ARG:NE	1.88	0.87
3:P:233:ASN:HD22	3:P:234:ASN:H	1.23	0.87
3:P:199:ILE:HG22	3:P:200:GLN:H	1.38	0.87
4:Q:149:ALA:HB2	4:Q:178:TRP:CZ2	2.09	0.87
1:A:21:VAL:HG12	1:A:22:THR:H	1.40	0.87
2:O:75:ILE:HG22	2:O:76:LEU:H	1.39	0.87
2:B:32:TRP:O	2:B:32:TRP:HE3	1.56	0.87
7:G:21:TYR:HA	7:G:24:TYR:CE1	2.10	0.87
1:N:101:VAL:HG11	12:O:1201:CLA:HMA2	1.57	0.87
2:O:124:PHE:HE1	5:R:26:ILE:HG21	1.37	0.87
1:N:32:ILE:CG2	1:N:33:PHE:H	1.88	0.86
10:N:1305:OPC:HB1	10:N:1305:OPC:HAP1	1.54	0.86
2:O:32:TRP:HE3	2:O:32:TRP:O	1.56	0.86
7:T:20:ALA:HB1	7:T:24:TYR:OH	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:28:LEU:HA	6:F:31:GLN:HE21	1.38	0.86
1:N:31:ASN:HB3	1:N:34:TYR:HE2	1.38	0.86
5:E:7:PHE:HA	5:E:10:VAL:HG12	1.54	0.86
2:B:62:VAL:HG23	2:B:63:GLY:H	1.39	0.86
1:N:47:GLN:HE22	1:N:89:SER:HB3	1.39	0.86
4:Q:154:THR:HB	4:Q:161:VAL:CG2	2.06	0.86
3:P:101:VAL:HB	3:P:118:PRO:HG3	1.57	0.86
1:N:195:ILE:O	1:N:199:MET:HG3	1.76	0.86
1:A:114:ARG:C	1:A:116:LEU:H	1.83	0.85
4:D:67:SER:HA	4:D:70:LEU:HD21	1.55	0.85
2:B:135:PHE:C	2:B:137:THR:H	1.82	0.85
6:F:27:LEU:CD1	8:H:15:TRP:HE1	1.88	0.85
3:P:171:VAL:CG1	3:P:234:ASN:HB2	2.06	0.85
3:P:272:LEU:HD21	4:Q:24:PHE:CE1	2.10	0.85
3:C:188:ASP:HB3	3:C:192:ASN:C	2.02	0.85
7:G:20:ALA:HB1	7:G:24:TYR:OH	1.75	0.85
5:R:2:ILE:HG23	5:R:3:LEU:H	1.42	0.85
3:C:176:ALA:HB3	3:C:199:ILE:HG21	1.57	0.85
3:P:271:MET:HB3	4:Q:23:ALA:CA	2.03	0.85
4:Q:93:VAL:HA	4:Q:99:ILE:HG22	1.56	0.85
2:O:38:TYR:HB2	3:P:276:LYS:CD	2.07	0.85
5:R:9:ILE:HG21	6:S:10:ALA:O	1.77	0.85
5:E:11:PHE:HA	5:E:14:LEU:HD23	1.59	0.84
1:N:69:VAL:HA	1:N:72:ILE:HD13	1.59	0.84
1:A:53:ALA:HA	4:D:42:PHE:HZ	1.42	0.84
5:E:2:ILE:HG23	5:E:3:LEU:H	1.41	0.84
1:N:14:ILE:HB	1:N:17:LEU:HD11	1.58	0.84
3:P:101:VAL:HG23	3:P:103:PHE:HE2	1.42	0.84
3:C:101:VAL:HG23	3:C:103:PHE:CE2	2.11	0.84
7:G:28:ASN:HD21	7:G:30:LEU:HD22	1.42	0.84
1:N:62:VAL:HG13	1:N:177:GLN:OE1	1.77	0.84
3:P:188:ASP:HB3	3:P:192:ASN:C	2.01	0.84
2:B:125:ARG:O	2:B:127:PRO:HD3	1.76	0.84
3:C:101:VAL:HG23	3:C:103:PHE:HE2	1.41	0.84
3:C:233:ASN:HD22	3:C:234:ASN:H	1.20	0.84
3:C:274:LEU:O	3:C:278:GLN:HB2	1.77	0.84
1:A:39:ILE:HG23	2:B:47:THR:HG21	1.60	0.84
2:O:31:ALA:HB1	7:T:30:LEU:HB2	1.59	0.84
2:O:81:LEU:HD23	2:O:84:VAL:HG23	1.60	0.84
4:Q:105:ASN:O	4:Q:148:LEU:HD22	1.77	0.84
4:D:125:LYS:HA	4:D:131:SER:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:O	1:A:199:MET:HG3	1.78	0.84
4:D:60:LEU:HB2	4:D:62:ASN:ND2	1.92	0.84
1:N:112:LYS:H	1:N:113:PRO:CD	1.90	0.84
3:P:188:ASP:H	3:P:193:VAL:HG22	1.43	0.84
3:P:176:ALA:HB3	3:P:199:ILE:HG21	1.56	0.83
2:B:125:ARG:HA	2:B:125:ARG:NH1	1.93	0.83
2:O:34:ASN:HD22	2:O:35:ASP:H	1.27	0.83
1:A:209:GLN:CD	2:B:28:GLY:O	2.21	0.83
2:O:124:PHE:O	2:O:125:ARG:HB2	1.77	0.83
1:A:114:ARG:O	1:A:116:LEU:N	2.11	0.83
1:A:202:HIS:O	1:A:206:ILE:HG13	1.77	0.83
3:P:55:ASP:OD1	3:P:57:LYS:HD2	1.79	0.83
1:A:140:TRP:O	2:B:68:PRO:HG3	1.79	0.83
4:D:35:LEU:H	4:D:37:PRO:HD2	1.43	0.83
4:D:118:ASN:OD1	4:D:121:GLU:HG2	1.77	0.83
1:N:83:ARG:NH1	2:O:60:ALA:HB1	1.94	0.83
6:S:27:LEU:CD1	8:U:15:TRP:HE1	1.92	0.83
2:B:75:ILE:O	2:B:77:PRO:HD3	1.78	0.83
2:B:89:ARG:HG3	2:B:90:SER:N	1.90	0.83
3:C:199:ILE:HG22	3:C:200:GLN:H	1.44	0.83
4:D:73:HIS:CB	4:D:93:VAL:HG21	2.09	0.83
2:O:64:GLU:CG	2:O:65:PRO:HD3	2.09	0.83
1:A:52:PHE:O	1:A:55:THR:HG23	1.78	0.83
2:B:123:PRO:HB2	2:B:129:ALA:HB3	1.60	0.83
3:C:164:GLY:O	3:C:165:GLU:HG3	1.78	0.83
2:O:135:PHE:C	2:O:137:THR:H	1.80	0.83
10:B:305:OPC:HBA1	10:C:306:OPC:HBX2	1.60	0.82
7:G:26:ARG:N	7:G:27:PRO:HD2	1.93	0.82
1:N:32:ILE:HG22	1:N:33:PHE:N	1.90	0.82
4:Q:35:LEU:H	4:Q:37:PRO:HD2	1.44	0.82
1:A:29:HIS:HB3	1:A:211:ILE:HD12	1.58	0.82
3:C:55:ASP:O	3:C:58:LEU:HD13	1.79	0.82
3:P:164:GLY:O	3:P:165:GLU:HG3	1.79	0.82
3:C:101:VAL:HB	3:C:118:PRO:HG3	1.61	0.82
7:G:5:VAL:HG13	7:G:8:LEU:HB3	1.60	0.82
2:O:62:VAL:HG22	11:O:1309:BNT:HAM2	1.62	0.82
4:Q:129:HIS:HB2	13:Q:201:FES:S1	2.19	0.82
1:N:52:PHE:O	1:N:55:THR:HG23	1.79	0.82
1:N:112:LYS:N	1:N:113:PRO:HD2	1.94	0.82
3:P:98:VAL:HB	3:P:128:VAL:HG21	1.60	0.82
2:O:79:TRP:HB2	2:O:80:TYR:CE2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:124:PHE:CE1	5:R:26:ILE:HG21	2.15	0.81
4:Q:94:GLU:CD	4:Q:100:ARG:HG2	2.05	0.81
2:O:53:ALA:O	2:O:57:LEU:HB2	1.80	0.81
2:O:125:ARG:NH1	2:O:126:ARG:H	1.77	0.81
2:O:129:ALA:O	2:O:132:ILE:HG13	1.80	0.81
2:B:75:ILE:O	2:B:75:ILE:HG22	1.78	0.81
4:D:149:ALA:HB2	4:D:178:TRP:CZ2	2.14	0.81
1:N:28:PRO:HD2	2:O:33:PRO:HD3	1.62	0.81
10:O:1306:OPC:HAP2	10:O:1306:OPC:CAL	2.09	0.81
6:S:28:LEU:C	6:S:30:ILE:H	1.87	0.81
7:T:9:VAL:HG23	7:T:10:PHE:H	1.43	0.81
1:A:53:ALA:HA	4:D:42:PHE:CZ	2.16	0.81
3:C:233:ASN:ND2	3:C:234:ASN:H	1.77	0.81
1:A:155:PRO:HG2	1:A:166:SER:HB3	1.61	0.81
4:D:36:TYR:N	4:D:37:PRO:HD2	1.94	0.81
2:O:91:LEU:CD2	2:O:96:LEU:HD12	2.11	0.81
4:Q:36:TYR:N	4:Q:37:PRO:HD2	1.94	0.81
4:Q:38:LEU:O	4:Q:41:TYR:HB3	1.81	0.81
7:G:9:VAL:HG23	7:G:10:PHE:H	1.45	0.81
2:B:39:VAL:HA	2:B:42:VAL:HG23	1.62	0.81
3:C:10:PRO:HA	3:C:106:TYR:HE2	1.46	0.81
1:N:63:THR:C	1:N:65:ALA:H	1.84	0.81
2:O:125:ARG:HB3	2:O:125:ARG:CZ	2.07	0.81
6:S:28:LEU:HA	6:S:31:GLN:NE2	1.96	0.81
4:Q:118:ASN:OD1	4:Q:121:GLU:HG2	1.80	0.81
7:T:5:VAL:HG13	7:T:8:LEU:HB3	1.63	0.81
2:B:79:TRP:CH2	5:E:1:MET:HA	2.15	0.81
3:C:86:PRO:HD3	3:C:132:LEU:HD22	1.63	0.81
1:N:66:TYR:CG	2:O:65:PRO:HG2	2.16	0.81
1:N:72:ILE:O	1:N:76:VAL:HG12	1.80	0.80
1:N:202:HIS:O	1:N:206:ILE:HG13	1.81	0.80
1:A:89:SER:HB2	2:B:51:ILE:HG21	1.63	0.80
2:B:51:ILE:H	2:B:51:ILE:HD12	1.46	0.80
1:N:31:ASN:HB3	1:N:34:TYR:CE2	2.15	0.80
1:N:30:VAL:O	1:N:30:VAL:HG12	1.81	0.80
2:O:105:PRO:HG2	2:O:106:LEU:H	1.46	0.80
3:P:149:ILE:HB	3:P:245:THR:HG23	1.61	0.80
1:A:113:PRO:HG2	1:A:114:ARG:HD3	1.63	0.80
2:B:61:MET:HG3	3:C:146:LYS:O	1.82	0.80
3:C:176:ALA:HB1	3:C:201:THR:OG1	1.80	0.80
3:P:91:PRO:O	3:P:92:GLU:HG2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:15:PHE:HB3	5:R:19:ALA:HB3	1.63	0.80
4:Q:113:CYS:HG	4:Q:128:CYS:HG	0.82	0.80
7:T:16:LEU:O	7:T:16:LEU:HD22	1.82	0.80
2:O:32:TRP:H	2:O:33:PRO:HD2	1.47	0.80
2:O:117:VAL:HG13	2:O:118:ASN:N	1.96	0.80
1:A:142:GLN:HE21	2:B:68:PRO:CB	1.95	0.80
3:C:55:ASP:OD1	3:C:57:LYS:HD2	1.82	0.80
1:N:14:ILE:HB	1:N:17:LEU:CD1	2.11	0.80
2:O:122:ASN:HD22	5:R:27:LYS:N	1.79	0.80
7:T:6:LEU:H	7:T:6:LEU:HD22	1.46	0.80
3:P:55:ASP:O	3:P:58:LEU:HD13	1.82	0.79
4:Q:115:VAL:HG13	4:Q:126:CYS:HA	1.63	0.79
2:B:105:PRO:HG2	2:B:106:LEU:H	1.45	0.79
3:C:98:VAL:HB	3:C:128:VAL:HG21	1.64	0.79
2:B:61:MET:HE3	11:B:309:BNT:HAM2	1.64	0.79
2:B:72:PRO:HG2	2:B:75:ILE:HG13	1.64	0.79
4:D:56:ALA:HB1	4:D:81:VAL:HG11	1.64	0.79
3:P:101:VAL:HB	3:P:118:PRO:CB	2.11	0.79
3:P:196:GLN:HE22	3:P:210:THR:CB	1.95	0.79
2:B:84:VAL:HG13	12:B:201:CLA:OBD	1.82	0.79
6:F:28:LEU:C	6:F:30:ILE:H	1.90	0.79
1:N:17:LEU:HG	1:N:20:ASP:HB2	1.63	0.79
3:P:180:ILE:HD11	3:P:182:LYS:O	1.82	0.79
4:Q:139:VAL:HG21	4:Q:144:ALA:O	1.83	0.79
4:D:63:ASN:ND2	4:D:63:ASN:H	1.81	0.79
1:N:155:PRO:HG2	1:N:166:SER:HB3	1.65	0.79
3:P:280:GLU:C	3:P:282:VAL:H	1.90	0.79
3:C:10:PRO:HA	3:C:106:TYR:CE2	2.18	0.78
3:C:91:PRO:O	3:C:92:GLU:HG2	1.83	0.78
2:B:34:ASN:HD22	2:B:35:ASP:H	1.31	0.78
3:C:91:PRO:O	3:C:95:LYS:HG2	1.82	0.78
2:O:32:TRP:H	2:O:33:PRO:CD	1.95	0.78
4:D:19:MET:SD	4:D:20:ASN:N	2.57	0.78
4:Q:70:LEU:CD1	4:Q:71:GLU:H	1.97	0.78
4:Q:111:LEU:HB3	13:Q:201:FES:S2	2.23	0.78
3:C:180:ILE:HD11	3:C:182:LYS:O	1.82	0.78
3:P:176:ALA:HB1	3:P:201:THR:OG1	1.82	0.78
3:C:101:VAL:HB	3:C:118:PRO:CB	2.14	0.78
1:N:15:GLN:HE21	1:N:15:GLN:C	1.91	0.78
1:N:87:ARG:HD2	2:O:61:MET:CE	2.14	0.78
1:A:69:VAL:HA	1:A:72:ILE:HD13	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:TRP:HZ3	5:E:1:MET:HA	1.43	0.78
1:N:27:PRO:HA	2:O:33:PRO:HD3	1.64	0.78
1:A:77:SER:HB2	4:D:41:TYR:HA	1.66	0.78
3:C:171:VAL:HG13	3:C:234:ASN:CB	2.08	0.78
3:P:79:PRO:HG2	3:P:82:PHE:CD1	2.19	0.78
10:B:305:OPC:HAV	10:B:305:OPC:OAI	1.84	0.78
6:S:27:LEU:HD13	6:S:27:LEU:N	1.99	0.78
2:B:18:LEU:N	2:B:31:ALA:HB2	1.98	0.78
2:B:117:VAL:HG23	2:B:118:ASN:N	1.99	0.78
2:B:129:ALA:O	2:B:132:ILE:HG13	1.81	0.78
5:E:15:PHE:HB3	5:E:19:ALA:HB3	1.66	0.78
10:B:305:OPC:CAO	10:B:305:OPC:HAS2	2.13	0.77
3:C:275:LYS:NZ	10:C:306:OPC:HBG3	1.98	0.77
5:E:9:ILE:HG21	6:F:10:ALA:O	1.84	0.77
1:N:209:GLN:NE2	2:O:28:GLY:N	2.31	0.77
5:R:11:PHE:CA	5:R:14:LEU:HD23	2.13	0.77
1:A:156:GLU:O	1:A:163:VAL:HG22	1.84	0.77
3:C:60:GLN:OE1	3:C:156:GLY:HA2	1.84	0.77
3:C:78:LEU:HD21	3:C:131:VAL:HG21	1.66	0.77
4:D:115:VAL:HG13	4:D:126:CYS:HA	1.63	0.77
1:A:47:GLN:NE2	1:A:90:ALA:N	2.31	0.77
1:N:15:GLN:C	1:N:17:LEU:H	1.92	0.77
3:C:192:ASN:O	3:C:193:VAL:HG23	1.84	0.77
3:C:280:GLU:C	3:C:282:VAL:H	1.89	0.77
4:Q:56:ALA:HB1	4:Q:81:VAL:HG11	1.66	0.77
3:C:267:LEU:O	3:C:270:LEU:HB3	1.84	0.77
2:B:79:TRP:CH2	5:E:1:MET:SD	2.78	0.77
3:C:23:ALA:C	3:C:25:CYS:H	1.93	0.77
4:D:154:THR:HB	4:D:161:VAL:CG2	2.14	0.77
2:O:89:ARG:CG	2:O:90:SER:H	1.96	0.77
1:A:41:LEU:HD23	1:A:42:THR:N	2.00	0.77
1:A:141:ASP:HA	2:B:65:PRO:HG2	1.65	0.77
8:H:18:ALA:O	8:H:21:VAL:HG22	1.84	0.77
1:N:15:GLN:N	1:N:15:GLN:NE2	2.33	0.77
3:P:267:LEU:O	3:P:270:LEU:HB3	1.84	0.77
4:D:50:VAL:HG21	4:D:164:PRO:HG2	1.67	0.77
1:A:29:HIS:CD2	1:A:211:ILE:HB	2.20	0.76
2:B:65:PRO:C	2:B:68:PRO:HD3	2.10	0.76
5:E:9:ILE:O	5:E:12:ILE:HG22	1.85	0.76
2:O:40:PHE:HA	2:O:43:VAL:HG23	1.66	0.76
3:P:271:MET:HE2	4:Q:26:THR:HG21	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:18:TYR:HA	7:T:21:TYR:CD2	2.20	0.76
8:U:18:ALA:O	8:U:21:VAL:HG22	1.85	0.76
1:A:28:PRO:CG	2:B:32:TRP:HB3	2.15	0.76
4:D:93:VAL:HA	4:D:99:ILE:HG22	1.66	0.76
6:F:26:LEU:HD23	6:F:26:LEU:O	1.85	0.76
1:N:20:ASP:O	1:N:21:VAL:HG13	1.82	0.76
3:P:9:TYR:C	3:P:11:PRO:HD2	2.10	0.76
2:B:108:LEU:O	2:B:111:VAL:HG23	1.85	0.76
2:B:91:LEU:CD2	2:B:96:LEU:HD12	2.14	0.76
3:P:154:ASN:O	3:P:155:ARG:HB3	1.86	0.76
1:A:121:GLY:O	1:A:124:LEU:HB2	1.85	0.76
4:D:51:GLY:CA	4:D:54:THR:HB	2.15	0.76
4:D:70:LEU:CD1	4:D:71:GLU:H	1.97	0.76
6:F:26:LEU:HD22	8:H:15:TRP:HZ2	1.51	0.76
3:P:233:ASN:ND2	3:P:234:ASN:H	1.82	0.76
8:U:1:ILE:HG23	8:U:2:ASP:H	1.50	0.76
2:O:32:TRP:N	2:O:33:PRO:CD	2.48	0.76
2:O:38:TYR:CD1	3:P:276:LYS:NZ	2.51	0.76
2:B:32:TRP:N	2:B:33:PRO:CD	2.48	0.76
1:N:123:ILE:H	1:N:123:ILE:CD1	1.99	0.76
1:N:135:GLY:HA2	1:N:138:LEU:CD1	2.16	0.76
6:S:26:LEU:HD22	8:U:15:TRP:HZ2	1.50	0.76
7:G:16:LEU:O	7:G:16:LEU:HD22	1.85	0.76
3:C:196:GLN:HE22	3:C:210:THR:CB	1.97	0.76
3:P:63:ALA:HA	3:P:157:ARG:NH1	2.01	0.76
3:C:205:LYS:HZ3	3:C:207:VAL:HG12	1.51	0.75
4:D:94:GLU:CD	4:D:100:ARG:HG2	2.10	0.75
1:N:121:GLY:O	1:N:124:LEU:HB2	1.86	0.75
4:D:139:VAL:HG21	4:D:144:ALA:O	1.85	0.75
1:A:52:PHE:HB2	1:N:189:PHE:CE2	2.21	0.75
10:N:1305:OPC:HAY2	10:N:1305:OPC:HBZ1	1.68	0.75
2:O:91:LEU:HD22	2:O:96:LEU:HD12	1.68	0.75
5:E:18:ILE:HA	5:E:22:ILE:CG2	2.14	0.75
8:H:4:LEU:C	8:H:6:TRP:N	2.44	0.75
10:B:305:OPC:HBT1	10:C:306:OPC:HBR	1.68	0.75
3:C:9:TYR:C	3:C:11:PRO:HD2	2.11	0.75
1:N:28:PRO:HD2	2:O:33:PRO:CD	2.17	0.75
1:N:63:THR:O	1:N:65:ALA:N	2.18	0.75
1:A:176:GLY:O	1:A:177:GLN:C	2.30	0.75
4:D:40:LYS:O	4:D:43:ILE:HB	1.87	0.75
7:G:18:TYR:HA	7:G:21:TYR:CD2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:171:VAL:HG13	3:P:234:ASN:CB	2.12	0.75
8:U:4:LEU:C	8:U:6:TRP:N	2.43	0.75
2:B:39:VAL:HA	2:B:42:VAL:CG2	2.17	0.75
2:B:112:PRO:O	2:B:116:ASN:HB2	1.87	0.75
3:P:10:PRO:HA	3:P:106:TYR:CE2	2.22	0.75
2:B:122:ASN:HB2	2:B:123:PRO:HD2	1.68	0.75
1:N:185:SER:O	1:N:189:PHE:HB3	1.87	0.75
5:R:24:PHE:C	5:R:26:ILE:H	1.93	0.75
3:C:249:LEU:H	3:C:249:LEU:HD12	1.52	0.75
3:P:86:PRO:HD3	3:P:132:LEU:HD22	1.69	0.75
3:C:79:PRO:HG2	3:C:82:PHE:CD1	2.22	0.74
3:C:188:ASP:OD2	3:C:192:ASN:HB3	1.87	0.74
4:D:50:VAL:C	4:D:84:LEU:HD21	2.12	0.74
5:E:22:ILE:CG2	5:E:23:ILE:N	2.50	0.74
1:A:124:LEU:HB3	9:A:302:HEC:CBB	2.16	0.74
1:A:138:LEU:N	1:A:139:PRO:HD2	2.01	0.74
2:O:39:VAL:HA	2:O:42:VAL:HG23	1.67	0.74
3:P:78:LEU:HD21	3:P:131:VAL:HG21	1.67	0.74
4:Q:125:LYS:HA	4:Q:131:SER:O	1.86	0.74
3:C:219:VAL:HG12	3:C:220:SER:H	1.52	0.74
2:O:81:LEU:O	2:O:85:PHE:HB2	1.88	0.74
3:P:60:GLN:OE1	3:P:156:GLY:HA2	1.86	0.74
3:P:271:MET:HA	3:P:274:LEU:HD12	1.68	0.74
1:A:158:ILE:O	1:A:163:VAL:HG23	1.87	0.74
3:P:219:VAL:HG12	3:P:220:SER:H	1.52	0.74
4:Q:27:VAL:C	4:Q:29:GLY:H	1.96	0.74
4:D:50:VAL:HB	4:D:84:LEU:HD13	1.67	0.74
1:N:188:THR:C	1:N:192:PRO:HG3	2.12	0.74
2:O:29:GLU:N	2:O:30:PRO:HD3	2.01	0.74
1:A:111:LYS:CB	1:A:114:ARG:HH22	2.00	0.74
7:G:8:LEU:HD23	7:G:8:LEU:O	1.88	0.74
2:O:51:ILE:HD12	2:O:51:ILE:N	2.03	0.74
10:O:1306:OPC:HBT2	10:O:1306:OPC:HBX2	1.67	0.74
2:B:79:TRP:O	2:B:80:TYR:CD1	2.41	0.74
2:B:91:LEU:HD22	2:B:96:LEU:HD12	1.67	0.74
1:N:47:GLN:NE2	1:N:90:ALA:N	2.36	0.74
4:Q:19:MET:SD	4:Q:20:ASN:N	2.61	0.74
5:R:9:ILE:O	5:R:12:ILE:HG22	1.87	0.74
1:A:102:PHE:O	1:A:106:LEU:HB2	1.88	0.74
2:B:57:LEU:HD13	7:G:10:PHE:CD2	2.23	0.74
2:B:133:PHE:CE2	2:B:137:THR:HG21	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:41:LEU:HD23	1:N:42:THR:N	2.02	0.74
3:P:271:MET:HE3	4:Q:22:LEU:HG	1.68	0.74
5:E:10:VAL:O	5:E:11:PHE:HB3	1.87	0.73
6:F:28:LEU:HA	6:F:31:GLN:NE2	2.01	0.73
3:P:2:PRO:HB3	3:P:115:LEU:HD22	1.70	0.73
1:A:111:LYS:HB3	1:A:114:ARG:HH22	1.53	0.73
1:A:147:ALA:HB2	2:B:75:ILE:HG23	1.69	0.73
3:C:2:PRO:HB3	3:C:115:LEU:HD22	1.68	0.73
5:E:24:PHE:C	5:E:26:ILE:H	1.96	0.73
1:A:60:PRO:C	1:A:180:LEU:HD21	2.12	0.73
2:B:57:LEU:HD11	7:G:10:PHE:HA	1.68	0.73
1:N:15:GLN:N	1:N:15:GLN:CD	2.43	0.73
6:S:8:TYR:HA	6:S:11:LEU:HD11	1.70	0.73
3:P:10:PRO:HA	3:P:106:TYR:HE2	1.52	0.73
4:Q:22:LEU:HD23	4:Q:23:ALA:N	2.03	0.73
1:A:28:PRO:HG3	2:B:32:TRP:HB3	1.70	0.73
1:A:135:GLY:HA2	1:A:138:LEU:CD1	2.18	0.73
2:O:93:ASN:OD1	2:O:94:LYS:N	2.18	0.73
1:A:114:ARG:HG3	1:A:208:LYS:CD	2.19	0.73
3:C:185:LYS:CD	3:C:195:TYR:HB3	2.19	0.73
4:D:73:HIS:HB3	4:D:93:VAL:HG21	1.71	0.73
5:E:5:ALA:HB1	6:F:10:ALA:CB	2.19	0.73
6:F:8:TYR:HA	6:F:11:LEU:HD11	1.68	0.73
3:P:70:LEU:HD11	3:P:122:GLU:HB2	1.71	0.73
3:P:231:LEU:HD13	3:P:233:ASN:N	2.02	0.73
1:A:188:THR:C	1:A:192:PRO:HG3	2.13	0.73
2:B:83:PRO:HB2	12:B:201:CLA:HMD2	1.70	0.73
3:P:176:ALA:CB	3:P:199:ILE:HG21	2.19	0.73
4:Q:73:HIS:CB	4:Q:93:VAL:HG21	2.18	0.73
2:B:89:ARG:CG	2:B:90:SER:H	2.01	0.73
5:E:11:PHE:CA	5:E:14:LEU:HD23	2.19	0.73
10:N:1305:OPC:HAT1	10:N:1305:OPC:CAX	2.18	0.73
2:O:79:TRP:CD1	2:O:79:TRP:H	2.07	0.73
3:P:282:VAL:O	3:P:285:ALA:HB3	1.89	0.73
2:B:122:ASN:HD21	2:B:124:PHE:HB3	1.51	0.72
3:C:185:LYS:HD2	3:C:195:TYR:CD2	2.24	0.72
1:N:21:VAL:HG23	1:N:22:THR:H	1.53	0.72
1:N:29:HIS:NE2	1:N:31:ASN:ND2	2.35	0.72
1:N:45:LEU:HB2	10:N:1305:OPC:OBH	1.89	0.72
3:P:23:ALA:C	3:P:25:CYS:H	1.94	0.72
4:Q:171:ARG:HH11	4:Q:171:ARG:HB2	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:O	1:A:23:SER:N	2.21	0.72
1:A:103:ARG:HH11	1:A:103:ARG:HG3	1.53	0.72
3:C:63:ALA:HA	3:C:157:ARG:NH1	2.03	0.72
3:C:154:ASN:O	3:C:155:ARG:HB3	1.88	0.72
1:N:149:LYS:O	1:N:149:LYS:HD3	1.89	0.72
2:O:39:VAL:HA	2:O:42:VAL:CG2	2.18	0.72
4:Q:60:LEU:HB2	4:Q:62:ASN:HD22	1.48	0.72
2:B:62:VAL:HG23	2:B:63:GLY:N	2.04	0.72
4:D:22:LEU:HD23	4:D:23:ALA:N	2.04	0.72
4:D:88:PRO:HB3	2:O:69:PHE:HD2	1.55	0.72
4:D:105:ASN:O	4:D:148:LEU:HD22	1.90	0.72
2:O:52:VAL:O	2:O:56:VAL:HG22	1.88	0.72
3:P:215:PRO:HB3	3:P:235:PRO:HD3	1.72	0.72
2:B:93:ASN:OD1	2:B:94:LYS:N	2.22	0.72
2:O:119:LYS:O	2:O:123:PRO:HB3	1.89	0.72
3:P:249:LEU:H	3:P:249:LEU:HD12	1.53	0.72
4:Q:51:GLY:O	4:Q:54:THR:HG22	1.88	0.72
5:R:10:VAL:HG13	5:R:10:VAL:O	1.90	0.72
1:A:148:VAL:HA	1:A:151:VAL:CG2	2.18	0.72
3:C:185:LYS:HD2	3:C:195:TYR:HB3	1.71	0.72
2:O:74:GLU:O	2:O:75:ILE:O	2.06	0.72
1:A:114:ARG:H	1:A:114:ARG:HH11	0.84	0.72
1:A:123:ILE:H	1:A:123:ILE:CD1	2.01	0.72
3:C:70:LEU:HD11	3:C:122:GLU:HB2	1.72	0.72
3:C:170:ASN:O	3:C:235:PRO:HD2	1.89	0.72
3:C:282:VAL:O	3:C:285:ALA:HB3	1.90	0.72
1:N:51:GLY:HA2	1:N:54:MET:HE3	1.71	0.72
4:D:104:ILE:HD12	4:D:104:ILE:O	1.90	0.72
7:G:5:VAL:O	7:G:5:VAL:HG12	1.89	0.72
1:N:159:PRO:C	1:N:161:VAL:H	1.97	0.72
1:N:196:ALA:O	1:N:200:LEU:HD23	1.89	0.72
2:O:108:LEU:O	2:O:111:VAL:HG23	1.88	0.72
7:T:8:LEU:HD23	7:T:8:LEU:O	1.88	0.72
1:A:99:LEU:N	1:A:99:LEU:HD23	2.05	0.72
2:B:65:PRO:HB3	2:B:68:PRO:CB	2.19	0.72
5:E:10:VAL:O	5:E:10:VAL:HG13	1.89	0.72
1:N:19:ASP:O	1:N:21:VAL:N	2.22	0.72
10:O:1306:OPC:HBB2	10:O:1306:OPC:HCB3	1.70	0.72
2:B:18:LEU:N	2:B:31:ALA:CB	2.53	0.72
3:C:271:MET:HG3	3:C:274:LEU:HD12	1.70	0.72
1:N:58:TYR:HD2	1:N:184:TYR:HE1	1.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:106:LEU:O	2:O:109:ILE:HG22	1.90	0.71
3:P:185:LYS:HD2	3:P:195:TYR:HB3	1.69	0.71
4:Q:67:SER:HA	4:Q:70:LEU:CD2	2.20	0.71
1:A:158:ILE:CG2	1:A:159:PRO:HD2	2.20	0.71
10:C:306:OPC:CAP	10:C:306:OPC:HAL2	2.20	0.71
3:C:233:ASN:ND2	3:C:234:ASN:N	2.38	0.71
7:G:16:LEU:HD13	7:G:16:LEU:C	2.15	0.71
3:P:34:VAL:CG1	3:P:151:LEU:HD13	2.21	0.71
1:A:21:VAL:HG12	1:A:22:THR:N	2.04	0.71
1:A:25:TYR:O	1:A:26:VAL:HG22	1.91	0.71
1:A:171:GLY:HA3	1:A:178:ALA:HB1	1.71	0.71
2:B:122:ASN:HD22	2:B:124:PHE:HB3	1.52	0.71
3:C:231:LEU:HD13	3:C:233:ASN:N	2.04	0.71
4:D:88:PRO:HB3	2:O:69:PHE:CD2	2.26	0.71
1:N:208:LYS:HG2	2:O:27:TYR:CZ	2.25	0.71
2:O:133:PHE:CE2	2:O:137:THR:HG21	2.25	0.71
2:B:74:GLU:O	2:B:75:ILE:HB	1.90	0.71
3:C:271:MET:HA	3:C:274:LEU:HD12	1.72	0.71
7:G:26:ARG:HD3	7:G:27:PRO:CD	2.15	0.71
4:Q:21:LEU:O	4:Q:25:GLY:HA3	1.90	0.71
5:R:10:VAL:O	5:R:11:PHE:HB3	1.89	0.71
3:C:34:VAL:CG1	3:C:151:LEU:HD13	2.20	0.71
3:P:188:ASP:OD2	3:P:192:ASN:HB3	1.89	0.71
3:P:271:MET:HG3	3:P:274:LEU:HD12	1.72	0.71
3:C:233:ASN:HD22	3:C:234:ASN:N	1.89	0.71
5:E:7:PHE:HA	5:E:10:VAL:CG1	2.20	0.71
1:N:111:LYS:HB3	1:N:113:PRO:HD2	1.72	0.71
1:N:127:ILE:HD13	1:N:194:LEU:HB2	1.71	0.71
3:P:91:PRO:O	3:P:95:LYS:HG2	1.90	0.71
3:P:192:ASN:O	3:P:193:VAL:HG23	1.90	0.71
1:A:149:LYS:O	1:A:149:LYS:HD3	1.88	0.71
3:C:159:GLN:HG3	3:C:169:ASN:O	1.90	0.71
1:N:16:ALA:O	1:N:17:LEU:O	2.08	0.71
3:C:282:VAL:HG23	3:C:283:GLN:H	1.55	0.71
6:F:27:LEU:HD11	8:H:15:TRP:NE1	2.06	0.71
1:A:185:SER:O	1:A:189:PHE:HB3	1.91	0.70
3:P:83:LYS:NZ	3:P:132:LEU:O	2.24	0.70
5:R:9:ILE:HG21	6:S:10:ALA:C	2.16	0.70
6:S:26:LEU:O	6:S:26:LEU:HD23	1.90	0.70
7:T:16:LEU:C	7:T:16:LEU:HD13	2.16	0.70
10:C:306:OPC:HAP1	10:C:306:OPC:OBJ	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:84:LEU:O	4:D:85:LYS:HB2	1.90	0.70
4:D:154:THR:HG22	4:D:155:VAL:N	2.04	0.70
5:R:15:PHE:HB3	5:R:19:ALA:CB	2.21	0.70
1:N:123:ILE:HD12	1:N:123:ILE:N	2.05	0.70
2:O:38:TYR:HB2	3:P:276:LYS:CE	2.21	0.70
3:P:25:CYS:HA	3:P:160:ILE:HD12	1.73	0.70
2:B:77:PRO:O	2:B:78:GLU:C	2.33	0.70
6:F:23:LEU:O	6:F:27:LEU:HD13	1.90	0.70
1:N:80:TRP:CZ3	1:N:81:LEU:HD23	2.27	0.70
1:A:52:PHE:O	1:A:54:MET:N	2.25	0.70
2:B:43:VAL:HA	7:G:23:GLN:OE1	1.91	0.70
2:B:102:ALA:C	2:B:105:PRO:HD2	2.15	0.70
1:N:167:ASP:C	1:N:169:LEU:H	1.99	0.70
3:C:25:CYS:HA	3:C:160:ILE:HD12	1.74	0.70
4:D:51:GLY:C	4:D:54:THR:HB	2.17	0.70
6:F:27:LEU:HD13	6:F:27:LEU:N	2.05	0.70
1:N:15:GLN:O	1:N:17:LEU:N	2.20	0.70
2:O:62:VAL:HG22	11:O:1309:BNT:CAM	2.21	0.70
3:P:185:LYS:CD	3:P:195:TYR:HB3	2.21	0.70
4:Q:154:THR:HB	4:Q:161:VAL:HG23	1.72	0.70
6:S:26:LEU:HD22	8:U:15:TRP:CZ2	2.27	0.70
7:T:16:LEU:C	7:T:18:TYR:H	2.00	0.70
4:D:27:VAL:C	4:D:29:GLY:H	1.99	0.70
6:F:16:LEU:HD13	6:F:19:VAL:HG21	1.73	0.70
1:A:47:GLN:HE22	1:A:89:SER:CB	2.04	0.70
2:B:55:SER:O	2:B:58:ASP:C	2.35	0.70
3:C:154:ASN:CG	3:C:155:ARG:H	1.98	0.70
3:C:266:MET:HA	3:C:269:GLN:NE2	2.07	0.70
1:N:101:VAL:CG1	12:O:1201:CLA:HMA2	2.22	0.70
3:P:169:ASN:ND2	3:P:237:VAL:H	1.90	0.70
4:Q:65:LYS:O	4:Q:68:LYS:HG2	1.91	0.70
5:R:22:ILE:CG2	5:R:23:ILE:N	2.54	0.70
7:T:5:VAL:O	7:T:5:VAL:HG12	1.91	0.70
1:N:142:GLN:HG2	2:O:64:GLU:CD	2.16	0.70
2:O:102:ALA:C	2:O:105:PRO:HD2	2.15	0.70
2:O:104:VAL:N	2:O:105:PRO:HD2	2.07	0.70
2:O:122:ASN:ND2	5:R:27:LYS:N	2.40	0.70
2:B:124:PHE:CZ	5:E:27:LYS:HB2	2.27	0.70
5:E:5:ALA:O	6:F:10:ALA:HA	1.92	0.70
1:N:56:PHE:O	1:N:57:TYR:HD2	1.75	0.70
1:N:85:ILE:HA	2:O:51:ILE:HG22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:104:VAL:H	2:O:105:PRO:HD2	1.56	0.69
1:A:142:GLN:N	2:B:65:PRO:HG2	2.06	0.69
2:B:32:TRP:O	2:B:32:TRP:CE3	2.44	0.69
3:C:28:ALA:HB1	3:C:238:GLY:O	1.91	0.69
7:G:20:ALA:CB	7:G:24:TYR:OH	2.40	0.69
1:N:124:LEU:HB3	9:N:302:HEC:HBB3	1.72	0.69
2:O:57:LEU:HD21	7:T:9:VAL:O	1.91	0.69
5:E:22:ILE:HG22	5:E:23:ILE:H	1.58	0.69
7:G:10:PHE:C	7:G:12:THR:H	2.00	0.69
8:H:22:TRP:NE1	8:H:26:GLY:HA3	2.06	0.69
2:O:117:VAL:CG1	2:O:118:ASN:H	2.00	0.69
4:Q:116:PRO:HD2	4:Q:127:PRO:HD3	1.74	0.69
7:T:10:PHE:C	7:T:12:THR:H	1.97	0.69
1:N:139:PRO:HG3	9:N:301:HEC:O1A	1.92	0.69
2:O:31:ALA:HB3	7:T:30:LEU:C	2.18	0.69
2:O:42:VAL:HG13	3:P:269:GLN:CB	2.20	0.69
7:T:28:ASN:OD1	7:T:30:LEU:HD21	1.92	0.69
2:B:125:ARG:HH11	2:B:125:ARG:CA	1.98	0.69
7:G:8:LEU:O	7:G:12:THR:HG23	1.92	0.69
3:P:89:ARG:HG3	3:P:89:ARG:HH11	1.57	0.69
3:P:233:ASN:HD22	3:P:234:ASN:N	1.91	0.69
4:Q:18:PHE:O	4:Q:21:LEU:HG	1.92	0.69
4:Q:126:CYS:SG	4:Q:127:PRO:HD2	2.32	0.69
1:A:152:SER:HB2	1:A:170:ARG:HD2	1.74	0.69
2:B:106:LEU:O	2:B:109:ILE:HG22	1.92	0.69
2:O:51:ILE:H	2:O:51:ILE:CD1	2.05	0.69
6:S:23:LEU:O	6:S:27:LEU:HD13	1.91	0.69
1:A:160:VAL:HG12	1:A:161:VAL:H	1.58	0.69
2:B:49:ALA:O	2:B:52:VAL:HB	1.93	0.69
3:P:154:ASN:CG	3:P:155:ARG:H	2.00	0.69
8:U:1:ILE:HG23	8:U:2:ASP:N	2.08	0.69
1:A:114:ARG:C	1:A:116:LEU:N	2.51	0.69
1:A:158:ILE:CG2	1:A:162:GLY:HA3	2.23	0.69
4:D:53:GLY:CA	4:D:57:LYS:HD3	2.20	0.69
7:G:10:PHE:C	7:G:12:THR:N	2.47	0.69
3:P:179:THR:HB	3:P:225:VAL:HG22	1.74	0.69
5:R:9:ILE:HG13	6:S:14:PHE:HB2	1.73	0.69
6:S:27:LEU:HD23	7:T:25:LYS:HD2	1.73	0.69
7:T:10:PHE:O	7:T:12:THR:N	2.26	0.69
10:B:305:OPC:HAG2	10:B:305:OPC:HBX1	1.74	0.69
4:D:59:LYS:HB2	4:D:59:LYS:NZ	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:PHE:C	5:E:17:GLY:H	1.99	0.69
1:N:211:ILE:CD1	1:N:212:SER:H	2.06	0.69
1:A:66:TYR:CB	1:A:140:TRP:HE3	2.06	0.69
1:A:155:PRO:HG2	1:A:166:SER:CB	2.22	0.69
3:C:84:ILE:HD12	3:C:130:PRO:O	1.93	0.69
5:E:15:PHE:HB3	5:E:19:ALA:CB	2.23	0.69
1:N:103:ARG:HH11	1:N:103:ARG:HG3	1.56	0.69
3:P:263:CYS:O	3:P:267:LEU:HD13	1.93	0.69
3:C:36:VAL:HB	3:C:37:PRO:HD2	1.75	0.68
3:C:45:VAL:HG13	3:C:85:ALA:HB2	1.75	0.68
3:C:219:VAL:HG12	3:C:220:SER:N	2.08	0.68
5:R:11:PHE:O	5:R:14:LEU:HB2	1.91	0.68
5:R:13:ALA:HA	6:S:14:PHE:HE1	1.58	0.68
1:A:124:LEU:HB3	9:A:302:HEC:HBB2	1.74	0.68
3:C:263:CYS:O	3:C:267:LEU:HD13	1.93	0.68
1:N:104:VAL:HG12	1:N:105:TYR:N	2.07	0.68
3:P:188:ASP:N	3:P:193:VAL:HA	2.08	0.68
1:A:214:PRO:HD3	5:E:29:ILE:HG21	1.76	0.68
5:E:16:PHE:HE2	14:E:101:BCR:H373	1.56	0.68
5:R:5:ALA:HB1	6:S:10:ALA:CB	2.20	0.68
1:A:61:THR:HG21	1:A:64:GLU:OE1	1.91	0.68
3:C:241:GLY:O	3:C:242:GLN:HB2	1.93	0.68
4:D:67:SER:HA	4:D:70:LEU:CD2	2.23	0.68
1:N:118:TRP:CZ3	2:O:109:ILE:HA	2.29	0.68
2:O:42:VAL:CG2	3:P:272:LEU:HB3	2.23	0.68
10:C:306:OPC:HAP2	10:C:306:OPC:OBH	1.94	0.68
5:E:13:ALA:HA	6:F:14:PHE:HE1	1.59	0.68
1:N:139:PRO:HG2	1:N:141:ASP:OD1	1.94	0.68
2:O:40:PHE:HA	2:O:43:VAL:CG2	2.23	0.68
4:Q:104:ILE:HD12	4:Q:104:ILE:O	1.94	0.68
1:A:33:PHE:HB3	1:A:103:ARG:HG2	1.76	0.68
1:A:49:ALA:O	1:A:50:THR:C	2.37	0.68
3:C:176:ALA:CB	3:C:199:ILE:HG21	2.22	0.68
5:E:9:ILE:HG21	6:F:10:ALA:C	2.19	0.68
7:T:20:ALA:CB	7:T:24:TYR:OH	2.41	0.68
2:B:123:PRO:HB2	2:B:129:ALA:CB	2.23	0.68
4:D:154:THR:HB	4:D:161:VAL:HG23	1.76	0.68
5:E:5:ALA:CB	6:F:10:ALA:HB2	2.22	0.68
1:N:52:PHE:O	1:N:54:MET:N	2.27	0.68
1:N:111:LYS:NZ	1:N:112:LYS:HG3	2.09	0.68
3:P:185:LYS:HD2	3:P:195:TYR:CD2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:282:VAL:HG23	3:P:283:GLN:H	1.57	0.68
6:S:8:TYR:CD2	6:S:9:ALA:N	2.62	0.68
1:A:104:VAL:HG12	1:A:105:TYR:N	2.06	0.68
3:C:89:ARG:HH11	3:C:89:ARG:HG3	1.58	0.68
1:N:190:VAL:C	1:N:192:PRO:HD2	2.19	0.68
10:N:1305:OPC:HBN2	10:N:1305:OPC:CBR	2.24	0.68
2:O:81:LEU:O	2:O:85:PHE:CB	2.42	0.68
4:Q:40:LYS:O	4:Q:43:ILE:HB	1.94	0.68
4:Q:67:SER:O	4:Q:70:LEU:HD11	1.94	0.68
4:D:63:ASN:HD22	4:D:63:ASN:N	1.92	0.68
1:N:111:LYS:HE2	2:O:118:ASN:O	1.93	0.68
1:N:167:ASP:CA	1:N:170:ARG:HE	1.97	0.68
6:S:16:LEU:HD13	6:S:19:VAL:HG21	1.75	0.68
7:T:8:LEU:O	7:T:12:THR:HG23	1.94	0.68
2:B:18:LEU:O	2:B:18:LEU:HD12	1.94	0.67
2:B:38:TYR:HB2	3:C:276:LYS:NZ	2.08	0.67
1:A:127:ILE:HD13	1:A:194:LEU:HB2	1.75	0.67
1:A:141:ASP:CA	2:B:65:PRO:HG2	2.23	0.67
2:B:132:ILE:HA	2:B:135:PHE:HD2	1.59	0.67
2:B:133:PHE:O	2:B:135:PHE:N	2.26	0.67
3:C:154:ASN:OD1	3:C:155:ARG:N	2.26	0.67
4:D:18:PHE:O	4:D:21:LEU:HG	1.95	0.67
5:E:9:ILE:HG13	6:F:14:PHE:HB2	1.76	0.67
2:O:40:PHE:CA	2:O:43:VAL:HG23	2.24	0.67
5:R:18:ILE:HA	5:R:22:ILE:CG2	2.18	0.67
4:D:53:GLY:HA2	4:D:57:LYS:CD	2.22	0.67
1:N:188:THR:O	1:N:192:PRO:HG3	1.94	0.67
5:E:26:ILE:HG23	5:E:30:LYS:HE2	1.76	0.67
1:N:165:ILE:CG2	1:N:166:SER:N	2.57	0.67
1:A:77:SER:O	1:A:78:PHE:HB2	1.94	0.67
1:A:140:TRP:CH2	2:B:67:ASN:HA	2.29	0.67
2:B:77:PRO:O	2:B:78:GLU:O	2.12	0.67
3:C:78:LEU:HG	3:C:79:PRO:HD2	1.76	0.67
3:P:82:PHE:HA	3:P:83:LYS:HZ2	1.59	0.67
6:F:26:LEU:HD22	8:H:15:TRP:CZ2	2.29	0.67
1:N:170:ARG:HA	1:N:179:THR:HA	1.75	0.67
2:O:32:TRP:O	2:O:32:TRP:CE3	2.44	0.67
5:R:7:PHE:HA	5:R:10:VAL:CG1	2.24	0.67
2:B:75:ILE:O	2:B:77:PRO:CD	2.42	0.67
7:G:16:LEU:O	7:G:16:LEU:HD13	1.95	0.67
7:T:26:ARG:N	7:T:27:PRO:HD3	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:CG2	1:A:166:SER:N	2.57	0.67
3:C:121:GLY:C	3:C:123:GLN:H	2.02	0.67
1:N:111:LYS:HZ2	1:N:112:LYS:HG3	1.60	0.67
1:N:162:GLY:HA2	1:N:165:ILE:HG21	1.76	0.67
2:O:38:TYR:CB	3:P:276:LYS:HD3	2.25	0.67
2:O:132:ILE:HA	2:O:135:PHE:HD2	1.59	0.67
3:P:233:ASN:ND2	3:P:234:ASN:N	2.43	0.67
4:Q:154:THR:HG22	4:Q:155:VAL:N	2.06	0.67
2:B:40:PHE:HA	2:B:43:VAL:HG23	1.75	0.67
2:B:150:PRO:HB2	2:B:153:LYS:O	1.94	0.67
1:N:99:LEU:N	1:N:99:LEU:HD23	2.09	0.67
1:N:114:ARG:HG3	1:N:117:THR:CG2	2.24	0.67
2:O:24:HIS:HD1	2:O:24:HIS:C	2.03	0.67
2:O:78:GLU:HB3	2:O:80:TYR:CE1	2.29	0.67
2:O:105:PRO:HG3	12:O:1201:CLA:H112	1.77	0.67
3:P:45:VAL:HG13	3:P:85:ALA:HB2	1.76	0.67
3:P:91:PRO:O	3:P:95:LYS:HE2	1.94	0.67
7:T:17:PHE:HB3	7:T:21:TYR:CE1	2.29	0.67
8:U:3:VAL:O	8:U:6:TRP:HB2	1.95	0.67
1:A:114:ARG:HG3	1:A:208:LYS:HD2	1.74	0.67
8:H:1:ILE:HG23	8:H:2:ASP:H	1.60	0.67
1:N:25:TYR:O	1:N:26:VAL:HG22	1.95	0.67
1:N:80:TRP:HZ3	2:O:56:VAL:HG12	1.59	0.67
3:P:6:GLN:O	3:P:10:PRO:HB3	1.95	0.67
5:R:16:PHE:HE2	14:R:1101:BCR:H373	1.58	0.67
1:A:167:ASP:C	1:A:169:LEU:H	2.03	0.66
8:H:3:VAL:O	8:H:6:TRP:HB2	1.94	0.66
1:N:85:ILE:HG23	2:O:51:ILE:HG21	1.78	0.66
4:Q:92:VAL:HG12	4:Q:93:VAL:H	1.59	0.66
5:E:22:ILE:HG22	5:E:23:ILE:N	2.10	0.66
10:N:1305:OPC:HBU1	10:O:1306:OPC:HBE2	1.76	0.66
10:B:305:OPC:HAV	10:B:305:OPC:CAG	2.25	0.66
4:D:116:PRO:HD2	4:D:127:PRO:HD3	1.77	0.66
8:H:7:VAL:HG12	8:H:11:VAL:HG21	1.76	0.66
1:N:17:LEU:HA	1:N:20:ASP:OD1	1.95	0.66
1:N:158:ILE:HG23	1:N:159:PRO:HD2	1.78	0.66
2:O:118:ASN:OD1	2:O:123:PRO:HA	1.96	0.66
2:O:122:ASN:C	2:O:124:PHE:N	2.53	0.66
2:O:149:LEU:C	2:O:151:LEU:H	2.03	0.66
3:P:44:THR:C	3:P:132:LEU:HD12	2.20	0.66
3:P:148:ALA:HB1	3:P:150:HIS:NE2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:5:ALA:O	6:S:10:ALA:HA	1.94	0.66
6:S:27:LEU:HD11	8:U:15:TRP:NE1	2.09	0.66
1:A:121:GLY:HA2	1:A:124:LEU:HD12	1.76	0.66
2:B:56:VAL:O	2:B:59:PRO:HD3	1.95	0.66
2:B:79:TRP:O	2:B:80:TYR:HD1	1.79	0.66
4:D:22:LEU:HD23	4:D:23:ALA:H	1.61	0.66
4:D:50:VAL:HG21	4:D:164:PRO:CG	2.25	0.66
4:Q:63:ASN:ND2	4:Q:63:ASN:H	1.91	0.66
1:A:189:PHE:CE2	1:N:52:PHE:HB2	2.31	0.66
3:C:179:THR:HB	3:C:225:VAL:HG22	1.77	0.66
1:N:114:ARG:HG3	1:N:117:THR:HG23	1.77	0.66
1:A:33:PHE:O	1:A:34:TYR:C	2.38	0.66
3:C:271:MET:HA	3:C:274:LEU:CG	2.26	0.66
4:D:60:LEU:HB2	4:D:62:ASN:HD22	1.60	0.66
4:Q:149:ALA:HB2	4:Q:178:TRP:CH2	2.31	0.66
5:R:9:ILE:HB	6:S:10:ALA:HB1	1.77	0.66
3:C:27:LEU:HD12	3:C:27:LEU:O	1.96	0.66
11:O:1309:BNT:HAM1	3:P:148:ALA:N	2.10	0.66
7:G:16:LEU:C	7:G:18:TYR:H	2.02	0.66
2:O:123:PRO:HG2	2:O:124:PHE:CE2	2.30	0.66
3:P:52:ILE:HG23	3:P:155:ARG:NH2	2.11	0.66
4:Q:90:TYR:HB2	4:Q:104:ILE:CD1	2.26	0.66
1:A:41:LEU:O	1:A:44:PHE:HB3	1.96	0.66
1:A:213:GLY:HA2	5:E:30:LYS:NZ	2.10	0.66
2:B:45:MET:HE1	3:C:272:LEU:HD12	1.78	0.66
3:C:273:ILE:HG21	7:G:22:GLN:HB3	1.78	0.66
7:G:17:PHE:HB3	7:G:21:TYR:CE1	2.31	0.66
2:O:46:GLY:HA3	7:T:19:ALA:CB	2.26	0.66
3:P:154:ASN:OD1	3:P:155:ARG:N	2.27	0.66
1:N:41:LEU:O	1:N:44:PHE:HB3	1.96	0.66
2:O:133:PHE:O	2:O:135:PHE:N	2.22	0.66
4:Q:94:GLU:OE1	4:Q:100:ARG:NE	2.28	0.66
4:Q:171:ARG:HB2	4:Q:171:ARG:NH1	2.10	0.66
3:C:82:PHE:HA	3:C:83:LYS:HZ2	1.59	0.65
3:P:78:LEU:HG	3:P:79:PRO:HD2	1.78	0.65
1:A:32:ILE:HD11	7:G:26:ARG:NE	2.11	0.65
1:A:51:GLY:HA2	1:A:54:MET:HE3	1.78	0.65
5:E:3:LEU:HD12	5:E:6:VAL:HB	1.79	0.65
1:N:146:TRP:HZ2	2:O:69:PHE:HA	1.61	0.65
3:P:28:ALA:HB1	3:P:238:GLY:O	1.95	0.65
8:U:22:TRP:NE1	8:U:26:GLY:HA3	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HA	1:A:39:ILE:HB	1.78	0.65
1:A:188:THR:O	1:A:192:PRO:HG3	1.96	0.65
4:D:21:LEU:O	4:D:25:GLY:HA3	1.95	0.65
1:N:33:PHE:CE1	1:N:34:TYR:HE1	2.15	0.65
3:P:219:VAL:HG12	3:P:220:SER:N	2.10	0.65
4:Q:145:PRO:O	4:Q:146:LEU:HB2	1.97	0.65
1:A:190:VAL:C	1:A:192:PRO:HD2	2.21	0.65
2:B:104:VAL:N	2:B:105:PRO:HD2	2.10	0.65
2:B:149:LEU:HB3	2:B:150:PRO:CD	2.26	0.65
3:C:159:GLN:N	3:C:159:GLN:OE1	2.29	0.65
4:D:23:ALA:O	4:D:27:VAL:HG23	1.97	0.65
8:H:7:VAL:CG1	8:H:11:VAL:HG21	2.26	0.65
1:N:141:ASP:HB2	1:N:144:GLY:H	1.61	0.65
1:N:159:PRO:O	1:N:161:VAL:N	2.29	0.65
2:O:41:PRO:HG2	3:P:272:LEU:HD13	1.78	0.65
3:P:78:LEU:HD23	3:P:82:PHE:HB3	1.77	0.65
3:P:84:ILE:HD12	3:P:130:PRO:O	1.97	0.65
4:Q:36:TYR:N	4:Q:37:PRO:CD	2.58	0.65
5:R:23:ILE:C	5:R:23:ILE:HD12	2.21	0.65
7:T:10:PHE:C	7:T:12:THR:N	2.47	0.65
2:B:98:VAL:O	2:B:101:MET:HG2	1.97	0.65
2:O:57:LEU:HD21	7:T:9:VAL:C	2.20	0.65
2:O:94:LYS:C	2:O:96:LEU:H	2.04	0.65
1:A:46:ILE:O	1:A:50:THR:HG23	1.97	0.65
2:B:42:VAL:HG22	3:C:272:LEU:CB	2.24	0.65
2:B:64:GLU:HG2	11:B:309:BNT:BRAI	2.52	0.65
2:B:144:GLY:O	2:B:145:ILE:HD13	1.97	0.65
6:F:4:GLU:HG3	6:F:5:GLU:OE1	1.97	0.65
1:N:119:ILE:O	1:N:122:VAL:HB	1.96	0.65
1:N:155:PRO:HG2	1:N:166:SER:CB	2.26	0.65
3:P:278:GLN:O	3:P:279:VAL:HG23	1.95	0.65
1:N:47:GLN:HE22	1:N:89:SER:CB	2.08	0.65
1:N:52:PHE:HA	9:N:301:HEC:HAC	1.77	0.65
2:O:24:HIS:ND1	2:O:24:HIS:O	2.26	0.65
2:O:78:GLU:C	2:O:80:TYR:H	2.05	0.65
5:R:17:GLY:O	5:R:18:ILE:HG23	1.97	0.65
1:A:104:VAL:O	1:A:107:THR:N	2.22	0.65
1:A:214:PRO:CG	5:E:29:ILE:HD13	2.27	0.65
2:B:91:LEU:HD12	2:B:91:LEU:O	1.97	0.65
1:N:165:ILE:O	1:N:168:LEU:HG	1.96	0.65
1:A:28:PRO:HD2	2:B:33:PRO:CD	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:65:LYS:O	4:D:68:LYS:HG2	1.96	0.65
4:D:149:ALA:HB2	4:D:178:TRP:CH2	2.31	0.65
7:G:21:TYR:CD1	7:G:21:TYR:N	2.62	0.65
1:N:125:ALA:O	1:N:129:VAL:HG23	1.96	0.65
2:O:75:ILE:O	2:O:76:LEU:HB2	1.95	0.65
3:P:121:GLY:C	3:P:123:GLN:H	2.05	0.65
6:F:35:LYS:O	6:F:36:GLU:HG2	1.97	0.65
8:H:9:LEU:HB3	8:H:13:PHE:CE1	2.32	0.65
3:P:91:PRO:HB2	3:P:95:LYS:HE3	1.79	0.65
3:C:52:ILE:HG23	3:C:155:ARG:NH2	2.12	0.64
3:C:139:ASP:HB3	3:C:142:ILE:HD12	1.79	0.64
4:D:94:GLU:OE1	4:D:100:ARG:NE	2.30	0.64
5:E:15:PHE:C	5:E:17:GLY:N	2.50	0.64
1:N:141:ASP:O	1:N:145:TYR:N	2.27	0.64
2:O:135:PHE:C	2:O:137:THR:N	2.50	0.64
3:P:26:HIS:CG	3:P:154:ASN:HD21	2.15	0.64
3:P:157:ARG:HB2	3:P:169:ASN:HB2	1.78	0.64
7:T:26:ARG:H	7:T:27:PRO:HD3	1.62	0.64
2:B:40:PHE:N	2:B:41:PRO:HD2	2.12	0.64
2:B:79:TRP:HH2	5:E:1:MET:SD	2.19	0.64
3:C:188:ASP:N	3:C:193:VAL:HA	2.12	0.64
2:O:64:GLU:N	2:O:65:PRO:HD2	2.11	0.64
2:O:122:ASN:OD1	2:O:124:PHE:HB2	1.96	0.64
3:P:252:PRO:C	3:P:254:ARG:H	2.04	0.64
1:A:58:TYR:HD2	1:A:184:TYR:HE1	1.44	0.64
3:C:185:LYS:HD2	3:C:195:TYR:HD2	1.62	0.64
7:G:29:GLU:HG3	7:G:30:LEU:H	1.62	0.64
1:N:209:GLN:HE22	2:O:28:GLY:H	1.44	0.64
2:O:131:THR:O	2:O:135:PHE:HB3	1.96	0.64
3:P:1:TYR:O	3:P:4:TRP:HB2	1.98	0.64
3:P:54:TYR:HB2	3:P:58:LEU:HD22	1.79	0.64
3:P:205:LYS:HZ3	3:P:207:VAL:HG12	1.62	0.64
5:R:15:PHE:C	5:R:17:GLY:H	2.05	0.64
2:B:94:LYS:C	2:B:96:LEU:H	2.05	0.64
3:C:91:PRO:O	3:C:95:LYS:HE2	1.98	0.64
3:C:268:ALA:C	3:C:270:LEU:H	2.05	0.64
4:D:108:CYS:HB2	4:D:115:VAL:HG23	1.79	0.64
1:N:211:ILE:HG23	1:N:212:SER:N	2.12	0.64
3:P:241:GLY:O	3:P:242:GLN:HB2	1.96	0.64
3:P:277:LYS:CE	7:T:27:PRO:HD2	2.28	0.64
4:Q:23:ALA:O	4:Q:27:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:O	1:A:17:LEU:HD12	1.98	0.64
1:A:123:ILE:HD12	1:A:123:ILE:N	2.07	0.64
5:R:22:ILE:HG22	5:R:23:ILE:H	1.62	0.64
7:T:16:LEU:O	7:T:16:LEU:HD13	1.98	0.64
3:C:278:GLN:O	3:C:279:VAL:HG23	1.97	0.64
7:G:24:TYR:O	7:G:26:ARG:HG3	1.97	0.64
1:N:121:GLY:HA2	1:N:124:LEU:HD12	1.79	0.64
3:P:159:GLN:HG3	3:P:169:ASN:O	1.97	0.64
4:Q:84:LEU:O	4:Q:85:LYS:HB2	1.97	0.64
1:A:106:LEU:CG	5:E:18:ILE:HD12	2.15	0.64
3:P:36:VAL:HB	3:P:37:PRO:HD2	1.78	0.64
4:D:36:TYR:N	4:D:37:PRO:CD	2.59	0.64
1:N:137:SER:HB2	1:N:144:GLY:O	1.98	0.64
2:O:112:PRO:O	2:O:116:ASN:HB2	1.98	0.64
2:O:130:THR:O	2:O:133:PHE:HB3	1.98	0.64
5:R:26:ILE:HG23	5:R:30:LYS:HE2	1.80	0.64
3:C:6:GLN:O	3:C:10:PRO:HB3	1.97	0.64
3:C:61:VAL:HG23	3:C:62:ALA:H	1.63	0.64
3:C:103:PHE:HB3	3:C:114:LEU:HD22	1.79	0.64
3:C:172:PHE:HB2	3:C:211:ILE:HG13	1.79	0.64
6:F:16:LEU:HA	6:F:19:VAL:CG2	2.27	0.64
1:N:28:PRO:HD2	2:O:33:PRO:N	2.12	0.64
3:P:187:GLU:HA	3:P:193:VAL:HG13	1.80	0.64
4:Q:175:LYS:HD3	4:Q:176:PRO:CD	2.28	0.64
5:R:5:ALA:CB	6:S:10:ALA:HB2	2.24	0.64
2:B:131:THR:O	2:B:135:PHE:HB3	1.98	0.64
4:D:90:TYR:HB2	4:D:104:ILE:CD1	2.27	0.64
6:F:27:LEU:HD23	7:G:25:LYS:HD2	1.80	0.64
4:Q:118:ASN:ND2	4:Q:120:ALA:H	1.95	0.64
7:T:21:TYR:N	7:T:21:TYR:CD1	2.62	0.64
2:B:117:VAL:HG23	2:B:118:ASN:H	1.62	0.63
2:B:117:VAL:CG2	2:B:118:ASN:N	2.61	0.63
7:G:5:VAL:O	7:G:9:VAL:HG13	1.99	0.63
3:P:110:GLN:OE1	3:P:113:VAL:HG21	1.97	0.63
3:P:281:LYS:HA	3:P:284:ALA:HB3	1.80	0.63
7:T:8:LEU:HA	7:T:11:ALA:HB3	1.80	0.63
1:A:25:TYR:C	1:A:26:VAL:HG22	2.23	0.63
3:C:148:ALA:HB1	3:C:150:HIS:NE2	2.13	0.63
1:N:38:GLY:N	15:N:1306:HOH:O	2.29	0.63
1:N:111:LYS:NZ	1:N:112:LYS:HE3	2.13	0.63
3:C:252:PRO:C	3:C:254:ARG:H	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:27:LYS:O	5:R:27:LYS:HD3	1.98	0.63
1:A:148:VAL:O	1:A:148:VAL:HG12	1.97	0.63
5:E:27:LYS:O	5:E:27:LYS:HD3	1.99	0.63
1:N:71:TYR:HD2	1:N:71:TYR:O	1.80	0.63
4:Q:22:LEU:HD23	4:Q:23:ALA:H	1.62	0.63
4:Q:53:GLY:HA2	4:Q:57:LYS:CD	2.23	0.63
1:A:102:PHE:CE1	5:E:15:PHE:HZ	2.17	0.63
4:D:88:PRO:HG3	4:D:114:VAL:HG22	1.80	0.63
5:E:9:ILE:HB	6:F:10:ALA:HB1	1.80	0.63
5:E:22:ILE:O	5:E:24:PHE:N	2.31	0.63
5:E:23:ILE:C	5:E:23:ILE:HD12	2.24	0.63
1:N:95:LEU:HD11	5:R:7:PHE:HB2	1.81	0.63
2:O:39:VAL:H	2:O:41:PRO:HD2	1.64	0.63
2:O:68:PRO:HG2	2:O:69:PHE:H	1.64	0.63
5:R:15:PHE:C	5:R:17:GLY:N	2.56	0.63
6:S:27:LEU:CD1	6:S:27:LEU:N	2.62	0.63
1:A:80:TRP:CZ3	1:A:81:LEU:HD23	2.34	0.63
3:C:182:LYS:HG2	3:C:198:SER:HB3	1.79	0.63
4:D:63:ASN:H	4:D:63:ASN:HD22	1.42	0.63
2:O:39:VAL:O	2:O:42:VAL:HB	1.98	0.63
2:O:91:LEU:HD21	2:O:96:LEU:HD12	1.79	0.63
1:A:117:THR:HG22	1:A:205:MET:CB	2.29	0.63
3:C:28:ALA:HB1	3:C:238:GLY:C	2.24	0.63
3:C:83:LYS:NZ	3:C:132:LEU:O	2.31	0.63
4:D:63:ASN:ND2	4:D:63:ASN:N	2.46	0.63
4:D:165:TRP:O	4:D:166:THR:HG23	1.99	0.63
5:E:17:GLY:O	5:E:18:ILE:HG23	1.99	0.63
14:E:101:BCR:HC21	7:G:23:GLN:HE22	1.64	0.63
1:N:49:ALA:O	1:N:50:THR:C	2.41	0.63
1:N:97:MET:O	1:N:100:HIS:HB3	1.99	0.63
2:O:98:VAL:O	2:O:101:MET:HG2	1.97	0.63
1:N:95:LEU:HD11	5:R:7:PHE:CB	2.29	0.63
2:O:82:TYR:HB2	2:O:83:PRO:CD	2.29	0.63
2:O:116:ASN:C	2:O:116:ASN:HD22	2.07	0.63
2:B:149:LEU:HD11	6:F:2:MET:HB2	1.80	0.63
3:C:26:HIS:CG	3:C:154:ASN:HD21	2.17	0.63
8:H:4:LEU:O	8:H:6:TRP:N	2.31	0.63
1:N:90:ALA:C	1:N:92:MET:H	2.07	0.63
3:P:266:MET:HE1	7:T:15:GLY:O	1.99	0.63
3:P:271:MET:HA	3:P:274:LEU:CD1	2.29	0.63
1:A:66:TYR:HB2	1:A:140:TRP:HE3	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:CYS:O	3:C:26:HIS:C	2.42	0.62
3:C:157:ARG:HB2	3:C:169:ASN:HB2	1.80	0.62
4:D:57:LYS:HG2	4:D:62:ASN:O	1.99	0.62
7:G:8:LEU:HA	7:G:11:ALA:HB3	1.81	0.62
7:G:10:PHE:O	7:G:12:THR:N	2.31	0.62
1:N:27:PRO:CA	2:O:33:PRO:HD3	2.28	0.62
3:P:28:ALA:HB3	3:P:240:PHE:N	2.14	0.62
2:O:122:ASN:HD22	5:R:26:ILE:C	2.08	0.62
3:P:34:VAL:O	3:P:34:VAL:HG23	1.99	0.62
3:P:104:GLN:NE2	3:P:104:GLN:H	1.97	0.62
3:P:182:LYS:HG2	3:P:198:SER:HB3	1.81	0.62
4:Q:80:LEU:HB2	4:Q:90:TYR:HA	1.80	0.62
4:Q:108:CYS:HB2	4:Q:113:CYS:O	1.98	0.62
6:S:14:PHE:O	6:S:17:ILE:HG12	2.00	0.62
6:S:16:LEU:HA	6:S:19:VAL:CG2	2.29	0.62
1:A:29:HIS:HD2	1:A:211:ILE:HB	1.65	0.62
1:A:165:ILE:O	1:A:168:LEU:HG	2.00	0.62
1:A:183:TYR:O	1:A:186:ALA:HB3	1.98	0.62
1:A:196:ALA:O	1:A:200:LEU:HD23	1.99	0.62
4:D:129:HIS:HB2	13:D:201:FES:S1	2.39	0.62
4:D:145:PRO:O	4:D:146:LEU:HB2	1.98	0.62
5:E:6:VAL:HG12	5:E:6:VAL:O	1.98	0.62
6:F:14:PHE:O	6:F:17:ILE:HG12	1.99	0.62
1:N:162:GLY:C	1:N:165:ILE:HG22	2.22	0.62
2:O:22:MET:O	2:O:24:HIS:N	2.32	0.62
5:R:22:ILE:HG22	5:R:23:ILE:N	2.14	0.62
3:C:34:VAL:HG12	3:C:151:LEU:HD13	1.81	0.62
3:C:251:ASP:O	3:C:254:ARG:HB3	1.99	0.62
1:N:117:THR:HG22	1:N:205:MET:CB	2.30	0.62
2:O:40:PHE:N	2:O:41:PRO:HD2	2.14	0.62
5:R:6:VAL:O	5:R:6:VAL:HG12	1.99	0.62
2:B:82:TYR:HB2	2:B:83:PRO:CD	2.29	0.62
3:C:54:TYR:HB2	3:C:58:LEU:HD22	1.81	0.62
1:N:31:ASN:CB	1:N:34:TYR:HE2	2.12	0.62
1:N:162:GLY:HA2	1:N:165:ILE:CG2	2.30	0.62
10:O:1306:OPC:HBB2	10:O:1306:OPC:CCB	2.28	0.62
1:A:39:ILE:HD11	2:B:43:VAL:CG1	2.29	0.62
2:B:104:VAL:H	2:B:105:PRO:HD2	1.63	0.62
3:C:187:GLU:HA	3:C:193:VAL:HG13	1.80	0.62
4:D:67:SER:O	4:D:70:LEU:HD11	2.00	0.62
3:P:48:ALA:HB3	3:P:129:PHE:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:271:MET:HG2	4:Q:22:LEU:HG	1.81	0.62
4:Q:70:LEU:HD12	4:Q:71:GLU:H	1.64	0.62
3:C:28:ALA:HB3	3:C:240:PHE:N	2.15	0.62
1:N:46:ILE:O	1:N:50:THR:HG23	1.99	0.62
3:P:10:PRO:N	3:P:11:PRO:HD2	2.14	0.62
3:P:34:VAL:HG12	3:P:151:LEU:HD13	1.82	0.62
1:A:29:HIS:CE1	2:B:30:PRO:HG3	2.35	0.62
3:C:172:PHE:H	3:C:231:LEU:HG	1.63	0.62
3:C:191:GLY:O	3:C:192:ASN:HB2	1.99	0.62
4:D:175:LYS:HD3	4:D:176:PRO:CD	2.30	0.62
1:N:105:TYR:OH	2:O:129:ALA:CB	2.42	0.62
1:N:148:VAL:HG12	1:N:148:VAL:O	1.98	0.62
2:O:78:GLU:O	2:O:80:TYR:N	2.32	0.62
3:P:28:ALA:HB1	3:P:238:GLY:C	2.24	0.62
3:P:280:GLU:C	3:P:282:VAL:N	2.58	0.62
4:D:35:LEU:HD23	4:D:35:LEU:C	2.24	0.62
4:D:50:VAL:HB	4:D:84:LEU:CD1	2.29	0.62
5:E:11:PHE:O	5:E:14:LEU:HB2	1.99	0.62
3:P:251:ASP:O	3:P:254:ARG:HB3	1.99	0.62
3:P:266:MET:HA	3:P:269:GLN:NE2	2.14	0.62
3:P:271:MET:HA	3:P:274:LEU:CG	2.30	0.62
4:Q:92:VAL:HG12	4:Q:93:VAL:N	2.15	0.62
5:R:24:PHE:C	5:R:26:ILE:N	2.58	0.62
8:U:7:VAL:HG12	8:U:11:VAL:HG21	1.82	0.62
1:A:78:PHE:CE1	4:D:37:PRO:HA	2.35	0.62
1:A:116:LEU:H	1:A:116:LEU:HD12	1.65	0.62
2:B:124:PHE:HZ	5:E:27:LYS:HB2	1.62	0.62
2:B:129:ALA:HA	2:B:132:ILE:HD11	1.82	0.62
3:C:45:VAL:HG13	3:C:85:ALA:CB	2.29	0.62
1:N:110:PHE:CD1	2:O:112:PRO:HB3	2.35	0.62
1:N:148:VAL:HA	1:N:151:VAL:CG2	2.22	0.62
2:O:34:ASN:ND2	2:O:35:ASP:N	2.42	0.62
1:A:27:PRO:HB3	2:B:33:PRO:HD3	1.82	0.61
1:A:44:PHE:O	1:A:47:GLN:N	2.33	0.61
1:A:136:TYR:HA	9:A:301:HEC:HAA2	1.80	0.61
3:C:193:VAL:O	3:C:193:VAL:HG12	2.00	0.61
1:N:44:PHE:O	1:N:47:GLN:N	2.33	0.61
3:P:117:GLY:N	3:P:118:PRO:HD2	2.13	0.61
3:P:172:PHE:H	3:P:231:LEU:HG	1.63	0.61
6:S:4:GLU:HG3	6:S:5:GLU:OE1	2.00	0.61
7:T:29:GLU:C	7:T:30:LEU:HD13	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:TYR:H	2:B:83:PRO:HD2	1.64	0.61
3:C:10:PRO:N	3:C:11:PRO:HD2	2.15	0.61
3:C:104:GLN:NE2	3:C:104:GLN:H	1.98	0.61
1:N:114:ARG:HB2	1:N:116:LEU:CD1	2.30	0.61
10:O:1306:OPC:HBX2	10:O:1306:OPC:CBT	2.30	0.61
1:A:28:PRO:CD	2:B:33:PRO:HD3	2.24	0.61
1:A:47:GLN:HE22	1:A:90:ALA:N	1.97	0.61
2:O:104:VAL:N	2:O:105:PRO:CD	2.63	0.61
3:P:136:PRO:HB3	3:P:142:ILE:HG22	1.81	0.61
3:P:139:ASP:OD2	3:P:142:ILE:HG13	2.00	0.61
3:P:191:GLY:O	3:P:192:ASN:HB2	1.99	0.61
2:B:39:VAL:O	2:B:43:VAL:HG23	2.00	0.61
2:B:86:GLN:HG3	2:B:90:SER:OG	2.01	0.61
6:F:28:LEU:C	6:F:30:ILE:N	2.58	0.61
1:N:112:LYS:HE2	2:O:116:ASN:HD21	1.64	0.61
1:N:191:LEU:O	1:N:195:ILE:HG22	2.00	0.61
2:O:37:LEU:HB2	2:O:38:TYR:CE1	2.35	0.61
2:O:123:PRO:HD2	2:O:124:PHE:CE1	2.36	0.61
2:O:127:PRO:C	2:O:129:ALA:H	2.08	0.61
3:P:25:CYS:O	3:P:26:HIS:C	2.42	0.61
3:P:79:PRO:HG2	3:P:82:PHE:CG	2.35	0.61
3:P:283:GLN:C	3:P:285:ALA:H	2.08	0.61
1:A:106:LEU:HG	5:E:18:ILE:CD1	2.14	0.61
1:A:158:ILE:HG21	1:A:162:GLY:HA3	1.82	0.61
3:C:78:LEU:HD23	3:C:82:PHE:HB3	1.82	0.61
4:D:22:LEU:O	4:D:26:THR:HG23	2.00	0.61
4:D:70:LEU:HD13	4:D:71:GLU:H	1.65	0.61
3:P:268:ALA:C	3:P:270:LEU:H	2.08	0.61
4:Q:108:CYS:HB2	4:Q:115:VAL:HG23	1.83	0.61
5:R:21:GLY:O	5:R:22:ILE:HD12	2.00	0.61
14:R:1101:BCR:H362	6:S:18:PHE:CE2	2.36	0.61
2:B:39:VAL:O	2:B:42:VAL:HB	2.01	0.61
2:B:117:VAL:CG2	2:B:118:ASN:H	2.13	0.61
3:C:172:PHE:H	3:C:231:LEU:CD2	2.12	0.61
4:D:171:ARG:HH11	4:D:171:ARG:HB2	1.64	0.61
2:O:86:GLN:HG3	2:O:90:SER:OG	2.00	0.61
2:O:118:ASN:HD21	2:O:123:PRO:HB2	1.65	0.61
4:D:92:VAL:HG12	4:D:93:VAL:H	1.65	0.61
5:E:9:ILE:HG23	5:E:10:VAL:N	2.16	0.61
1:N:59:LYS:O	1:N:64:GLU:O	2.17	0.61
2:O:78:GLU:HB3	2:O:80:TYR:CD1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:126:CYS:O	4:Q:130:GLY:HA2	2.01	0.61
5:R:9:ILE:CG2	5:R:10:VAL:N	2.64	0.61
8:U:9:LEU:HB3	8:U:13:PHE:CE1	2.35	0.61
1:A:66:TYR:HB3	1:A:140:TRP:CE3	2.35	0.61
1:A:104:VAL:HG13	1:A:108:GLY:O	2.01	0.61
2:B:39:VAL:H	2:B:41:PRO:HD2	1.65	0.61
3:C:271:MET:HA	3:C:274:LEU:CD1	2.30	0.61
2:O:95:LEU:O	2:O:99:LEU:N	2.33	0.61
3:P:102:TYR:O	3:P:118:PRO:HD2	2.01	0.61
3:P:281:LYS:HD3	3:P:281:LYS:N	2.16	0.61
5:R:2:ILE:O	5:R:4:GLY:N	2.34	0.61
8:U:7:VAL:CG1	8:U:11:VAL:HG21	2.31	0.61
1:A:76:VAL:O	1:A:78:PHE:N	2.34	0.61
2:B:61:MET:SD	2:B:62:VAL:HG22	2.41	0.61
3:C:257:TRP:HE3	3:C:257:TRP:HA	1.66	0.61
2:O:20:LYS:NZ	2:O:20:LYS:HB2	2.15	0.61
4:Q:73:HIS:HB3	4:Q:93:VAL:HG21	1.82	0.61
5:R:22:ILE:O	5:R:24:PHE:N	2.34	0.61
2:B:65:PRO:HD3	11:B:309:BNT:BRAI	2.56	0.61
10:B:305:OPC:HBX1	10:C:306:OPC:HBX1	1.82	0.61
5:E:9:ILE:CG2	5:E:10:VAL:N	2.64	0.61
14:E:101:BCR:HC21	7:G:23:GLN:NE2	2.15	0.61
2:O:73:LEU:HD11	3:P:244:ASP:OD2	2.01	0.61
2:O:86:GLN:HG2	2:O:143:LEU:HD22	1.83	0.61
4:Q:116:PRO:CD	4:Q:127:PRO:HD3	2.31	0.61
1:A:30:VAL:H	1:A:211:ILE:CD1	2.13	0.60
1:A:142:GLN:NE2	2:B:68:PRO:HB2	2.10	0.60
6:F:8:TYR:CD2	6:F:9:ALA:N	2.69	0.60
4:Q:22:LEU:O	4:Q:26:THR:HG23	2.00	0.60
4:Q:132:GLN:O	4:Q:133:TYR:HD2	1.84	0.60
6:S:27:LEU:HD13	6:S:27:LEU:H	1.63	0.60
3:C:91:PRO:HB2	3:C:95:LYS:HE3	1.82	0.60
4:D:111:LEU:HB3	13:D:201:FES:S2	2.40	0.60
5:E:21:GLY:O	5:E:22:ILE:HD12	2.02	0.60
2:O:39:VAL:C	2:O:42:VAL:H	2.09	0.60
2:O:83:PRO:HA	2:O:143:LEU:HB3	1.82	0.60
8:U:4:LEU:O	8:U:6:TRP:N	2.32	0.60
1:N:159:PRO:HG2	1:N:161:VAL:CG2	2.31	0.60
2:O:25:ASN:O	2:O:26:TYR:HB3	2.01	0.60
3:P:61:VAL:HG23	3:P:62:ALA:H	1.66	0.60
4:Q:35:LEU:HD23	4:Q:35:LEU:C	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:16:LEU:C	7:T:18:TYR:N	2.56	0.60
1:A:191:LEU:O	1:A:195:ILE:HG22	2.01	0.60
1:A:195:ILE:HG23	1:A:196:ALA:N	2.16	0.60
2:B:65:PRO:HB3	2:B:68:PRO:CG	2.32	0.60
10:B:305:OPC:HBW1	10:C:306:OPC:HBW2	1.82	0.60
1:N:61:THR:O	1:N:62:VAL:C	2.43	0.60
2:O:62:VAL:CG2	11:O:1309:BNT:HAM2	2.32	0.60
3:P:45:VAL:HG13	3:P:85:ALA:CB	2.31	0.60
1:A:116:LEU:N	1:A:116:LEU:HD12	2.16	0.60
1:A:193:TRP:O	1:A:196:ALA:HB3	2.02	0.60
2:B:57:LEU:CD1	7:G:10:PHE:HA	2.31	0.60
5:E:2:ILE:O	5:E:4:GLY:N	2.34	0.60
3:P:159:GLN:N	3:P:159:GLN:OE1	2.34	0.60
3:P:171:VAL:HG12	3:P:231:LEU:CD1	2.28	0.60
3:C:281:LYS:HA	3:C:284:ALA:HB3	1.84	0.60
1:N:135:GLY:HA2	1:N:138:LEU:HG	1.83	0.60
2:O:133:PHE:C	2:O:135:PHE:H	2.10	0.60
2:O:147:ALA:O	2:O:149:LEU:HD23	2.01	0.60
3:P:122:GLU:O	3:P:122:GLU:HG2	2.01	0.60
3:P:185:LYS:HD2	3:P:195:TYR:HD2	1.65	0.60
7:T:5:VAL:O	7:T:9:VAL:HG13	2.01	0.60
2:B:85:PHE:O	2:B:86:GLN:C	2.44	0.60
3:C:117:GLY:N	3:C:118:PRO:HD2	2.16	0.60
4:D:126:CYS:SG	4:D:127:PRO:HD2	2.41	0.60
4:D:126:CYS:O	4:D:130:GLY:HA2	2.00	0.60
4:D:146:LEU:HD13	4:D:177:TRP:CE3	2.37	0.60
7:G:18:TYR:HA	7:G:21:TYR:CG	2.36	0.60
7:G:26:ARG:H	7:G:27:PRO:HD2	1.65	0.60
1:N:80:TRP:CG	3:P:254:ARG:HH21	2.19	0.60
1:N:114:ARG:HB2	1:N:116:LEU:HD11	1.84	0.60
2:O:57:LEU:HD13	7:T:10:PHE:CD2	2.37	0.60
2:O:70:ALA:O	2:O:71:THR:CB	2.49	0.60
2:O:79:TRP:CD1	2:O:80:TYR:HH	2.20	0.60
3:P:139:ASP:HB3	3:P:142:ILE:HD12	1.84	0.60
6:S:28:LEU:C	6:S:30:ILE:N	2.57	0.60
2:B:63:GLY:HA2	11:B:309:BNT:CAK	2.32	0.60
2:B:79:TRP:C	2:B:80:TYR:HD1	2.08	0.60
2:B:86:GLN:HG2	2:B:143:LEU:HD22	1.83	0.60
4:D:107:VAL:O	4:D:107:VAL:HG12	2.02	0.60
5:R:9:ILE:HG23	5:R:10:VAL:N	2.17	0.60
1:A:66:TYR:CB	1:A:140:TRP:CE3	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ALA:O	1:A:129:VAL:HG23	2.02	0.60
2:B:73:LEU:HD23	3:C:18:GLY:HA3	1.84	0.60
2:B:95:LEU:O	2:B:99:LEU:N	2.35	0.60
3:C:217:LEU:HA	3:C:232:THR:HB	1.83	0.60
4:D:35:LEU:H	4:D:37:PRO:CD	2.15	0.60
4:Q:88:PRO:HG3	4:Q:114:VAL:HG22	1.83	0.60
1:A:127:ILE:HG21	1:A:195:ILE:HB	1.83	0.60
1:A:135:GLY:H	1:A:187:HIS:HD1	1.49	0.60
2:B:114:ILE:HG22	2:B:115:GLU:N	2.16	0.60
4:D:155:VAL:O	4:D:155:VAL:HG12	2.02	0.60
1:N:52:PHE:N	9:N:301:HEC:HAC	2.17	0.60
1:N:58:TYR:O	1:N:60:PRO:HD3	2.00	0.60
2:O:39:VAL:O	2:O:43:VAL:HG23	2.01	0.60
3:P:55:ASP:OD2	3:P:55:ASP:N	2.31	0.60
3:P:271:MET:CE	4:Q:26:THR:HG21	2.32	0.60
3:P:280:GLU:O	3:P:280:GLU:HG2	2.02	0.60
1:A:132:GLY:O	1:A:134:THR:N	2.35	0.59
4:D:108:CYS:HB2	4:D:113:CYS:O	2.02	0.59
5:E:18:ILE:HG13	5:E:19:ALA:H	1.67	0.59
2:O:81:LEU:HA	2:O:84:VAL:CG2	2.32	0.59
3:P:257:TRP:HA	3:P:257:TRP:CE3	2.35	0.59
1:A:16:ALA:O	1:A:17:LEU:HB2	2.02	0.59
2:B:38:TYR:HB2	3:C:276:LYS:CE	2.30	0.59
2:B:63:GLY:C	2:B:65:PRO:CD	2.75	0.59
3:C:251:ASP:HB3	3:C:254:ARG:HB2	1.83	0.59
3:C:283:GLN:C	3:C:285:ALA:H	2.09	0.59
1:N:52:PHE:CA	9:N:301:HEC:HAC	2.31	0.59
1:N:137:SER:HB3	1:N:148:VAL:HG21	1.83	0.59
2:O:39:VAL:O	2:O:43:VAL:N	2.35	0.59
10:O:1306:OPC:CAL	10:O:1306:OPC:CAP	2.78	0.59
4:Q:70:LEU:HD13	4:Q:71:GLU:HG2	1.83	0.59
1:A:119:ILE:O	1:A:122:VAL:HB	2.01	0.59
1:A:191:LEU:H	1:A:191:LEU:CD1	2.10	0.59
2:B:34:ASN:ND2	2:B:35:ASP:N	2.45	0.59
3:C:281:LYS:HD3	3:C:281:LYS:N	2.17	0.59
4:D:38:LEU:HD11	4:D:42:PHE:CE1	2.37	0.59
5:E:15:PHE:HA	5:E:18:ILE:HG13	1.84	0.59
7:G:16:LEU:C	7:G:18:TYR:N	2.58	0.59
8:H:1:ILE:HG23	8:H:2:ASP:N	2.15	0.59
2:O:59:PRO:HG2	3:P:146:LYS:HG3	1.84	0.59
6:S:28:LEU:O	6:S:30:ILE:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:29:HIS:CE1	1:N:31:ASN:HD21	2.20	0.59
3:P:26:HIS:CE1	3:P:154:ASN:HD21	2.19	0.59
3:P:40:VAL:CG1	3:P:247:ILE:HD11	2.28	0.59
1:A:47:GLN:NE2	1:A:89:SER:HB3	2.15	0.59
1:A:90:ALA:C	1:A:92:MET:H	2.11	0.59
1:A:113:PRO:HD2	1:A:114:ARG:NH1	2.16	0.59
2:B:32:TRP:H	2:B:33:PRO:HD2	1.64	0.59
2:B:125:ARG:NH1	2:B:125:ARG:CA	2.62	0.59
3:P:257:TRP:HA	3:P:257:TRP:HE3	1.67	0.59
4:Q:35:LEU:H	4:Q:37:PRO:CD	2.14	0.59
8:U:9:LEU:O	8:U:10:LEU:C	2.46	0.59
1:A:105:TYR:HA	1:A:110:PHE:CE2	2.37	0.59
3:C:34:VAL:O	3:C:34:VAL:HG23	2.02	0.59
8:U:18:ALA:O	8:U:21:VAL:CG2	2.49	0.59
2:B:85:PHE:C	2:B:85:PHE:CD1	2.79	0.59
3:C:188:ASP:H	3:C:193:VAL:CG2	2.12	0.59
3:C:277:LYS:C	3:C:279:VAL:H	2.11	0.59
1:N:27:PRO:O	2:O:29:GLU:HA	2.02	0.59
1:N:88:TRP:O	1:N:89:SER:C	2.46	0.59
2:O:57:LEU:HD11	7:T:10:PHE:HA	1.84	0.59
7:G:21:TYR:N	7:G:21:TYR:HD1	2.00	0.59
3:P:10:PRO:C	3:P:106:TYR:HE2	2.11	0.59
4:Q:65:LYS:HB2	4:Q:68:LYS:NZ	2.17	0.59
5:R:9:ILE:CG1	6:S:14:PHE:HB2	2.32	0.59
7:T:20:ALA:O	7:T:24:TYR:CE2	2.56	0.59
1:A:39:ILE:HD11	2:B:43:VAL:HG12	1.85	0.59
2:B:93:ASN:CG	2:B:94:LYS:H	2.03	0.59
3:C:44:THR:C	3:C:132:LEU:HD12	2.28	0.59
3:C:79:PRO:HG2	3:C:82:PHE:CG	2.37	0.59
3:C:139:ASP:OD2	3:C:142:ILE:HG13	2.03	0.59
3:C:280:GLU:C	3:C:282:VAL:N	2.56	0.59
4:D:80:LEU:HB2	4:D:90:TYR:HA	1.85	0.59
14:E:101:BCR:H362	6:F:18:PHE:CE2	2.38	0.59
1:N:160:VAL:HG13	1:N:164:LEU:HB2	1.83	0.59
2:O:85:PHE:C	2:O:85:PHE:CD1	2.81	0.59
2:O:127:PRO:O	2:O:129:ALA:N	2.35	0.59
2:O:133:PHE:C	2:O:135:PHE:N	2.60	0.59
3:P:172:PHE:HB2	3:P:211:ILE:HG13	1.85	0.59
5:R:3:LEU:HD12	5:R:6:VAL:HB	1.84	0.59
1:A:47:GLN:HG3	1:A:86:HIS:CE1	2.38	0.59
1:A:110:PHE:HB2	2:B:112:PRO:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:TRP:HA	2:B:82:TYR:CE2	2.38	0.59
3:C:26:HIS:CE1	3:C:154:ASN:HD21	2.21	0.59
3:C:122:GLU:O	3:C:122:GLU:HG2	2.03	0.59
4:D:123:LYS:O	4:D:125:LYS:HG3	2.03	0.59
6:F:26:LEU:HD23	6:F:26:LEU:C	2.28	0.59
1:N:114:ARG:HD3	1:N:208:LYS:HB3	1.85	0.59
1:N:157:ALA:HB1	2:O:95:LEU:HD22	1.84	0.59
2:O:129:ALA:HA	2:O:132:ILE:HD11	1.84	0.59
2:O:147:ALA:O	2:O:149:LEU:N	2.34	0.59
3:P:83:LYS:NZ	3:P:83:LYS:H	2.01	0.59
3:P:251:ASP:HB3	3:P:254:ARG:HB2	1.84	0.59
4:Q:70:LEU:HD13	4:Q:71:GLU:H	1.67	0.59
4:Q:165:TRP:O	4:Q:166:THR:HG23	2.03	0.59
1:A:24:LYS:HG3	1:A:24:LYS:O	2.02	0.58
1:A:39:ILE:HD12	2:B:47:THR:CG2	2.28	0.58
2:B:61:MET:HE2	3:C:146:LYS:O	2.03	0.58
4:D:38:LEU:O	4:D:38:LEU:HD12	2.02	0.58
4:D:132:GLN:O	4:D:133:TYR:HD2	1.85	0.58
7:G:8:LEU:HD23	7:G:12:THR:CG2	2.33	0.58
7:G:20:ALA:C	7:G:24:TYR:CE2	2.81	0.58
1:N:183:TYR:O	1:N:186:ALA:HB3	2.02	0.58
2:O:122:ASN:O	2:O:124:PHE:N	2.35	0.58
3:P:103:PHE:HB3	3:P:114:LEU:HD22	1.85	0.58
3:P:116:VAL:HG13	3:P:118:PRO:HG2	1.85	0.58
4:Q:36:TYR:O	4:Q:40:LYS:HB2	2.03	0.58
1:A:21:VAL:CG1	1:A:22:THR:H	2.14	0.58
1:A:57:TYR:HE1	1:A:76:VAL:HG13	1.67	0.58
1:A:119:ILE:O	1:A:120:SER:C	2.46	0.58
2:B:111:VAL:N	2:B:112:PRO:HD2	2.18	0.58
2:B:141:ILE:C	2:B:143:LEU:H	2.09	0.58
4:D:171:ARG:HB2	4:D:171:ARG:NH1	2.18	0.58
1:N:47:GLN:HG3	1:N:86:HIS:CE1	2.37	0.58
8:U:9:LEU:O	8:U:11:VAL:N	2.36	0.58
1:A:33:PHE:HE1	5:E:18:ILE:CD1	2.12	0.58
1:A:141:ASP:C	2:B:65:PRO:HG2	2.28	0.58
3:C:257:TRP:HA	3:C:257:TRP:CE3	2.35	0.58
5:R:5:ALA:C	5:R:7:PHE:H	2.12	0.58
1:A:124:LEU:HB3	9:A:302:HEC:HBB3	1.83	0.58
2:B:40:PHE:HA	2:B:43:VAL:CG2	2.31	0.58
4:D:65:LYS:HB2	4:D:68:LYS:NZ	2.18	0.58
4:D:94:GLU:C	4:D:96:LYS:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:113:CYS:HG	4:D:128:CYS:HG	0.75	0.58
1:N:83:ARG:HH12	2:O:60:ALA:HB1	1.67	0.58
2:O:34:ASN:CG	2:O:35:ASP:H	2.03	0.58
7:T:10:PHE:O	7:T:13:LEU:N	2.35	0.58
1:A:70:GLN:O	1:A:74:ASN:HB2	2.03	0.58
1:A:137:SER:HB2	1:A:144:GLY:O	2.02	0.58
1:N:17:LEU:HG	1:N:20:ASP:CB	2.30	0.58
1:N:94:VAL:O	1:N:98:ILE:HG13	2.03	0.58
1:N:115:GLU:O	1:N:118:TRP:HB3	2.03	0.58
2:O:82:TYR:O	2:O:86:GLN:N	2.34	0.58
2:O:145:ILE:HG22	2:O:145:ILE:O	2.04	0.58
3:P:50:VAL:HG21	3:P:129:PHE:CE1	2.38	0.58
3:P:127:ILE:HD12	3:P:127:ILE:N	2.18	0.58
2:B:126:ARG:CZ	2:B:128:VAL:HB	2.34	0.58
11:O:1309:BNT:CAM	3:P:148:ALA:H	2.15	0.58
5:R:18:ILE:HG13	5:R:19:ALA:H	1.68	0.58
1:A:154:VAL:HB	1:A:155:PRO:HD3	1.86	0.58
10:B:305:OPC:HBX1	10:B:305:OPC:HAE2	1.84	0.58
3:C:23:ALA:C	3:C:25:CYS:N	2.60	0.58
3:C:217:LEU:O	3:C:218:ILE:HG23	2.04	0.58
1:N:38:GLY:HA3	9:N:303:HEC:NC	2.19	0.58
2:O:85:PHE:O	2:O:86:GLN:C	2.45	0.58
1:A:95:LEU:CD2	1:A:99:LEU:HD21	2.34	0.58
1:A:97:MET:O	1:A:100:HIS:HB3	2.03	0.58
1:A:162:GLY:O	1:A:165:ILE:HG22	2.03	0.58
2:B:18:LEU:HD12	2:B:18:LEU:C	2.29	0.58
3:C:110:GLN:OE1	3:C:113:VAL:HG21	2.04	0.58
3:C:187:GLU:HG3	3:C:188:ASP:N	2.19	0.58
7:G:20:ALA:O	7:G:24:TYR:CE2	2.56	0.58
2:O:111:VAL:N	2:O:112:PRO:HD2	2.18	0.58
3:P:169:ASN:HD21	3:P:237:VAL:HG22	1.67	0.58
4:Q:38:LEU:HD11	4:Q:42:PHE:CE1	2.39	0.58
4:Q:63:ASN:HD22	4:Q:63:ASN:N	2.02	0.58
5:R:13:ALA:HA	6:S:14:PHE:CE1	2.39	0.58
7:T:18:TYR:HA	7:T:21:TYR:CG	2.38	0.58
1:A:71:TYR:O	1:A:71:TYR:HD2	1.87	0.58
4:D:70:LEU:HD12	4:D:71:GLU:H	1.67	0.58
4:D:146:LEU:HD13	4:D:177:TRP:CZ3	2.38	0.58
1:N:27:PRO:HA	2:O:33:PRO:CD	2.32	0.58
1:N:191:LEU:N	1:N:192:PRO:HD2	2.19	0.58
1:N:209:GLN:OE1	2:O:28:GLY:O	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:49:ALA:O	2:O:52:VAL:HB	2.03	0.58
2:O:64:GLU:CD	2:O:65:PRO:HD3	2.29	0.58
2:O:141:ILE:C	2:O:143:LEU:H	2.12	0.58
1:A:194:LEU:O	1:A:195:ILE:C	2.47	0.58
3:C:188:ASP:HB3	3:C:192:ASN:O	2.04	0.58
6:F:14:PHE:C	6:F:17:ILE:HG12	2.29	0.58
2:O:41:PRO:O	2:O:45:MET:HE2	2.04	0.58
2:O:87:ILE:O	2:O:88:LEU:C	2.46	0.58
3:P:102:TYR:H	3:P:118:PRO:CG	2.11	0.58
4:Q:154:THR:CG2	4:Q:155:VAL:H	2.08	0.58
5:R:25:ALA:C	5:R:26:ILE:HD12	2.28	0.58
14:R:1101:BCR:HC21	7:T:23:GLN:HE22	1.68	0.58
1:A:27:PRO:HG2	2:B:20:LYS:NZ	2.19	0.57
2:B:31:ALA:O	2:B:32:TRP:HB2	2.03	0.57
2:B:130:THR:O	2:B:133:PHE:HB3	2.03	0.57
3:C:118:PRO:C	3:C:120:PRO:HD3	2.29	0.57
4:D:125:LYS:HG2	4:D:132:GLN:HG2	1.86	0.57
5:E:3:LEU:O	5:E:4:GLY:C	2.47	0.57
5:E:26:ILE:HG23	5:E:30:LYS:CE	2.34	0.57
9:N:303:HEC:HBD2	9:N:303:HEC:HHA	1.85	0.57
3:P:3:PHE:N	3:P:3:PHE:CD1	2.72	0.57
3:P:60:GLN:NE2	3:P:157:ARG:HG3	2.19	0.57
1:A:165:ILE:HG23	1:A:166:SER:N	2.19	0.57
3:C:40:VAL:CG1	3:C:247:ILE:HD11	2.31	0.57
3:C:282:VAL:HG23	3:C:283:GLN:N	2.19	0.57
4:D:35:LEU:HD23	4:D:36:TYR:N	2.19	0.57
1:N:158:ILE:CG2	1:N:159:PRO:HD2	2.33	0.57
1:N:195:ILE:HG23	1:N:196:ALA:N	2.19	0.57
1:N:205:MET:O	1:N:207:ARG:N	2.37	0.57
10:O:1306:OPC:HAP2	10:O:1306:OPC:CAT	2.31	0.57
3:P:14:ARG:HG3	3:P:14:ARG:NH1	2.19	0.57
3:P:14:ARG:HG3	3:P:14:ARG:HH11	1.69	0.57
7:T:7:GLY:C	7:T:9:VAL:H	2.10	0.57
1:A:34:TYR:CD1	1:A:103:ARG:HD3	2.40	0.57
3:C:10:PRO:C	3:C:106:TYR:HE2	2.11	0.57
7:G:10:PHE:O	7:G:13:LEU:N	2.37	0.57
1:N:190:VAL:HG12	1:N:191:LEU:N	2.17	0.57
2:O:75:ILE:HG22	2:O:76:LEU:N	2.14	0.57
2:O:91:LEU:HD12	2:O:91:LEU:O	2.04	0.57
3:P:34:VAL:HG11	3:P:151:LEU:HD13	1.86	0.57
3:P:126:GLU:C	3:P:127:ILE:HD12	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:146:LEU:HD13	4:Q:177:TRP:CE3	2.39	0.57
1:A:189:PHE:O	1:A:193:TRP:HE3	1.87	0.57
2:B:39:VAL:C	2:B:42:VAL:H	2.10	0.57
2:B:94:LYS:C	2:B:96:LEU:N	2.59	0.57
2:B:104:VAL:N	2:B:105:PRO:CD	2.67	0.57
3:C:93:GLU:C	3:C:95:LYS:N	2.61	0.57
2:O:63:GLY:O	2:O:64:GLU:CB	2.52	0.57
3:P:277:LYS:C	3:P:279:VAL:H	2.11	0.57
4:Q:57:LYS:HG2	4:Q:62:ASN:O	2.04	0.57
4:Q:123:LYS:O	4:Q:125:LYS:HG3	2.04	0.57
1:A:117:THR:HG22	1:A:205:MET:HB2	1.86	0.57
1:A:205:MET:O	1:A:207:ARG:HG2	2.05	0.57
3:C:180:ILE:HG13	3:C:198:SER:O	2.05	0.57
3:C:275:LYS:HZ2	10:C:306:OPC:HGB3	1.69	0.57
1:N:119:ILE:HG23	2:O:109:ILE:CD1	2.31	0.57
2:O:94:LYS:C	2:O:96:LEU:N	2.57	0.57
2:O:127:PRO:C	2:O:129:ALA:N	2.62	0.57
4:Q:155:VAL:O	4:Q:155:VAL:HG12	2.03	0.57
5:R:3:LEU:O	5:R:4:GLY:C	2.45	0.57
3:C:136:PRO:HB3	3:C:142:ILE:HG22	1.85	0.57
3:C:136:PRO:HA	3:C:142:ILE:HB	1.87	0.57
4:D:45:PRO:O	4:D:46:SER:HB2	2.05	0.57
1:N:32:ILE:CG2	1:N:33:PHE:N	2.57	0.57
1:N:159:PRO:O	1:N:161:VAL:HG22	2.04	0.57
1:N:160:VAL:C	1:N:162:GLY:N	2.60	0.57
2:O:20:LYS:HB2	2:O:20:LYS:HZ2	1.69	0.57
3:P:217:LEU:HA	3:P:232:THR:HB	1.87	0.57
1:A:62:VAL:HG23	1:A:63:THR:N	2.14	0.57
2:B:79:TRP:CH2	5:E:1:MET:CA	2.87	0.57
1:N:83:ARG:HG3	1:N:84:SER:N	2.18	0.57
1:N:174:SER:O	1:N:175:VAL:HG23	2.05	0.57
4:Q:146:LEU:HD13	4:Q:177:TRP:CZ3	2.40	0.57
6:S:29:LYS:HG2	6:S:29:LYS:O	2.05	0.57
1:A:21:VAL:HG12	1:A:22:THR:HG22	1.86	0.57
2:B:40:PHE:CA	2:B:43:VAL:HG23	2.34	0.57
10:B:305:OPC:HAH1	10:B:305:OPC:HBP2	1.86	0.57
4:D:116:PRO:CD	4:D:127:PRO:HD3	2.35	0.57
1:N:85:ILE:HG23	2:O:51:ILE:CG2	2.35	0.57
2:O:64:GLU:CG	2:O:65:PRO:CD	2.81	0.57
8:U:2:ASP:O	8:U:4:LEU:N	2.37	0.57
1:N:33:PHE:CE1	1:N:34:TYR:CE1	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:43:VAL:HA	7:T:23:GLN:OE1	2.04	0.57
5:R:26:ILE:HG23	5:R:30:LYS:CE	2.35	0.57
1:A:88:TRP:O	1:A:89:SER:C	2.47	0.57
2:B:96:LEU:HD11	2:B:100:LEU:HD12	1.86	0.57
3:C:176:ALA:H	3:C:228:GLY:HA3	1.70	0.57
4:D:36:TYR:O	4:D:40:LYS:HB2	2.05	0.57
4:D:92:VAL:HG12	4:D:93:VAL:N	2.18	0.57
8:H:9:LEU:O	8:H:10:LEU:C	2.47	0.57
2:O:77:PRO:CG	2:O:81:LEU:HB3	2.34	0.57
2:O:125:ARG:HB3	2:O:125:ARG:HH11	1.67	0.57
3:P:188:ASP:HB3	3:P:192:ASN:O	2.04	0.57
4:Q:107:VAL:O	4:Q:107:VAL:HG12	2.04	0.57
4:Q:175:LYS:HD3	4:Q:176:PRO:HD2	1.86	0.57
6:S:26:LEU:HD23	6:S:26:LEU:C	2.30	0.57
2:B:84:VAL:HG11	12:B:201:CLA:H42	1.86	0.56
3:C:279:VAL:O	3:C:279:VAL:HG12	2.04	0.56
5:E:13:ALA:HA	6:F:14:PHE:CE1	2.40	0.56
6:F:28:LEU:O	6:F:30:ILE:N	2.37	0.56
7:G:29:GLU:HG3	7:G:30:LEU:N	2.19	0.56
1:N:132:GLY:O	1:N:134:THR:N	2.38	0.56
1:N:154:VAL:HB	1:N:155:PRO:HD3	1.87	0.56
11:O:1309:BNT:CAM	3:P:148:ALA:N	2.67	0.56
7:T:20:ALA:C	7:T:24:TYR:CE2	2.83	0.56
2:B:56:VAL:HG12	2:B:57:LEU:N	2.19	0.56
2:B:124:PHE:CZ	5:E:23:ILE:HD11	2.40	0.56
3:C:157:ARG:O	3:C:159:GLN:NE2	2.38	0.56
6:F:25:VAL:O	6:F:28:LEU:HB2	2.04	0.56
7:G:7:GLY:C	7:G:9:VAL:H	2.10	0.56
10:B:305:OPC:HCB3	10:B:305:OPC:HAU1	1.87	0.56
3:C:1:TYR:O	3:C:4:TRP:HB2	2.05	0.56
3:C:34:VAL:HG11	3:C:151:LEU:HD13	1.86	0.56
3:C:60:GLN:NE2	3:C:157:ARG:HG3	2.19	0.56
3:C:120:PRO:CB	3:C:124:TYR:HB2	2.35	0.56
6:F:35:LYS:H	6:F:35:LYS:HD2	1.70	0.56
6:F:35:LYS:HD2	6:F:35:LYS:N	2.20	0.56
1:N:104:VAL:O	1:N:105:TYR:C	2.48	0.56
9:N:302:HEC:HMD3	9:N:302:HEC:HBD2	1.87	0.56
3:P:187:GLU:HG3	3:P:188:ASP:N	2.20	0.56
5:R:26:ILE:HG23	5:R:30:LYS:NZ	2.20	0.56
8:U:7:VAL:O	8:U:8:ALA:C	2.49	0.56
1:A:78:PHE:HD1	4:D:37:PRO:O	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:VAL:O	1:A:98:ILE:HG13	2.05	0.56
2:B:91:LEU:HD21	2:B:96:LEU:HD12	1.86	0.56
2:B:109:ILE:HG23	2:B:110:LEU:HD23	1.88	0.56
3:C:66:SER:O	3:C:68:VAL:HG22	2.06	0.56
4:D:123:LYS:O	4:D:125:LYS:N	2.38	0.56
4:D:132:GLN:NE2	4:D:141:ARG:HB2	2.21	0.56
8:H:18:ALA:O	8:H:21:VAL:CG2	2.52	0.56
1:A:31:ASN:CG	1:A:211:ILE:HD11	2.31	0.56
2:B:39:VAL:O	2:B:43:VAL:N	2.36	0.56
8:H:9:LEU:HD22	8:H:13:PHE:HZ	1.69	0.56
1:N:117:THR:HG22	1:N:205:MET:HB2	1.87	0.56
2:O:127:PRO:HA	2:O:130:THR:HB	1.87	0.56
3:P:272:LEU:HD21	4:Q:24:PHE:CZ	2.41	0.56
4:Q:27:VAL:C	4:Q:29:GLY:N	2.62	0.56
4:Q:123:LYS:O	4:Q:125:LYS:N	2.39	0.56
6:S:8:TYR:HD2	6:S:9:ALA:N	2.03	0.56
3:C:169:ASN:ND2	3:C:237:VAL:H	2.03	0.56
3:C:188:ASP:CG	3:C:192:ASN:HB3	2.30	0.56
6:F:27:LEU:CD1	6:F:27:LEU:N	2.68	0.56
7:G:8:LEU:HD23	7:G:12:THR:HG23	1.88	0.56
1:N:25:TYR:O	1:N:26:VAL:CG2	2.54	0.56
1:N:41:LEU:O	1:N:42:THR:C	2.49	0.56
1:N:114:ARG:CD	1:N:208:LYS:HE2	2.35	0.56
3:P:205:LYS:HE2	3:P:206:THR:N	2.20	0.56
1:A:30:VAL:O	1:A:211:ILE:HD13	2.05	0.56
1:A:52:PHE:O	1:A:55:THR:N	2.32	0.56
2:B:34:ASN:ND2	2:B:35:ASP:OD1	2.37	0.56
2:B:127:PRO:C	2:B:129:ALA:H	2.13	0.56
2:B:133:PHE:C	2:B:135:PHE:H	2.11	0.56
3:C:102:TYR:O	3:C:118:PRO:HD2	2.05	0.56
5:E:17:GLY:O	5:E:22:ILE:HG21	2.06	0.56
8:H:2:ASP:O	8:H:4:LEU:N	2.38	0.56
1:N:189:PHE:O	1:N:193:TRP:HE3	1.88	0.56
2:O:116:ASN:C	2:O:116:ASN:ND2	2.61	0.56
2:O:133:PHE:HB2	12:O:1201:CLA:CAB	2.36	0.56
10:B:305:OPC:CAO	10:B:305:OPC:CAS	2.84	0.56
4:D:81:VAL:HG12	4:D:82:GLN:N	2.15	0.56
5:E:9:ILE:CG1	6:F:14:PHE:HB2	2.36	0.56
1:N:47:GLN:HE22	1:N:90:ALA:N	2.03	0.56
1:N:47:GLN:HB3	9:N:301:HEC:HBB2	1.88	0.56
2:O:35:ASP:HB3	3:P:276:LYS:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:38:TYR:C	3:P:272:LEU:HD22	2.30	0.56
3:P:118:PRO:C	3:P:120:PRO:HD3	2.31	0.56
1:A:14:ILE:O	1:A:15:GLN:O	2.24	0.56
1:A:122:VAL:HA	9:A:302:HEC:HMC1	1.86	0.56
2:B:40:PHE:N	2:B:41:PRO:CD	2.69	0.56
2:B:89:ARG:O	2:B:91:LEU:N	2.39	0.56
3:C:146:LYS:HG2	3:C:248:VAL:CG2	2.32	0.56
4:D:154:THR:CG2	4:D:155:VAL:H	2.07	0.56
4:D:175:LYS:HD3	4:D:176:PRO:HD2	1.88	0.56
1:N:66:TYR:CB	2:O:65:PRO:HG2	2.35	0.56
2:O:42:VAL:HG23	3:P:272:LEU:HB3	1.87	0.56
2:O:89:ARG:O	2:O:91:LEU:N	2.38	0.56
2:O:122:ASN:ND2	5:R:27:LYS:HB2	2.21	0.56
3:P:93:GLU:O	3:P:95:LYS:N	2.39	0.56
1:A:43:CYS:HA	1:A:46:ILE:HD12	1.88	0.56
1:A:104:VAL:O	1:A:105:TYR:C	2.49	0.56
2:B:82:TYR:O	2:B:83:PRO:C	2.48	0.56
3:C:127:ILE:HD12	3:C:127:ILE:N	2.21	0.56
1:A:170:ARG:HA	1:A:179:THR:HG23	1.87	0.55
3:C:241:GLY:O	3:C:242:GLN:CB	2.54	0.55
1:N:15:GLN:NE2	1:N:15:GLN:CA	2.67	0.55
1:N:90:ALA:O	1:N:92:MET:N	2.39	0.55
1:N:113:PRO:HB3	2:O:27:TYR:HE1	1.70	0.55
1:N:157:ALA:O	1:N:158:ILE:HB	2.06	0.55
3:P:120:PRO:CB	3:P:124:TYR:HB2	2.36	0.55
1:A:74:ASN:HB3	1:A:75:GLU:OE2	2.06	0.55
4:D:137:GLY:O	4:D:138:ARG:C	2.48	0.55
1:N:61:THR:HG22	1:N:64:GLU:HB3	1.89	0.55
1:N:167:ASP:O	1:N:169:LEU:N	2.38	0.55
3:P:180:ILE:HG13	3:P:198:SER:O	2.05	0.55
3:P:271:MET:CG	4:Q:23:ALA:HA	2.36	0.55
1:A:214:PRO:CG	5:E:29:ILE:HG21	2.36	0.55
3:C:55:ASP:OD2	3:C:55:ASP:N	2.32	0.55
3:C:177:THR:HA	3:C:227:ALA:HA	1.88	0.55
3:P:27:LEU:HD12	3:P:27:LEU:O	2.06	0.55
5:R:14:LEU:O	5:R:17:GLY:C	2.49	0.55
10:B:305:OPC:HBT1	10:C:306:OPC:CBR	2.35	0.55
3:C:161:TYR:CE1	3:C:167:SER:HA	2.42	0.55
3:C:249:LEU:HD12	3:C:249:LEU:N	2.20	0.55
7:G:14:GLY:C	7:G:16:LEU:H	2.14	0.55
7:G:30:LEU:H	7:G:30:LEU:CD1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:165:ILE:O	1:N:165:ILE:HD13	2.06	0.55
1:N:191:LEU:H	1:N:191:LEU:CD1	2.10	0.55
3:P:93:GLU:C	3:P:95:LYS:N	2.60	0.55
1:A:190:VAL:HG12	1:A:191:LEU:N	2.19	0.55
2:B:65:PRO:O	2:B:68:PRO:HD3	2.06	0.55
3:C:14:ARG:HH11	3:C:14:ARG:HG3	1.69	0.55
3:C:172:PHE:H	3:C:231:LEU:CG	2.19	0.55
5:E:28:SER:C	5:E:30:LYS:N	2.63	0.55
6:F:10:ALA:C	6:F:12:LEU:N	2.63	0.55
8:H:3:VAL:O	8:H:6:TRP:N	2.39	0.55
1:N:33:PHE:O	1:N:35:CYS:SG	2.64	0.55
1:N:47:GLN:NE2	1:N:89:SER:HB3	2.16	0.55
1:N:61:THR:O	1:N:63:THR:N	2.39	0.55
1:N:119:ILE:CG2	2:O:109:ILE:HD11	2.31	0.55
2:O:114:ILE:HG22	2:O:115:GLU:N	2.19	0.55
3:P:197:VAL:HG13	3:P:211:ILE:HG22	1.87	0.55
6:S:9:ALA:HA	6:S:12:LEU:HD12	1.87	0.55
3:C:169:ASN:HD21	3:C:237:VAL:HG22	1.72	0.55
1:N:116:LEU:H	1:N:116:LEU:HD12	1.71	0.55
3:P:161:TYR:CE1	3:P:167:SER:HA	2.42	0.55
4:Q:59:LYS:HB2	4:Q:59:LYS:NZ	2.21	0.55
6:S:14:PHE:C	6:S:17:ILE:HG12	2.32	0.55
7:T:21:TYR:N	7:T:21:TYR:HD1	2.02	0.55
3:C:34:VAL:CG1	3:C:151:LEU:HD22	2.36	0.55
4:D:58:ASP:O	4:D:59:LYS:HB2	2.07	0.55
2:O:24:HIS:C	2:O:24:HIS:ND1	2.61	0.55
3:P:241:GLY:O	3:P:242:GLN:CB	2.54	0.55
6:S:24:GLY:CA	6:S:27:LEU:HD22	2.37	0.55
8:U:2:ASP:OD1	8:U:3:VAL:N	2.39	0.55
3:C:10:PRO:CA	3:C:106:TYR:HE2	2.18	0.55
3:C:48:ALA:HB3	3:C:129:PHE:HB2	1.87	0.55
6:F:29:LYS:HG2	6:F:29:LYS:O	2.07	0.55
2:O:38:TYR:HB2	3:P:276:LYS:HE2	1.88	0.55
6:S:10:ALA:C	6:S:12:LEU:N	2.64	0.55
2:B:96:LEU:O	2:B:96:LEU:HD13	2.07	0.55
11:B:309:BNT:HAM3	3:C:148:ALA:HB2	1.89	0.55
3:C:102:TYR:H	3:C:118:PRO:CG	2.09	0.55
3:C:171:VAL:HG12	3:C:231:LEU:CD1	2.31	0.55
1:N:170:ARG:HB3	1:N:179:THR:HG23	1.88	0.55
2:O:40:PHE:N	2:O:41:PRO:CD	2.70	0.55
2:O:63:GLY:O	2:O:64:GLU:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:85:ALA:HA	3:P:132:LEU:HB2	1.89	0.55
3:P:180:ILE:HA	3:P:200:GLN:HB2	1.89	0.55
3:P:200:GLN:O	3:P:206:THR:HA	2.07	0.55
4:Q:143:PRO:O	4:Q:145:PRO:HD3	2.07	0.55
1:A:41:LEU:O	1:A:42:THR:C	2.50	0.55
1:A:114:ARG:HG3	1:A:208:LYS:HD3	1.86	0.55
1:A:191:LEU:N	1:A:192:PRO:HD2	2.21	0.55
8:H:9:LEU:HD22	8:H:13:PHE:CZ	2.41	0.55
1:N:52:PHE:C	1:N:54:MET:N	2.63	0.55
1:N:63:THR:C	1:N:65:ALA:N	2.54	0.55
3:P:188:ASP:CG	3:P:192:ASN:HB3	2.32	0.55
3:P:249:LEU:HD12	3:P:249:LEU:N	2.20	0.55
4:Q:51:GLY:C	4:Q:54:THR:HG22	2.32	0.55
4:Q:63:ASN:H	4:Q:63:ASN:HD22	1.53	0.55
1:A:214:PRO:CD	5:E:29:ILE:HG21	2.36	0.54
2:B:135:PHE:C	2:B:135:PHE:CD1	2.83	0.54
3:C:22:CYS:HB2	3:C:240:PHE:CZ	2.42	0.54
3:C:280:GLU:HA	3:C:282:VAL:HG22	1.89	0.54
4:D:51:GLY:CA	4:D:84:LEU:HD21	2.36	0.54
1:N:113:PRO:HB3	2:O:27:TYR:CE1	2.42	0.54
1:N:167:ASP:C	1:N:169:LEU:N	2.63	0.54
6:S:25:VAL:O	6:S:28:LEU:HB2	2.07	0.54
1:A:60:PRO:HB3	1:A:184:TYR:CD1	2.42	0.54
3:C:120:PRO:HB2	3:C:124:TYR:HB2	1.89	0.54
3:C:217:LEU:HD23	3:C:232:THR:OG1	2.07	0.54
7:G:19:ALA:O	7:G:20:ALA:C	2.50	0.54
1:N:108:GLY:O	1:N:111:LYS:HB2	2.06	0.54
1:N:165:ILE:HG23	1:N:166:SER:N	2.21	0.54
2:O:53:ALA:O	2:O:57:LEU:CB	2.52	0.54
2:O:98:VAL:O	2:O:99:LEU:C	2.50	0.54
3:P:199:ILE:HG22	3:P:200:GLN:N	2.15	0.54
3:P:252:PRO:C	3:P:254:ARG:N	2.64	0.54
1:A:52:PHE:HA	1:A:55:THR:HG23	1.89	0.54
1:A:62:VAL:HG13	1:A:177:GLN:CG	2.25	0.54
1:A:103:ARG:NH1	1:A:103:ARG:HG3	2.21	0.54
1:A:202:HIS:O	1:A:206:ILE:CG1	2.53	0.54
2:B:133:PHE:C	2:B:135:PHE:N	2.62	0.54
10:B:305:OPC:HAV	10:B:305:OPC:HAG1	1.89	0.54
3:C:205:LYS:HE2	3:C:205:LYS:C	2.32	0.54
6:F:27:LEU:HD13	6:F:27:LEU:H	1.71	0.54
3:P:280:GLU:HA	3:P:282:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:64:VAL:HG13	4:Q:68:LYS:HG3	1.88	0.54
4:Q:115:VAL:HG11	4:Q:124:PHE:O	2.07	0.54
4:Q:145:PRO:O	4:Q:146:LEU:CB	2.55	0.54
4:Q:165:TRP:HE3	4:Q:167:GLU:OE2	1.89	0.54
7:T:28:ASN:CG	7:T:30:LEU:HD21	2.31	0.54
1:A:137:SER:HB3	1:A:148:VAL:HG21	1.88	0.54
2:B:96:LEU:HD13	2:B:100:LEU:HB2	1.88	0.54
2:B:115:GLU:OE2	2:B:126:ARG:NH2	2.41	0.54
4:D:50:VAL:O	4:D:84:LEU:HD11	2.06	0.54
5:E:25:ALA:O	5:E:29:ILE:HD12	2.07	0.54
1:N:103:ARG:HG3	1:N:103:ARG:NH1	2.23	0.54
2:O:62:VAL:HG22	11:O:1309:BNT:CAL	2.36	0.54
2:O:82:TYR:O	2:O:83:PRO:C	2.48	0.54
3:P:140:LYS:H	3:P:140:LYS:HD2	1.73	0.54
14:R:1101:BCR:HC21	7:T:23:GLN:NE2	2.23	0.54
2:B:36:LEU:C	2:B:39:VAL:HG13	2.32	0.54
2:B:135:PHE:C	2:B:137:THR:N	2.52	0.54
3:C:26:HIS:CD2	3:C:158:GLY:HA2	2.43	0.54
3:C:54:TYR:CD1	3:C:58:LEU:HD22	2.42	0.54
3:C:61:VAL:HG23	3:C:62:ALA:N	2.23	0.54
5:E:5:ALA:C	5:E:7:PHE:H	2.15	0.54
6:F:9:ALA:HA	6:F:12:LEU:HD12	1.87	0.54
6:F:16:LEU:HA	6:F:19:VAL:HB	1.90	0.54
3:P:89:ARG:O	3:P:90:ILE:C	2.50	0.54
5:R:2:ILE:O	5:R:3:LEU:C	2.49	0.54
1:A:35:CYS:HA	9:A:303:HEC:C3B	2.36	0.54
2:B:100:LEU:HD23	2:B:100:LEU:O	2.08	0.54
2:B:125:ARG:O	2:B:127:PRO:CD	2.52	0.54
3:C:116:VAL:HG13	3:C:118:PRO:HG2	1.90	0.54
3:C:262:ILE:O	3:C:265:VAL:N	2.40	0.54
4:D:118:ASN:C	4:D:120:ALA:N	2.66	0.54
5:E:14:LEU:O	5:E:17:GLY:C	2.50	0.54
1:N:28:PRO:O	2:O:30:PRO:HB2	2.08	0.54
1:N:119:ILE:O	1:N:120:SER:C	2.51	0.54
5:R:15:PHE:HA	5:R:18:ILE:HG13	1.89	0.54
1:A:135:GLY:HA2	1:A:138:LEU:HG	1.89	0.54
2:B:87:ILE:O	2:B:88:LEU:C	2.51	0.54
4:D:143:PRO:O	4:D:145:PRO:HD3	2.08	0.54
2:O:45:MET:HE3	3:P:269:GLN:HB3	1.89	0.54
5:R:24:PHE:O	5:R:26:ILE:N	2.41	0.54
1:A:90:ALA:O	1:A:92:MET:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:C	1:A:116:LEU:HD12	2.33	0.54
1:A:157:ALA:C	1:A:158:ILE:HG13	2.32	0.54
1:A:173:SER:HB2	4:Q:85:LYS:O	2.07	0.54
2:B:41:PRO:O	2:B:45:MET:HE2	2.08	0.54
3:C:14:ARG:HG3	3:C:14:ARG:NH1	2.21	0.54
5:E:7:PHE:C	5:E:9:ILE:N	2.66	0.54
1:N:43:CYS:HA	1:N:46:ILE:HD12	1.90	0.54
2:O:43:VAL:CG2	7:T:23:GLN:OE1	2.50	0.54
2:O:78:GLU:C	2:O:80:TYR:N	2.65	0.54
2:O:135:PHE:HA	2:O:138:LEU:HB2	1.90	0.54
3:P:120:PRO:HB2	3:P:124:TYR:HB2	1.89	0.54
1:A:52:PHE:C	1:A:54:MET:N	2.62	0.54
2:B:83:PRO:HB2	12:B:201:CLA:CMD	2.38	0.54
3:C:31:PRO:O	3:C:32:ALA:HB2	2.08	0.54
3:C:54:TYR:HD2	3:C:155:ARG:HH11	1.56	0.54
4:D:27:VAL:C	4:D:29:GLY:N	2.64	0.54
7:G:28:ASN:ND2	7:G:30:LEU:HD22	2.18	0.54
8:H:9:LEU:O	8:H:11:VAL:N	2.41	0.54
3:P:46:PHE:CE1	3:P:131:VAL:HG13	2.43	0.54
3:P:61:VAL:HG23	3:P:62:ALA:N	2.23	0.54
3:P:188:ASP:H	3:P:193:VAL:CG2	2.17	0.54
3:P:282:VAL:HG23	3:P:283:GLN:N	2.21	0.54
4:Q:106:ALA:HB1	4:Q:114:VAL:HG13	1.90	0.54
6:S:24:GLY:HA2	6:S:27:LEU:HD22	1.89	0.54
3:C:76:LEU:HD23	3:C:76:LEU:C	2.33	0.54
3:C:83:LYS:NZ	3:C:83:LYS:H	2.06	0.54
3:C:205:LYS:HE2	3:C:206:THR:N	2.23	0.54
3:C:268:ALA:C	3:C:270:LEU:N	2.65	0.54
8:H:6:TRP:O	8:H:9:LEU:HB2	2.07	0.54
1:N:88:TRP:HB2	2:O:51:ILE:HG23	1.90	0.54
1:N:90:ALA:C	1:N:92:MET:N	2.63	0.54
1:N:106:LEU:HD21	2:O:133:PHE:CE1	2.43	0.54
1:N:194:LEU:O	1:N:195:ILE:C	2.51	0.54
2:O:38:TYR:CD1	2:O:38:TYR:N	2.75	0.54
2:O:53:ALA:HA	3:P:258:MET:HE2	1.90	0.54
2:O:100:LEU:HD23	2:O:100:LEU:O	2.07	0.54
5:R:16:PHE:CE2	14:R:1101:BCR:H373	2.41	0.54
1:A:178:ALA:O	1:A:179:THR:C	2.52	0.53
2:B:127:PRO:C	2:B:129:ALA:N	2.66	0.53
3:C:91:PRO:C	3:C:92:GLU:HG2	2.33	0.53
5:E:16:PHE:CE2	14:E:101:BCR:H373	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:58:TYR:CE2	1:N:60:PRO:HB3	2.42	0.53
1:N:135:GLY:HA2	1:N:138:LEU:CG	2.37	0.53
1:A:52:PHE:C	1:A:54:MET:H	2.17	0.53
1:A:167:ASP:C	1:A:169:LEU:N	2.66	0.53
1:N:127:ILE:HG21	1:N:195:ILE:HB	1.90	0.53
3:P:277:LYS:HE3	7:T:27:PRO:HD2	1.90	0.53
1:A:14:ILE:HD12	1:A:14:ILE:C	2.33	0.53
1:A:24:LYS:NZ	1:A:26:VAL:H	2.06	0.53
2:B:34:ASN:HD22	2:B:35:ASP:CG	2.17	0.53
2:B:41:PRO:HB3	10:B:305:OPC:HBI2	1.90	0.53
3:C:85:ALA:HA	3:C:132:LEU:HB2	1.89	0.53
3:C:126:GLU:C	3:C:127:ILE:HD12	2.34	0.53
4:D:90:TYR:HD2	4:D:104:ILE:HD11	1.73	0.53
5:E:28:SER:C	5:E:30:LYS:H	2.16	0.53
7:G:9:VAL:HG23	7:G:10:PHE:N	2.20	0.53
3:P:104:GLN:NE2	3:P:104:GLN:N	2.57	0.53
3:P:231:LEU:HD21	3:P:233:ASN:O	2.09	0.53
4:Q:90:TYR:CD2	4:Q:104:ILE:HD11	2.44	0.53
7:T:19:ALA:O	7:T:20:ALA:C	2.51	0.53
1:A:90:ALA:C	1:A:92:MET:N	2.66	0.53
1:A:116:LEU:C	1:A:118:TRP:N	2.63	0.53
1:A:146:TRP:CB	2:B:75:ILE:HD11	2.39	0.53
1:A:176:GLY:O	1:A:178:ALA:N	2.41	0.53
1:A:205:MET:O	1:A:207:ARG:N	2.41	0.53
2:B:34:ASN:CG	2:B:35:ASP:H	2.03	0.53
10:B:305:OPC:HBA1	10:C:306:OPC:CBX	2.36	0.53
3:C:53:PRO:O	3:C:54:TYR:CD2	2.60	0.53
5:E:2:ILE:O	5:E:3:LEU:C	2.51	0.53
1:N:170:ARG:NH1	1:N:173:SER:O	2.41	0.53
1:N:193:TRP:O	1:N:197:VAL:HG23	2.08	0.53
10:N:1305:OPC:HCB2	10:N:1305:OPC:CAY	2.39	0.53
2:O:26:TYR:O	2:O:26:TYR:CD1	2.60	0.53
3:P:44:THR:O	3:P:132:LEU:HA	2.08	0.53
3:P:54:TYR:CD1	3:P:58:LEU:HD22	2.44	0.53
3:P:101:VAL:HB	3:P:118:PRO:HB2	1.87	0.53
4:Q:115:VAL:HG22	4:Q:126:CYS:CB	2.37	0.53
5:R:7:PHE:C	5:R:9:ILE:N	2.66	0.53
8:U:6:TRP:O	8:U:9:LEU:HB2	2.07	0.53
1:A:39:ILE:HG23	2:B:47:THR:CG2	2.35	0.53
1:A:194:LEU:N	1:A:194:LEU:HD23	2.22	0.53
9:A:303:HEC:HBC2	2:B:44:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:7:PHE:C	5:E:9:ILE:H	2.17	0.53
1:N:78:PHE:O	1:N:79:GLY:C	2.51	0.53
1:N:116:LEU:C	1:N:118:TRP:H	2.17	0.53
1:N:211:ILE:O	1:N:212:SER:OG	2.23	0.53
2:O:93:ASN:O	2:O:94:LYS:HB2	2.08	0.53
2:O:130:THR:O	2:O:133:PHE:N	2.39	0.53
3:P:17:THR:OG1	3:P:18:GLY:N	2.41	0.53
3:P:120:PRO:HG2	3:P:124:TYR:CD1	2.44	0.53
4:Q:58:ASP:O	4:Q:59:LYS:HB2	2.08	0.53
2:B:82:TYR:O	2:B:86:GLN:N	2.35	0.53
2:B:115:GLU:OE2	2:B:126:ARG:CZ	2.57	0.53
1:N:17:LEU:CG	1:N:20:ASP:HB2	2.35	0.53
1:N:27:PRO:HA	2:O:33:PRO:HG3	1.91	0.53
1:N:52:PHE:HA	1:N:55:THR:HG23	1.90	0.53
1:N:54:MET:C	1:N:56:PHE:N	2.64	0.53
1:N:118:TRP:HZ3	2:O:109:ILE:HA	1.70	0.53
2:O:95:LEU:N	2:O:95:LEU:HD23	2.24	0.53
4:Q:118:ASN:C	4:Q:120:ALA:N	2.64	0.53
1:A:34:TYR:OH	1:A:107:THR:HG21	2.09	0.53
1:A:113:PRO:HA	1:N:16:ALA:HB1	1.86	0.53
1:A:165:ILE:O	1:A:165:ILE:HD13	2.09	0.53
2:B:124:PHE:HZ	5:E:27:LYS:CB	2.21	0.53
3:C:89:ARG:HG3	3:C:89:ARG:NH1	2.23	0.53
3:C:213:ALA:O	3:C:215:PRO:HD2	2.08	0.53
3:C:280:GLU:O	3:C:280:GLU:HG2	2.08	0.53
10:C:306:OPC:HAL2	10:C:306:OPC:HAP2	1.90	0.53
1:N:166:SER:OG	1:N:170:ARG:NH2	2.42	0.53
2:O:57:LEU:CD1	7:T:10:PHE:HA	2.39	0.53
2:O:99:LEU:O	2:O:102:ALA:N	2.42	0.53
3:P:151:LEU:HG	3:P:152:GLY:N	2.23	0.53
3:P:277:LYS:NZ	7:T:27:PRO:HD2	2.24	0.53
6:S:23:LEU:O	6:S:24:GLY:C	2.52	0.53
7:T:9:VAL:HG23	7:T:10:PHE:N	2.18	0.53
1:A:42:THR:O	1:A:44:PHE:N	2.42	0.53
11:B:309:BNT:HAM1	3:C:148:ALA:N	2.24	0.53
3:C:118:PRO:O	3:C:120:PRO:HD3	2.09	0.53
3:C:168:ASN:C	3:C:168:ASN:HD22	2.16	0.53
4:D:115:VAL:HG13	4:D:126:CYS:CA	2.36	0.53
5:E:2:ILE:HG23	5:E:3:LEU:N	2.19	0.53
1:N:27:PRO:HD2	2:O:29:GLU:HB3	1.90	0.53
1:N:32:ILE:HD11	7:T:26:ARG:HH22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:41:LEU:HD21	1:N:45:LEU:HD11	1.90	0.53
1:N:170:ARG:HD2	1:N:171:GLY:N	2.23	0.53
2:O:75:ILE:CG2	2:O:76:LEU:H	2.11	0.53
2:O:125:ARG:O	2:O:126:ARG:HB3	2.07	0.53
3:P:22:CYS:HB2	3:P:240:PHE:CZ	2.44	0.53
3:P:91:PRO:HB2	3:P:95:LYS:CE	2.39	0.53
1:A:146:TRP:HB3	2:B:75:ILE:HD11	1.90	0.53
2:B:37:LEU:HB2	2:B:38:TYR:CE1	2.44	0.53
3:C:83:LYS:HZ1	3:C:133:SER:C	2.17	0.53
2:O:79:TRP:CZ3	5:R:4:GLY:HA3	2.43	0.53
3:P:61:VAL:O	3:P:62:ALA:HB2	2.07	0.53
4:Q:102:TYR:CG	4:Q:150:LEU:HD23	2.43	0.53
1:A:25:TYR:O	1:A:26:VAL:HG13	2.09	0.53
1:A:33:PHE:CE1	5:E:14:LEU:HD12	2.44	0.53
2:B:50:CYS:C	2:B:52:VAL:N	2.66	0.53
2:B:105:PRO:HG2	2:B:106:LEU:N	2.21	0.53
3:C:76:LEU:HD23	3:C:77:MET:N	2.23	0.53
3:C:90:ILE:HG22	3:C:90:ILE:O	2.07	0.53
3:C:91:PRO:HB2	3:C:95:LYS:CE	2.39	0.53
4:D:145:PRO:O	4:D:146:LEU:CB	2.57	0.53
1:N:17:LEU:HG	1:N:20:ASP:OD1	2.08	0.53
1:N:116:LEU:HD12	1:N:117:THR:H	1.74	0.53
2:O:52:VAL:O	2:O:53:ALA:C	2.52	0.53
3:P:53:PRO:O	3:P:54:TYR:CD2	2.62	0.53
4:Q:38:LEU:O	4:Q:38:LEU:HD12	2.08	0.53
3:C:101:VAL:HB	3:C:118:PRO:HB2	1.88	0.52
3:C:205:LYS:HZ3	3:C:207:VAL:CG1	2.21	0.52
3:C:219:VAL:CG1	3:C:220:SER:H	2.21	0.52
5:E:25:ALA:C	5:E:26:ILE:HD12	2.34	0.52
1:N:34:TYR:CD1	1:N:34:TYR:N	2.76	0.52
1:N:105:TYR:HH	2:O:129:ALA:HB1	1.68	0.52
2:O:96:LEU:HD11	2:O:100:LEU:HD12	1.91	0.52
3:P:83:LYS:HZ1	3:P:133:SER:C	2.18	0.52
3:P:89:ARG:HG3	3:P:89:ARG:NH1	2.24	0.52
4:Q:90:TYR:HD2	4:Q:104:ILE:HD11	1.75	0.52
1:A:212:SER:O	5:E:26:ILE:HG12	2.08	0.52
2:B:98:VAL:O	2:B:99:LEU:C	2.51	0.52
3:C:3:PHE:CD1	3:C:3:PHE:N	2.72	0.52
4:D:90:TYR:CD2	4:D:104:ILE:HD11	2.44	0.52
4:D:118:ASN:ND2	4:D:120:ALA:H	2.07	0.52
1:N:158:ILE:HG22	1:N:161:VAL:CG2	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:39:VAL:O	2:O:42:VAL:N	2.43	0.52
2:O:139:VAL:O	2:O:142:TRP:HB3	2.09	0.52
1:A:24:LYS:HB2	1:A:24:LYS:HZ2	1.73	0.52
1:A:102:PHE:O	1:A:103:ARG:C	2.51	0.52
1:A:114:ARG:NH1	1:A:114:ARG:HB2	2.24	0.52
2:B:135:PHE:HA	2:B:138:LEU:HB2	1.91	0.52
10:B:305:OPC:CAG	10:B:305:OPC:CAV	2.86	0.52
1:N:14:ILE:C	1:N:15:GLN:CD	2.77	0.52
1:N:58:TYR:CD2	1:N:184:TYR:HE1	2.22	0.52
1:N:194:LEU:N	1:N:194:LEU:HD23	2.23	0.52
2:O:78:GLU:C	2:O:82:TYR:CE2	2.87	0.52
3:P:205:LYS:HE2	3:P:205:LYS:C	2.35	0.52
7:T:14:GLY:C	7:T:16:LEU:H	2.17	0.52
1:A:52:PHE:HB2	1:N:189:PHE:CZ	2.44	0.52
5:E:5:ALA:HB1	6:F:10:ALA:CA	2.38	0.52
1:N:114:ARG:HD3	1:N:208:LYS:CB	2.39	0.52
1:N:116:LEU:C	1:N:118:TRP:N	2.65	0.52
2:O:71:THR:O	2:O:71:THR:HG22	2.08	0.52
1:A:24:LYS:HZ1	1:A:26:VAL:H	1.56	0.52
1:A:30:VAL:H	1:A:211:ILE:HD12	1.75	0.52
1:A:77:SER:O	1:A:78:PHE:CB	2.57	0.52
1:A:155:PRO:O	1:A:158:ILE:HD12	2.08	0.52
2:B:91:LEU:HD12	2:B:91:LEU:C	2.34	0.52
3:C:97:GLU:O	3:C:97:GLU:HG2	2.08	0.52
3:C:153:ALA:O	3:C:240:PHE:HA	2.10	0.52
3:C:180:ILE:HA	3:C:200:GLN:HB2	1.90	0.52
3:C:268:ALA:O	3:C:270:LEU:N	2.43	0.52
4:D:55:THR:O	4:D:64:VAL:HB	2.10	0.52
2:O:133:PHE:HE2	2:O:137:THR:HG21	1.71	0.52
3:P:23:ALA:C	3:P:25:CYS:N	2.60	0.52
3:P:136:PRO:HA	3:P:142:ILE:HB	1.91	0.52
3:C:61:VAL:O	3:C:62:ALA:HB2	2.08	0.52
3:C:172:PHE:N	3:C:231:LEU:HG	2.25	0.52
7:G:6:LEU:H	7:G:6:LEU:CD2	2.13	0.52
8:H:7:VAL:O	8:H:8:ALA:C	2.50	0.52
3:P:26:HIS:HA	3:P:159:GLN:OE1	2.09	0.52
3:P:34:VAL:CG1	3:P:151:LEU:HD22	2.40	0.52
3:P:255:VAL:O	3:P:258:MET:HG3	2.08	0.52
8:U:3:VAL:O	8:U:6:TRP:N	2.42	0.52
2:B:82:TYR:N	2:B:83:PRO:HD2	2.23	0.52
2:B:99:LEU:O	2:B:102:ALA:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:ARG:NH2	3:C:161:TYR:OH	2.43	0.52
4:D:102:TYR:CG	4:D:150:LEU:HD23	2.45	0.52
4:D:126:CYS:HB3	4:D:131:SER:H	1.75	0.52
4:D:165:TRP:HE3	4:D:167:GLU:OE2	1.91	0.52
6:F:23:LEU:O	6:F:24:GLY:C	2.51	0.52
8:H:7:VAL:O	8:H:9:LEU:N	2.43	0.52
1:N:160:VAL:HA	1:N:163:VAL:HB	1.91	0.52
2:O:72:PRO:C	2:O:74:GLU:H	2.18	0.52
11:O:1309:BNT:HAM3	3:P:148:ALA:H	1.75	0.52
2:B:69:PHE:CD2	2:B:69:PHE:O	2.63	0.52
2:B:127:PRO:HA	2:B:130:THR:HB	1.92	0.52
6:F:18:PHE:CD2	6:F:18:PHE:N	2.78	0.52
1:N:54:MET:C	1:N:56:PHE:H	2.17	0.52
3:P:219:VAL:CG1	3:P:220:SER:H	2.22	0.52
8:U:9:LEU:HD22	8:U:13:PHE:CZ	2.44	0.52
1:A:78:PHE:HE1	4:D:37:PRO:HA	1.74	0.52
2:B:45:MET:CE	3:C:272:LEU:HD12	2.40	0.52
4:D:55:THR:OG1	4:D:63:ASN:HA	2.09	0.52
6:F:10:ALA:O	6:F:12:LEU:N	2.43	0.52
7:G:28:ASN:HD21	7:G:30:LEU:CD2	2.18	0.52
1:N:15:GLN:NE2	1:N:15:GLN:H	2.06	0.52
1:N:201:LEU:C	1:N:205:MET:HE2	2.35	0.52
1:N:210:GLY:O	1:N:211:ILE:HB	2.09	0.52
2:O:36:LEU:HA	2:O:39:VAL:CG1	2.40	0.52
6:S:16:LEU:HA	6:S:19:VAL:HB	1.92	0.52
7:T:8:LEU:HD23	7:T:12:THR:CG2	2.39	0.52
1:A:15:GLN:O	1:A:16:ALA:C	2.53	0.52
3:C:159:GLN:N	3:C:159:GLN:CD	2.68	0.52
3:C:226:LYS:NZ	3:C:226:LYS:CB	2.73	0.52
4:D:35:LEU:C	4:D:37:PRO:HD2	2.35	0.52
1:N:178:ALA:O	1:N:179:THR:C	2.52	0.52
9:N:302:HEC:HAA2	9:N:303:HEC:CHA	2.40	0.52
10:N:1305:OPC:CBR	10:N:1305:OPC:CBN	2.86	0.52
2:O:36:LEU:HA	2:O:39:VAL:HG13	1.92	0.52
2:O:150:PRO:O	2:O:151:LEU:HB3	2.10	0.52
3:P:157:ARG:NH2	3:P:161:TYR:OH	2.43	0.52
3:P:245:THR:OG1	3:P:246:GLU:N	2.43	0.52
4:Q:152:HIS:HB2	4:Q:163:THR:OG1	2.09	0.52
5:R:10:VAL:O	5:R:10:VAL:CG1	2.58	0.52
5:R:11:PHE:CG	5:R:12:ILE:N	2.77	0.52
6:S:8:TYR:CD2	6:S:8:TYR:C	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:23:LEU:O	6:S:27:LEU:HD22	2.10	0.52
1:A:28:PRO:HG2	1:A:29:HIS:H	1.74	0.51
1:A:70:GLN:O	1:A:74:ASN:CB	2.58	0.51
1:A:116:LEU:HD12	1:A:117:THR:H	1.74	0.51
1:A:116:LEU:C	1:A:118:TRP:H	2.16	0.51
1:A:134:THR:HB	1:A:187:HIS:HB2	1.92	0.51
1:A:175:VAL:O	1:A:176:GLY:O	2.28	0.51
9:A:302:HEC:HMA1	15:A:304:HOH:O	2.09	0.51
2:B:49:ALA:O	2:B:52:VAL:CB	2.59	0.51
3:C:216:GLU:C	3:C:217:LEU:HG	2.36	0.51
4:D:90:TYR:O	4:D:103:GLY:HA3	2.10	0.51
7:G:30:LEU:H	7:G:30:LEU:HD12	1.75	0.51
1:N:160:VAL:C	1:N:162:GLY:H	2.17	0.51
1:N:184:TYR:CE2	1:N:188:THR:HG21	2.44	0.51
2:O:42:VAL:HG22	3:P:269:GLN:HA	1.92	0.51
3:P:161:TYR:HA	9:P:301:HEC:HMD1	1.91	0.51
3:P:177:THR:HA	3:P:227:ALA:HA	1.91	0.51
4:Q:94:GLU:OE1	4:Q:94:GLU:HA	2.10	0.51
3:C:271:MET:HA	3:C:274:LEU:HG	1.92	0.51
1:N:95:LEU:CD2	1:N:99:LEU:HD21	2.41	0.51
1:N:140:TRP:O	1:N:141:ASP:C	2.52	0.51
1:N:157:ALA:O	1:N:158:ILE:CB	2.57	0.51
3:P:66:SER:O	3:P:68:VAL:HG22	2.10	0.51
1:A:85:ILE:O	1:A:89:SER:N	2.44	0.51
1:A:141:ASP:O	1:A:145:TYR:HB2	2.10	0.51
2:B:51:ILE:HD12	2:B:51:ILE:N	2.22	0.51
10:B:305:OPC:HBZ2	10:B:305:OPC:CAX	2.40	0.51
3:C:54:TYR:OH	3:C:125:GLN:NE2	2.43	0.51
3:C:117:GLY:O	3:C:119:LEU:HG	2.11	0.51
3:C:255:VAL:O	3:C:258:MET:HG3	2.10	0.51
5:E:10:VAL:O	5:E:10:VAL:CG1	2.59	0.51
1:N:15:GLN:HE21	1:N:15:GLN:CA	2.20	0.51
1:N:41:LEU:HD23	1:N:41:LEU:C	2.35	0.51
1:N:87:ARG:HH12	3:P:146:LYS:HZ1	1.58	0.51
2:O:53:ALA:HA	3:P:258:MET:CE	2.40	0.51
2:O:64:GLU:N	2:O:65:PRO:CD	2.72	0.51
2:O:118:ASN:ND2	2:O:123:PRO:HB2	2.24	0.51
7:T:29:GLU:O	7:T:30:LEU:HD13	2.09	0.51
5:E:5:ALA:CB	6:F:6:MET:O	2.59	0.51
5:E:24:PHE:C	5:E:26:ILE:N	2.61	0.51
1:N:90:ALA:O	1:N:94:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:81:GLY:O	3:P:83:LYS:HD3	2.10	0.51
4:Q:110:HIS:CD2	4:Q:143:PRO:HB2	2.46	0.51
6:S:28:LEU:HB3	6:S:33:ALA:HB2	1.92	0.51
1:A:31:ASN:ND2	1:A:211:ILE:HD11	2.26	0.51
1:A:83:ARG:O	1:A:84:SER:C	2.53	0.51
1:A:142:GLN:N	2:B:65:PRO:CG	2.73	0.51
2:B:39:VAL:O	2:B:42:VAL:N	2.44	0.51
2:B:41:PRO:O	2:B:45:MET:HG3	2.11	0.51
3:C:102:TYR:HB3	3:C:118:PRO:HD3	1.91	0.51
3:C:120:PRO:HG2	3:C:124:TYR:CD1	2.46	0.51
4:D:19:MET:O	4:D:22:LEU:HD22	2.11	0.51
4:D:80:LEU:H	4:D:80:LEU:HD23	1.74	0.51
7:G:18:TYR:O	7:G:21:TYR:N	2.43	0.51
2:O:36:LEU:CA	2:O:39:VAL:HG13	2.41	0.51
4:Q:35:LEU:HD23	4:Q:36:TYR:N	2.26	0.51
4:Q:115:VAL:HG22	4:Q:126:CYS:HB2	1.91	0.51
8:U:9:LEU:HD22	8:U:13:PHE:HZ	1.75	0.51
3:C:110:GLN:HB3	3:C:113:VAL:CG2	2.40	0.51
3:C:168:ASN:O	3:C:170:ASN:N	2.44	0.51
1:N:25:TYR:C	1:N:26:VAL:HG22	2.35	0.51
1:N:87:ARG:HH12	3:P:146:LYS:NZ	2.08	0.51
1:N:163:VAL:C	1:N:165:ILE:H	2.18	0.51
3:P:168:ASN:HD22	3:P:168:ASN:C	2.18	0.51
4:Q:132:GLN:NE2	4:Q:141:ARG:HB2	2.25	0.51
5:R:13:ALA:HB2	6:S:14:PHE:HD1	1.75	0.51
1:A:41:LEU:HD21	1:A:45:LEU:HD11	1.93	0.51
1:A:117:THR:HA	1:A:205:MET:CE	2.41	0.51
1:A:158:ILE:HG22	1:A:162:GLY:HA3	1.92	0.51
2:B:50:CYS:C	2:B:54:LEU:HG	2.34	0.51
2:B:80:TYR:O	2:B:82:TYR:N	2.35	0.51
2:B:127:PRO:O	2:B:129:ALA:N	2.44	0.51
2:B:130:THR:O	2:B:133:PHE:N	2.42	0.51
3:C:41:LEU:O	3:C:133:SER:HB3	2.11	0.51
5:E:32:ILE:O	5:E:32:ILE:HG22	2.09	0.51
1:N:135:GLY:H	1:N:187:HIS:HD1	1.56	0.51
1:A:41:LEU:HD23	1:A:41:LEU:C	2.35	0.51
1:A:193:TRP:O	1:A:197:VAL:HG23	2.11	0.51
2:B:36:LEU:CA	2:B:39:VAL:HG13	2.40	0.51
3:C:44:THR:O	3:C:132:LEU:HA	2.11	0.51
3:C:181:THR:OG1	3:C:200:GLN:HG2	2.11	0.51
1:N:23:SER:HA	1:N:25:TYR:CE1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:32:ILE:HD11	7:T:26:ARG:NH2	2.26	0.51
1:N:191:LEU:C	1:N:193:TRP:H	2.19	0.51
3:P:169:ASN:C	3:P:236:ASN:HB2	2.36	0.51
4:Q:113:CYS:CB	4:Q:128:CYS:HG	2.20	0.51
1:A:33:PHE:CE2	14:E:101:BCR:H352	2.46	0.51
1:A:82:ILE:HD13	4:D:41:TYR:CD1	2.46	0.51
1:A:167:ASP:O	1:A:169:LEU:N	2.44	0.51
2:B:83:PRO:HA	2:B:143:LEU:HB3	1.92	0.51
3:C:26:HIS:HA	3:C:159:GLN:OE1	2.11	0.51
1:N:32:ILE:HG22	1:N:33:PHE:HD1	1.75	0.51
2:O:20:LYS:NZ	2:O:20:LYS:CB	2.72	0.51
3:P:76:LEU:HD23	3:P:77:MET:N	2.26	0.51
3:P:81:GLY:C	3:P:134:PRO:HG2	2.36	0.51
3:P:91:PRO:C	3:P:92:GLU:HG2	2.35	0.51
3:P:117:GLY:O	3:P:119:LEU:HG	2.11	0.51
3:P:154:ASN:CG	3:P:155:ARG:N	2.69	0.51
4:Q:38:LEU:HD11	4:Q:42:PHE:HE1	1.75	0.51
1:A:102:PHE:HE1	5:E:11:PHE:HD1	1.59	0.51
3:C:81:GLY:O	3:C:83:LYS:HD3	2.11	0.51
3:C:265:VAL:O	3:C:269:GLN:HG3	2.11	0.51
1:N:146:TRP:CZ2	2:O:69:PHE:HA	2.43	0.51
1:N:202:HIS:O	1:N:206:ILE:CG1	2.57	0.51
2:O:96:LEU:HD13	2:O:100:LEU:HB2	1.92	0.51
3:P:83:LYS:HZ1	3:P:133:SER:CA	2.24	0.51
3:P:172:PHE:N	3:P:231:LEU:HG	2.26	0.51
4:Q:137:GLY:O	4:Q:138:ARG:C	2.53	0.51
5:R:2:ILE:HG23	5:R:3:LEU:N	2.19	0.51
6:S:24:GLY:HA2	6:S:27:LEU:CD2	2.41	0.51
8:U:7:VAL:O	8:U:9:LEU:N	2.44	0.51
1:A:52:PHE:N	9:A:301:HEC:HAC	2.26	0.50
1:A:77:SER:O	4:D:41:TYR:HA	2.10	0.50
1:A:140:TRP:CE3	2:B:68:PRO:HD2	2.46	0.50
1:A:191:LEU:C	1:A:193:TRP:H	2.18	0.50
4:D:41:TYR:C	4:D:41:TYR:CD2	2.89	0.50
1:N:14:ILE:C	1:N:15:GLN:CG	2.83	0.50
2:O:64:GLU:CD	2:O:65:PRO:N	2.69	0.50
3:P:54:TYR:OH	3:P:125:GLN:NE2	2.43	0.50
3:P:61:VAL:CG2	3:P:62:ALA:H	2.23	0.50
3:P:92:GLU:HG3	3:P:94:LEU:H	1.76	0.50
3:P:144:PHE:O	3:P:147:TYR:HE1	1.94	0.50
3:P:172:PHE:H	3:P:231:LEU:CD2	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:172:PHE:H	3:P:231:LEU:CG	2.23	0.50
3:P:189:GLU:O	3:P:190:TYR:HB2	2.10	0.50
3:P:199:ILE:HB	3:P:207:VAL:O	2.11	0.50
5:R:5:ALA:HB1	6:S:10:ALA:CA	2.40	0.50
1:A:47:GLN:OE1	1:A:47:GLN:HA	2.11	0.50
1:A:148:VAL:CG1	1:A:183:TYR:CE2	2.94	0.50
3:C:17:THR:OG1	3:C:18:GLY:N	2.44	0.50
3:C:87:GLU:HA	3:C:90:ILE:HD12	1.93	0.50
4:D:132:GLN:HB2	4:D:141:ARG:HB3	1.94	0.50
1:N:31:ASN:C	1:N:34:TYR:CE2	2.89	0.50
2:O:36:LEU:C	2:O:39:VAL:HG13	2.35	0.50
2:O:125:ARG:CZ	2:O:125:ARG:CB	2.85	0.50
3:P:269:GLN:HE22	7:T:18:TYR:HD2	1.57	0.50
6:S:9:ALA:HA	6:S:12:LEU:CD1	2.40	0.50
7:T:8:LEU:HD23	7:T:12:THR:HG23	1.94	0.50
8:U:7:VAL:C	8:U:9:LEU:N	2.66	0.50
1:A:110:PHE:HB3	1:A:118:TRP:CD1	2.46	0.50
2:B:79:TRP:C	2:B:80:TYR:CD1	2.88	0.50
2:B:81:LEU:HD12	2:B:81:LEU:N	2.26	0.50
3:C:70:LEU:HD12	3:C:70:LEU:O	2.11	0.50
4:D:70:LEU:HD13	4:D:71:GLU:HG2	1.92	0.50
4:D:132:GLN:NE2	4:D:141:ARG:CB	2.73	0.50
1:N:123:ILE:HG21	1:N:198:PHE:CE2	2.47	0.50
2:O:38:TYR:O	3:P:272:LEU:HD22	2.11	0.50
3:P:10:PRO:N	3:P:11:PRO:CD	2.74	0.50
3:P:46:PHE:HE2	3:P:133:SER:HB2	1.76	0.50
3:P:65:GLY:O	3:P:66:SER:C	2.54	0.50
3:P:118:PRO:O	3:P:120:PRO:HD3	2.11	0.50
3:P:168:ASN:C	3:P:168:ASN:ND2	2.67	0.50
1:A:30:VAL:C	1:A:211:ILE:HD13	2.37	0.50
1:A:152:SER:HB2	1:A:170:ARG:CG	2.41	0.50
1:A:152:SER:HB2	1:A:170:ARG:CD	2.40	0.50
2:B:31:ALA:O	2:B:32:TRP:CB	2.60	0.50
3:C:121:GLY:C	3:C:123:GLN:N	2.69	0.50
3:C:185:LYS:HD2	3:C:195:TYR:CB	2.40	0.50
4:D:115:VAL:HG11	4:D:124:PHE:O	2.12	0.50
5:E:2:ILE:HD11	6:F:9:ALA:CB	2.42	0.50
8:H:3:VAL:O	8:H:6:TRP:CB	2.59	0.50
1:N:197:VAL:O	1:N:200:LEU:HB2	2.11	0.50
2:O:130:THR:HG22	2:O:131:THR:N	2.24	0.50
4:Q:94:GLU:C	4:Q:96:LYS:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:32:ILE:O	5:R:32:ILE:HG22	2.10	0.50
7:T:16:LEU:O	7:T:18:TYR:N	2.44	0.50
7:T:28:ASN:O	7:T:29:GLU:HB2	2.11	0.50
1:A:81:LEU:HD13	1:A:81:LEU:C	2.35	0.50
2:B:141:ILE:C	2:B:143:LEU:N	2.66	0.50
3:C:140:LYS:H	3:C:140:LYS:HD2	1.76	0.50
5:E:26:ILE:HG23	5:E:30:LYS:NZ	2.25	0.50
6:F:11:LEU:N	6:F:11:LEU:HD12	2.26	0.50
8:H:2:ASP:OD1	8:H:3:VAL:N	2.44	0.50
1:N:52:PHE:C	1:N:54:MET:H	2.18	0.50
1:N:114:ARG:HD3	1:N:208:LYS:HE2	1.94	0.50
2:O:50:CYS:O	2:O:54:LEU:HG	2.12	0.50
2:O:73:LEU:HD23	2:O:73:LEU:N	2.26	0.50
5:R:3:LEU:O	5:R:7:PHE:CD2	2.64	0.50
1:A:78:PHE:O	1:A:79:GLY:C	2.53	0.50
2:B:71:THR:OG1	4:Q:114:VAL:HB	2.11	0.50
2:B:82:TYR:O	2:B:85:PHE:N	2.45	0.50
3:C:50:VAL:HG21	3:C:129:PHE:CE1	2.46	0.50
3:C:83:LYS:HZ1	3:C:133:SER:CA	2.25	0.50
3:C:277:LYS:NZ	3:C:278:GLN:OE1	2.40	0.50
1:N:56:PHE:C	1:N:57:TYR:CD2	2.89	0.50
2:O:105:PRO:HG2	2:O:106:LEU:N	2.23	0.50
2:O:105:PRO:CG	2:O:106:LEU:H	2.21	0.50
3:P:170:ASN:HA	3:P:236:ASN:HB2	1.93	0.50
3:P:262:ILE:O	3:P:265:VAL:N	2.45	0.50
4:Q:56:ALA:O	4:Q:57:LYS:C	2.55	0.50
4:Q:126:CYS:SG	4:Q:127:PRO:CD	3.00	0.50
5:R:2:ILE:HD11	6:S:9:ALA:CB	2.41	0.50
5:R:11:PHE:HA	5:R:14:LEU:CD2	2.37	0.50
5:R:11:PHE:C	5:R:14:LEU:HD23	2.36	0.50
1:A:27:PRO:O	2:B:29:GLU:CD	2.55	0.50
1:A:68:SER:O	1:A:71:TYR:HB3	2.11	0.50
2:B:66:ALA:O	2:B:67:ASN:ND2	2.45	0.50
4:D:41:TYR:HD2	4:D:42:PHE:N	2.09	0.50
1:N:39:ILE:O	1:N:40:THR:C	2.55	0.50
2:O:41:PRO:HB2	3:P:272:LEU:CD1	2.42	0.50
3:P:31:PRO:O	3:P:32:ALA:HB2	2.11	0.50
3:P:55:ASP:HB2	3:P:57:LYS:HD2	1.92	0.50
5:R:11:PHE:CD2	5:R:12:ILE:N	2.79	0.50
8:U:1:ILE:CG2	8:U:2:ASP:H	2.21	0.50
1:A:83:ARG:HG3	1:A:84:SER:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PHE:CE1	5:E:15:PHE:CZ	2.97	0.50
1:A:184:TYR:CE2	1:A:188:THR:HG21	2.47	0.50
2:B:31:ALA:HB1	7:G:30:LEU:O	2.11	0.50
3:C:189:GLU:O	3:C:190:TYR:HB2	2.12	0.50
3:C:252:PRO:C	3:C:254:ARG:N	2.67	0.50
1:N:17:LEU:CD2	1:N:20:ASP:HB2	2.42	0.50
1:N:114:ARG:O	1:N:114:ARG:HG2	2.10	0.50
2:O:59:PRO:HD2	3:P:248:VAL:HG21	1.93	0.50
5:R:12:ILE:HA	5:R:15:PHE:CE1	2.46	0.50
1:A:120:SER:O	1:A:121:GLY:C	2.54	0.50
2:B:34:ASN:CG	2:B:35:ASP:N	2.70	0.50
2:B:63:GLY:HA2	11:B:309:BNT:OAN	2.12	0.50
3:C:89:ARG:O	3:C:90:ILE:C	2.55	0.50
3:C:168:ASN:C	3:C:168:ASN:ND2	2.67	0.50
4:D:19:MET:C	4:D:21:LEU:H	2.20	0.50
6:F:35:LYS:C	6:F:36:GLU:HG2	2.37	0.50
7:G:18:TYR:O	7:G:21:TYR:HB2	2.12	0.50
1:N:56:PHE:C	1:N:57:TYR:HD2	2.20	0.50
1:N:117:THR:HA	1:N:205:MET:HE1	1.93	0.50
2:O:38:TYR:HA	2:O:41:PRO:CG	2.42	0.50
2:O:45:MET:HE1	3:P:269:GLN:CA	2.41	0.50
2:O:135:PHE:C	2:O:135:PHE:CD1	2.88	0.50
3:P:90:ILE:O	3:P:90:ILE:HG22	2.12	0.50
3:P:102:TYR:HB3	3:P:118:PRO:HD3	1.93	0.50
7:T:26:ARG:N	7:T:27:PRO:CD	2.73	0.50
1:A:79:GLY:O	1:A:80:TRP:C	2.55	0.49
2:B:36:LEU:HA	2:B:39:VAL:CG1	2.41	0.49
3:C:151:LEU:HG	3:C:152:GLY:N	2.27	0.49
4:D:38:LEU:HD12	4:D:38:LEU:C	2.36	0.49
4:D:51:GLY:HA2	4:D:54:THR:CB	2.33	0.49
5:E:2:ILE:HG13	5:E:6:VAL:CG2	2.42	0.49
7:G:24:TYR:N	7:G:24:TYR:CD2	2.80	0.49
8:H:7:VAL:C	8:H:9:LEU:N	2.67	0.49
1:N:111:LYS:HZ1	1:N:112:LYS:HE3	1.76	0.49
2:O:38:TYR:HA	2:O:41:PRO:HG3	1.94	0.49
2:O:91:LEU:HD12	2:O:91:LEU:C	2.37	0.49
3:P:86:PRO:HG2	3:P:89:ARG:HB2	1.94	0.49
3:P:159:GLN:N	3:P:159:GLN:CD	2.70	0.49
3:P:169:ASN:CG	3:P:236:ASN:HA	2.36	0.49
3:P:263:CYS:HA	3:P:266:MET:HB2	1.94	0.49
6:S:11:LEU:N	6:S:11:LEU:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:HD3	2:B:60:ALA:HB2	1.93	0.49
1:A:154:VAL:N	1:A:155:PRO:HD2	2.26	0.49
2:B:61:MET:HE2	3:C:147:TYR:HA	1.94	0.49
3:C:93:GLU:O	3:C:95:LYS:N	2.45	0.49
4:D:113:CYS:SG	13:D:201:FES:S2	3.09	0.49
4:D:155:VAL:HG13	4:D:158:ASP:HA	1.94	0.49
5:E:11:PHE:CD2	5:E:12:ILE:N	2.79	0.49
6:F:9:ALA:HA	6:F:12:LEU:CD1	2.41	0.49
7:G:29:GLU:O	7:G:30:LEU:O	2.30	0.49
2:O:36:LEU:O	2:O:40:PHE:N	2.44	0.49
3:P:146:LYS:HG2	3:P:248:VAL:CG2	2.34	0.49
3:P:193:VAL:O	3:P:193:VAL:HG12	2.10	0.49
3:P:217:LEU:HD23	3:P:232:THR:OG1	2.13	0.49
3:P:271:MET:CG	3:P:274:LEU:HD12	2.41	0.49
3:P:278:GLN:NE2	7:T:25:LYS:HE3	2.27	0.49
5:R:7:PHE:C	5:R:9:ILE:H	2.17	0.49
6:S:21:TRP:O	6:S:25:VAL:HG23	2.11	0.49
1:A:59:LYS:HD2	1:A:68:SER:HB2	1.93	0.49
1:A:85:ILE:HG23	2:B:51:ILE:HG22	1.93	0.49
1:A:88:TRP:HZ2	2:B:58:ASP:OD1	1.95	0.49
2:B:130:THR:HG22	2:B:131:THR:N	2.25	0.49
3:C:34:VAL:HG22	3:C:243:ASP:HB3	1.95	0.49
1:N:104:VAL:O	1:N:107:THR:N	2.45	0.49
1:N:116:LEU:CD1	1:N:117:THR:H	2.25	0.49
1:N:120:SER:O	1:N:121:GLY:C	2.55	0.49
1:N:140:TRP:C	1:N:141:ASP:O	2.51	0.49
1:N:209:GLN:NE2	2:O:27:TYR:C	2.70	0.49
2:O:64:GLU:CD	2:O:65:PRO:CD	2.86	0.49
2:O:79:TRP:CZ3	5:R:4:GLY:CA	2.95	0.49
3:P:110:GLN:HB3	3:P:113:VAL:CG2	2.41	0.49
4:Q:118:ASN:C	4:Q:120:ALA:H	2.21	0.49
3:C:11:PRO:HA	3:C:107:LYS:HD2	1.93	0.49
4:D:56:ALA:O	4:D:57:LYS:C	2.55	0.49
4:D:94:GLU:OE1	4:D:94:GLU:HA	2.12	0.49
4:D:106:ALA:HB1	4:D:114:VAL:HG13	1.95	0.49
3:P:10:PRO:O	3:P:106:TYR:CE2	2.65	0.49
3:P:176:ALA:H	3:P:228:GLY:HA3	1.77	0.49
1:A:135:GLY:HA2	1:A:138:LEU:CG	2.43	0.49
1:A:145:TYR:C	1:A:145:TYR:CD2	2.89	0.49
1:A:209:GLN:OE1	2:B:28:GLY:O	2.30	0.49
2:B:133:PHE:HE2	2:B:137:THR:HG21	1.72	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:TYR:HA	9:C:301:HEC:HMD1	1.95	0.49
3:C:175:SER:O	3:C:176:ALA:HB2	2.13	0.49
3:C:223:GLN:O	3:C:224:ALA:HB3	2.13	0.49
1:N:52:PHE:O	1:N:55:THR:N	2.36	0.49
1:N:103:ARG:HD2	1:N:103:ARG:O	2.12	0.49
1:N:193:TRP:O	1:N:196:ALA:HB3	2.12	0.49
10:O:1306:OPC:HCB3	10:O:1306:OPC:CBB	2.42	0.49
11:O:1309:BNT:HAM3	3:P:148:ALA:HB2	1.94	0.49
3:P:26:HIS:CD2	3:P:158:GLY:HA2	2.48	0.49
4:Q:125:LYS:HG2	4:Q:132:GLN:HG2	1.93	0.49
5:R:2:ILE:HG13	5:R:6:VAL:CG2	2.42	0.49
5:R:28:SER:C	5:R:30:LYS:H	2.21	0.49
7:T:18:TYR:O	7:T:21:TYR:N	2.45	0.49
1:A:116:LEU:CD1	1:A:117:THR:H	2.25	0.49
1:A:117:THR:HA	1:A:205:MET:HE1	1.93	0.49
1:A:158:ILE:CG2	1:A:159:PRO:CD	2.91	0.49
1:N:44:PHE:C	1:N:46:ILE:N	2.70	0.49
1:N:118:TRP:CH2	2:O:108:LEU:HD23	2.48	0.49
2:O:31:ALA:CB	7:T:30:LEU:C	2.85	0.49
2:O:141:ILE:C	2:O:143:LEU:N	2.68	0.49
3:P:61:VAL:HA	3:P:67:LYS:HA	1.95	0.49
3:P:272:LEU:O	3:P:276:LYS:HG2	2.12	0.49
4:Q:19:MET:C	4:Q:21:LEU:H	2.20	0.49
4:Q:55:THR:OG1	4:Q:63:ASN:HA	2.12	0.49
4:Q:81:VAL:HG12	4:Q:82:GLN:N	2.17	0.49
4:Q:83:GLY:HA3	4:Q:89:THR:OG1	2.13	0.49
5:R:17:GLY:O	5:R:22:ILE:HG21	2.12	0.49
6:S:22:GLY:O	6:S:25:VAL:N	2.44	0.49
1:A:52:PHE:HA	1:A:55:THR:CG2	2.43	0.49
1:A:105:TYR:HA	1:A:110:PHE:HE2	1.74	0.49
2:B:42:VAL:HA	2:B:45:MET:HE2	1.94	0.49
10:B:305:OPC:HBM1	10:B:305:OPC:OAB	2.12	0.49
3:C:34:VAL:HG11	3:C:151:LEU:HB3	1.94	0.49
3:C:81:GLY:C	3:C:134:PRO:HG2	2.38	0.49
3:C:83:LYS:O	3:C:131:VAL:HG23	2.12	0.49
3:C:153:ALA:O	3:C:240:PHE:HD1	1.96	0.49
3:C:270:LEU:O	3:C:273:ILE:HG12	2.13	0.49
5:E:18:ILE:O	5:E:19:ALA:O	2.31	0.49
1:N:27:PRO:CA	2:O:33:PRO:HG3	2.43	0.49
1:N:38:GLY:HA3	9:N:303:HEC:C4C	2.43	0.49
1:N:42:THR:O	1:N:44:PHE:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:51:GLY:HA2	1:N:54:MET:CE	2.41	0.49
1:N:145:TYR:C	1:N:145:TYR:CD2	2.89	0.49
1:N:175:VAL:HA	1:N:179:THR:OG1	2.12	0.49
3:P:86:PRO:O	3:P:90:ILE:HG13	2.12	0.49
3:P:155:ARG:HG2	3:P:239:GLY:CA	2.42	0.49
3:P:217:LEU:O	3:P:218:ILE:HG23	2.12	0.49
4:Q:115:VAL:HG13	4:Q:126:CYS:CA	2.37	0.49
5:R:7:PHE:O	5:R:11:PHE:HD2	1.96	0.49
6:S:18:PHE:O	6:S:19:VAL:C	2.55	0.49
1:A:77:SER:HB2	4:D:41:TYR:CA	2.41	0.49
1:A:201:LEU:C	1:A:205:MET:HE2	2.38	0.49
2:B:93:ASN:O	2:B:94:LYS:HB2	2.13	0.49
3:C:10:PRO:N	3:C:11:PRO:CD	2.75	0.49
3:C:25:CYS:O	3:C:27:LEU:N	2.45	0.49
5:E:3:LEU:O	5:E:7:PHE:CD2	2.65	0.49
5:E:5:ALA:O	5:E:9:ILE:HG22	2.11	0.49
1:N:62:VAL:HG23	1:N:63:THR:H	1.77	0.49
1:N:116:LEU:HD12	1:N:116:LEU:N	2.28	0.49
9:N:303:HEC:HBC3	10:N:1305:OPC:HAS1	1.94	0.49
2:O:64:GLU:OE1	2:O:65:PRO:N	2.45	0.49
7:T:18:TYR:O	7:T:19:ALA:C	2.55	0.49
1:A:34:TYR:O	1:A:35:CYS:HB2	2.12	0.49
2:B:65:PRO:CB	2:B:68:PRO:HB3	2.35	0.49
2:B:144:GLY:C	2:B:145:ILE:HG12	2.38	0.49
1:N:39:ILE:HD11	2:O:43:VAL:HG11	1.95	0.49
1:N:52:PHE:C	1:N:52:PHE:CD1	2.89	0.49
3:P:10:PRO:O	3:P:106:TYR:HE2	1.94	0.49
3:P:157:ARG:O	3:P:159:GLN:NE2	2.46	0.49
3:P:268:ALA:C	3:P:270:LEU:N	2.67	0.49
8:U:10:LEU:O	8:U:13:PHE:HB2	2.13	0.49
1:A:117:THR:O	1:A:202:HIS:CE1	2.66	0.49
1:A:121:GLY:O	1:A:122:VAL:C	2.56	0.49
1:A:135:GLY:HA2	1:A:138:LEU:HD12	1.94	0.49
1:A:158:ILE:O	1:A:163:VAL:CG2	2.60	0.49
2:B:139:VAL:O	2:B:142:TRP:HB3	2.12	0.49
3:C:79:PRO:HB3	3:C:147:TYR:HB3	1.94	0.49
4:D:38:LEU:HD11	4:D:42:PHE:HE1	1.78	0.49
5:E:11:PHE:CG	5:E:12:ILE:N	2.81	0.49
6:F:24:GLY:HA2	6:F:27:LEU:HD22	1.94	0.49
7:G:16:LEU:O	7:G:18:TYR:N	2.46	0.49
2:O:152:ASP:N	2:O:152:ASP:OD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:55:ASP:CB	3:P:57:LYS:HD2	2.43	0.49
4:Q:41:TYR:C	4:Q:41:TYR:CD2	2.91	0.49
1:A:85:ILE:HG23	2:B:51:ILE:CG2	2.43	0.48
2:B:55:SER:O	2:B:56:VAL:C	2.56	0.48
3:C:200:GLN:O	3:C:206:THR:HA	2.13	0.48
3:C:263:CYS:HA	3:C:266:MET:HB2	1.96	0.48
1:N:29:HIS:CE1	1:N:31:ASN:ND2	2.81	0.48
1:N:104:VAL:O	1:N:106:LEU:N	2.46	0.48
2:O:82:TYR:O	2:O:85:PHE:N	2.46	0.48
2:O:109:ILE:HG23	2:O:110:LEU:HD23	1.94	0.48
3:P:28:ALA:HB3	3:P:240:PHE:HB3	1.94	0.48
3:P:237:VAL:O	3:P:238:GLY:C	2.56	0.48
1:A:170:ARG:O	1:A:179:THR:N	2.45	0.48
2:B:120:PHE:O	2:B:121:GLN:C	2.56	0.48
3:C:277:LYS:HZ3	3:C:278:GLN:CD	2.21	0.48
4:D:118:ASN:C	4:D:120:ALA:H	2.21	0.48
5:E:13:ALA:HB2	6:F:14:PHE:HD1	1.78	0.48
6:F:24:GLY:CA	6:F:27:LEU:HD22	2.42	0.48
1:N:142:GLN:HG2	2:O:64:GLU:OE1	2.13	0.48
1:A:87:ARG:HD3	2:B:60:ALA:CB	2.43	0.48
1:A:112:LYS:NZ	2:B:27:TYR:CE1	2.80	0.48
1:A:112:LYS:NZ	2:B:27:TYR:HE1	2.11	0.48
1:A:140:TRP:CZ3	2:B:68:PRO:HD2	2.47	0.48
3:C:205:LYS:NZ	3:C:207:VAL:HA	2.28	0.48
3:C:221:GLU:C	3:C:223:GLN:H	2.22	0.48
5:E:14:LEU:O	5:E:17:GLY:CA	2.61	0.48
1:N:68:SER:O	1:N:71:TYR:HB3	2.13	0.48
1:N:73:MET:HE1	2:O:60:ALA:HB3	1.94	0.48
2:O:34:ASN:ND2	2:O:35:ASP:OD1	2.45	0.48
2:O:72:PRO:C	2:O:74:GLU:N	2.68	0.48
3:P:11:PRO:HA	3:P:107:LYS:HD2	1.95	0.48
3:P:270:LEU:O	3:P:273:ILE:HG12	2.13	0.48
4:Q:69:PHE:HA	4:Q:73:HIS:CE1	2.48	0.48
4:Q:90:TYR:HB2	4:Q:104:ILE:HD11	1.94	0.48
1:A:33:PHE:O	1:A:35:CYS:HB2	2.13	0.48
1:A:34:TYR:CD1	1:A:103:ARG:NE	2.81	0.48
1:A:165:ILE:O	1:A:167:ASP:N	2.46	0.48
2:B:64:GLU:N	2:B:65:PRO:CD	2.77	0.48
2:B:153:LYS:O	2:B:154:THR:O	2.31	0.48
10:B:305:OPC:CAO	10:B:305:OPC:OCC	2.62	0.48
3:C:61:VAL:CG2	3:C:62:ALA:H	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:PRO:O	3:C:92:GLU:O	2.32	0.48
3:C:270:LEU:O	3:C:274:LEU:HG	2.14	0.48
1:N:117:THR:HA	1:N:205:MET:CE	2.43	0.48
2:O:18:LEU:O	2:O:19:ALA:HB2	2.13	0.48
3:P:278:GLN:O	3:P:279:VAL:CG2	2.59	0.48
4:Q:163:THR:HB	4:Q:164:PRO:HD2	1.96	0.48
5:R:28:SER:C	5:R:30:LYS:N	2.68	0.48
2:B:59:PRO:O	3:C:146:LYS:NZ	2.46	0.48
10:B:305:OPC:HBW1	10:C:306:OPC:HBU2	1.96	0.48
3:C:219:VAL:CG1	3:C:220:SER:N	2.76	0.48
4:D:27:VAL:O	4:D:29:GLY:N	2.38	0.48
6:F:23:LEU:O	6:F:27:LEU:HD22	2.12	0.48
8:H:6:TRP:O	8:H:7:VAL:C	2.55	0.48
1:N:122:VAL:O	1:N:123:ILE:C	2.56	0.48
1:N:148:VAL:O	1:N:148:VAL:CG1	2.62	0.48
2:O:122:ASN:ND2	5:R:26:ILE:C	2.71	0.48
3:P:10:PRO:CA	3:P:106:TYR:HE2	2.22	0.48
3:P:15:GLU:HB2	3:P:19:ARG:O	2.12	0.48
3:P:126:GLU:O	3:P:127:ILE:C	2.55	0.48
3:P:196:GLN:HE22	3:P:210:THR:HB	1.78	0.48
4:Q:90:TYR:HB2	4:Q:104:ILE:HD12	1.95	0.48
1:A:129:VAL:HG13	2:B:81:LEU:HD11	1.94	0.48
4:D:152:HIS:HB2	4:D:163:THR:OG1	2.13	0.48
1:N:83:ARG:O	1:N:84:SER:C	2.56	0.48
1:N:85:ILE:O	1:N:89:SER:N	2.45	0.48
1:N:121:GLY:O	1:N:122:VAL:C	2.56	0.48
2:O:37:LEU:C	2:O:41:PRO:HD2	2.38	0.48
3:P:4:TRP:NE1	3:P:162:PRO:HG3	2.28	0.48
3:P:41:LEU:O	3:P:133:SER:HB3	2.14	0.48
3:P:76:LEU:HD23	3:P:76:LEU:C	2.38	0.48
3:P:199:ILE:CG1	3:P:208:VAL:HA	2.44	0.48
6:S:10:ALA:O	6:S:12:LEU:N	2.46	0.48
8:U:3:VAL:O	8:U:6:TRP:CB	2.60	0.48
1:A:42:THR:C	1:A:44:PHE:N	2.70	0.48
1:A:151:VAL:HA	1:A:154:VAL:HG23	1.96	0.48
2:B:41:PRO:HA	2:B:44:ILE:HD12	1.95	0.48
3:C:75:VAL:HG12	3:C:152:GLY:O	2.14	0.48
3:C:144:PHE:O	3:C:147:TYR:HE1	1.96	0.48
4:D:88:PRO:O	4:D:106:ALA:HB3	2.13	0.48
4:D:88:PRO:HD2	4:D:107:VAL:HG23	1.96	0.48
4:D:118:ASN:O	4:D:120:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:120:ALA:O	4:D:122:ASN:ND2	2.47	0.48
4:D:173:GLY:O	4:D:174:GLU:CD	2.57	0.48
1:N:82:ILE:CD1	1:N:82:ILE:H	2.27	0.48
1:N:85:ILE:HA	2:O:51:ILE:CG2	2.42	0.48
1:N:200:LEU:O	1:N:204:LEU:HG	2.14	0.48
2:O:43:VAL:O	2:O:44:ILE:C	2.56	0.48
2:O:122:ASN:HA	2:O:124:PHE:CD1	2.48	0.48
3:P:25:CYS:O	3:P:27:LEU:N	2.46	0.48
2:B:87:ILE:HA	2:B:90:SER:HB2	1.96	0.48
10:B:305:OPC:HB1	10:C:306:OPC:CBX	2.44	0.48
3:C:126:GLU:O	3:C:127:ILE:C	2.57	0.48
6:F:11:LEU:HD12	6:F:12:LEU:H	1.78	0.48
6:F:12:LEU:O	6:F:16:LEU:HD23	2.14	0.48
7:G:26:ARG:N	7:G:27:PRO:CD	2.73	0.48
1:N:28:PRO:HG2	2:O:32:TRP:CB	2.31	0.48
1:N:79:GLY:O	1:N:80:TRP:C	2.56	0.48
1:N:82:ILE:N	1:N:82:ILE:HD12	2.27	0.48
1:N:111:LYS:HZ2	1:N:112:LYS:CG	2.26	0.48
1:N:132:GLY:O	1:N:133:VAL:C	2.56	0.48
3:P:55:ASP:C	3:P:57:LYS:N	2.71	0.48
3:P:170:ASN:O	3:P:235:PRO:HD2	2.14	0.48
3:P:256:LYS:O	3:P:259:ILE:N	2.47	0.48
3:P:268:ALA:O	3:P:270:LEU:N	2.46	0.48
5:R:18:ILE:C	5:R:23:ILE:HG23	2.39	0.48
1:A:82:ILE:HD12	1:A:82:ILE:N	2.29	0.48
3:C:28:ALA:CB	3:C:238:GLY:C	2.87	0.48
3:C:86:PRO:O	3:C:90:ILE:HG13	2.14	0.48
4:D:67:SER:HA	4:D:70:LEU:CG	2.44	0.48
5:E:18:ILE:C	5:E:23:ILE:HG23	2.39	0.48
6:F:20:GLY:HA3	7:G:21:TYR:CE1	2.49	0.48
1:N:50:THR:OG1	1:N:51:GLY:N	2.46	0.48
1:N:151:VAL:HA	1:N:154:VAL:HG23	1.95	0.48
2:O:124:PHE:HB2	5:R:23:ILE:HD13	1.96	0.48
3:P:54:TYR:CD1	3:P:54:TYR:C	2.91	0.48
3:P:79:PRO:HB3	3:P:147:TYR:HB3	1.95	0.48
4:Q:80:LEU:CB	4:Q:90:TYR:HA	2.43	0.48
4:Q:173:GLY:O	4:Q:174:GLU:CD	2.57	0.48
7:T:4:LEU:N	7:T:6:LEU:HD11	2.29	0.48
7:T:9:VAL:HG23	7:T:10:PHE:HD1	1.77	0.48
1:A:148:VAL:HG11	1:A:183:TYR:CE2	2.49	0.48
2:B:121:GLN:O	2:B:121:GLN:CD	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:115:VAL:HG22	4:D:126:CYS:CB	2.44	0.48
4:D:131:SER:O	4:D:132:GLN:HG3	2.13	0.48
5:E:23:ILE:C	5:E:25:ALA:H	2.21	0.48
1:N:39:ILE:HD11	2:O:43:VAL:CG1	2.43	0.48
2:O:127:PRO:O	2:O:130:THR:N	2.47	0.48
3:P:41:LEU:HB3	3:P:42:PRO:HD2	1.95	0.48
3:P:97:GLU:O	3:P:97:GLU:HG2	2.14	0.48
3:P:256:LYS:HE2	3:P:257:TRP:CZ3	2.49	0.48
4:Q:27:VAL:O	4:Q:29:GLY:N	2.36	0.48
4:Q:83:GLY:N	4:Q:87:ASP:O	2.42	0.48
4:Q:131:SER:O	4:Q:132:GLN:HG3	2.14	0.48
4:Q:155:VAL:HG13	4:Q:158:ASP:HA	1.96	0.48
5:R:5:ALA:O	5:R:9:ILE:HG22	2.14	0.48
7:T:17:PHE:HB3	7:T:21:TYR:HE1	1.79	0.48
1:A:83:ARG:NH1	2:B:60:ALA:HB1	2.29	0.47
1:A:122:VAL:O	1:A:123:ILE:C	2.55	0.47
2:B:36:LEU:O	2:B:40:PHE:N	2.47	0.47
2:B:81:LEU:N	2:B:81:LEU:CD1	2.77	0.47
3:C:55:ASP:HB2	3:C:57:LYS:HD2	1.95	0.47
3:C:158:GLY:H	9:C:301:HEC:CAD	2.27	0.47
3:C:251:ASP:O	3:C:254:ARG:CB	2.62	0.47
3:C:262:ILE:O	3:C:264:LEU:N	2.47	0.47
7:G:9:VAL:HG23	7:G:10:PHE:HD1	1.78	0.47
1:N:165:ILE:HD11	1:N:168:LEU:HD12	1.96	0.47
3:P:28:ALA:HB3	3:P:240:PHE:CB	2.44	0.47
3:P:187:GLU:HB2	3:P:193:VAL:HG13	1.96	0.47
3:P:259:ILE:HD11	7:T:12:THR:CG2	2.44	0.47
3:P:273:ILE:O	3:P:278:GLN:CG	2.61	0.47
4:Q:110:HIS:HB2	4:Q:144:ALA:CA	2.34	0.47
4:Q:132:GLN:NE2	4:Q:141:ARG:CB	2.77	0.47
1:A:62:VAL:CG2	1:A:63:THR:H	2.17	0.47
1:A:138:LEU:N	1:A:139:PRO:CD	2.74	0.47
2:B:38:TYR:N	2:B:38:TYR:CD1	2.82	0.47
2:B:80:TYR:O	2:B:83:PRO:HD2	2.14	0.47
10:B:305:OPC:HAS2	10:B:305:OPC:OAD	2.12	0.47
3:C:176:ALA:N	3:C:228:GLY:HA3	2.28	0.47
3:C:199:ILE:HG22	3:C:200:GLN:N	2.20	0.47
3:C:278:GLN:O	3:C:279:VAL:CG2	2.62	0.47
4:D:82:GLN:HA	4:D:82:GLN:HE21	1.78	0.47
7:G:18:TYR:O	7:G:19:ALA:C	2.57	0.47
7:G:22:GLN:C	7:G:24:TYR:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:29:GLU:O	7:G:30:LEU:C	2.57	0.47
1:N:81:LEU:O	1:N:82:ILE:C	2.56	0.47
2:O:34:ASN:CG	2:O:35:ASP:N	2.68	0.47
2:O:67:ASN:HD22	3:P:16:PRO:HB3	1.79	0.47
3:P:153:ALA:O	3:P:240:PHE:HA	2.13	0.47
3:P:168:ASN:O	3:P:170:ASN:N	2.47	0.47
4:Q:132:GLN:HB2	4:Q:141:ARG:HB3	1.96	0.47
4:Q:154:THR:HB	4:Q:161:VAL:HG22	1.90	0.47
1:A:29:HIS:CB	1:A:211:ILE:HD12	2.38	0.47
1:A:197:VAL:O	1:A:200:LEU:HB2	2.13	0.47
2:B:37:LEU:O	10:B:305:OPC:HBL1	2.15	0.47
2:B:65:PRO:CA	2:B:68:PRO:HD3	2.44	0.47
3:C:55:ASP:C	3:C:57:LYS:H	2.22	0.47
3:C:258:MET:SD	3:C:258:MET:C	2.97	0.47
5:E:5:ALA:HB3	6:F:6:MET:O	2.14	0.47
1:N:134:THR:HB	1:N:187:HIS:HB2	1.96	0.47
2:O:79:TRP:HA	2:O:82:TYR:CE2	2.49	0.47
2:O:104:VAL:H	2:O:105:PRO:CD	2.24	0.47
3:P:70:LEU:HD12	3:P:70:LEU:O	2.14	0.47
7:T:20:ALA:O	7:T:24:TYR:CD2	2.67	0.47
1:A:29:HIS:ND1	2:B:30:PRO:HG3	2.29	0.47
1:A:66:TYR:HB2	1:A:140:TRP:CE3	2.45	0.47
1:A:112:LYS:HZ3	2:B:27:TYR:HE1	1.61	0.47
1:A:116:LEU:HD13	1:A:205:MET:SD	2.55	0.47
1:A:163:VAL:C	1:A:165:ILE:H	2.21	0.47
3:C:54:TYR:HD2	3:C:155:ARG:NH1	2.12	0.47
4:D:67:SER:CA	4:D:70:LEU:HD21	2.36	0.47
1:N:66:TYR:CE1	2:O:65:PRO:HD2	2.49	0.47
1:N:154:VAL:N	1:N:155:PRO:HD2	2.30	0.47
2:O:48:PHE:CD1	2:O:48:PHE:C	2.92	0.47
2:O:76:LEU:N	2:O:76:LEU:HD22	2.29	0.47
3:P:169:ASN:ND2	3:P:236:ASN:HA	2.29	0.47
3:P:205:LYS:NZ	3:P:207:VAL:HA	2.29	0.47
3:P:223:GLN:O	3:P:224:ALA:HB3	2.14	0.47
3:P:274:LEU:O	3:P:275:LYS:O	2.31	0.47
4:Q:19:MET:O	4:Q:22:LEU:HD22	2.13	0.47
4:Q:67:SER:HA	4:Q:70:LEU:CG	2.45	0.47
8:U:3:VAL:HA	8:U:6:TRP:HD1	1.79	0.47
1:A:118:TRP:HA	9:A:302:HEC:CHD	2.44	0.47
1:A:122:VAL:O	1:A:125:ALA:N	2.44	0.47
1:A:189:PHE:CZ	1:N:52:PHE:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:LEU:HA	2:B:39:VAL:HG13	1.95	0.47
12:B:201:CLA:HHC	12:B:201:CLA:HBB1	1.95	0.47
3:C:6:GLN:HB3	3:C:106:TYR:CE2	2.49	0.47
3:C:65:GLY:O	3:C:66:SER:C	2.58	0.47
4:D:178:TRP:O	4:D:179:VAL:C	2.58	0.47
2:O:82:TYR:O	2:O:85:PHE:HB3	2.15	0.47
2:O:99:LEU:O	2:O:100:LEU:C	2.57	0.47
7:T:18:TYR:O	7:T:21:TYR:HB2	2.15	0.47
1:A:39:ILE:O	1:A:40:THR:C	2.57	0.47
1:A:140:TRP:HH2	2:B:67:ASN:OD1	1.98	0.47
2:B:48:PHE:O	2:B:49:ALA:C	2.58	0.47
2:B:82:TYR:O	2:B:85:PHE:HB3	2.15	0.47
3:C:55:ASP:C	3:C:57:LYS:N	2.72	0.47
3:C:92:GLU:HG3	3:C:94:LEU:H	1.79	0.47
6:F:20:GLY:O	6:F:21:TRP:C	2.57	0.47
6:F:27:LEU:CD1	8:H:15:TRP:NE1	2.68	0.47
7:G:20:ALA:C	7:G:24:TYR:CZ	2.93	0.47
7:G:20:ALA:O	7:G:24:TYR:CD2	2.67	0.47
1:N:102:PHE:O	1:N:103:ARG:C	2.58	0.47
3:P:91:PRO:O	3:P:95:LYS:CG	2.61	0.47
3:P:92:GLU:HG3	3:P:94:LEU:CB	2.44	0.47
6:S:18:PHE:CD2	6:S:18:PHE:N	2.81	0.47
7:T:22:GLN:C	7:T:24:TYR:H	2.22	0.47
1:A:34:TYR:CG	1:A:103:ARG:HD3	2.49	0.47
1:A:165:ILE:C	1:A:167:ASP:N	2.72	0.47
1:A:175:VAL:O	1:A:176:GLY:C	2.58	0.47
2:B:64:GLU:N	2:B:65:PRO:HD3	2.30	0.47
3:C:54:TYR:HB2	3:C:58:LEU:CD2	2.45	0.47
3:C:54:TYR:CD1	3:C:54:TYR:C	2.91	0.47
3:C:91:PRO:O	3:C:95:LYS:CG	2.57	0.47
3:C:197:VAL:HG13	3:C:211:ILE:HG22	1.96	0.47
3:C:259:ILE:HD11	7:G:12:THR:HG21	1.97	0.47
3:C:275:LYS:O	3:C:276:LYS:C	2.57	0.47
4:D:73:HIS:HB2	4:D:93:VAL:HG21	1.94	0.47
4:D:90:TYR:HB2	4:D:104:ILE:HD12	1.96	0.47
6:F:22:GLY:O	6:F:25:VAL:N	2.45	0.47
1:N:28:PRO:CD	2:O:33:PRO:HD3	2.37	0.47
1:N:81:LEU:C	1:N:81:LEU:HD13	2.40	0.47
1:N:114:ARG:HG2	1:N:114:ARG:NH1	2.30	0.47
10:N:1305:OPC:HCB2	10:N:1305:OPC:HAY1	1.97	0.47
2:O:34:ASN:HD22	2:O:35:ASP:CG	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:48:PHE:O	2:O:49:ALA:C	2.56	0.47
2:O:64:GLU:HG3	2:O:65:PRO:CD	2.30	0.47
2:O:70:ALA:O	2:O:71:THR:HB	2.14	0.47
3:P:153:ALA:O	3:P:240:PHE:HD1	1.96	0.47
4:Q:118:ASN:O	4:Q:120:ALA:N	2.48	0.47
5:R:18:ILE:O	5:R:19:ALA:O	2.32	0.47
3:C:4:TRP:NE1	3:C:162:PRO:HG3	2.29	0.47
4:D:24:PHE:HA	4:D:27:VAL:HB	1.97	0.47
4:D:64:VAL:HG13	4:D:68:LYS:HG3	1.97	0.47
1:N:47:GLN:OE1	1:N:47:GLN:HA	2.14	0.47
1:N:95:LEU:HD11	5:R:7:PHE:HB3	1.97	0.47
1:N:105:TYR:HD2	1:N:106:LEU:HD23	1.80	0.47
2:O:42:VAL:HA	2:O:45:MET:HE2	1.96	0.47
3:P:4:TRP:N	3:P:4:TRP:HE3	2.13	0.47
4:Q:113:CYS:HG	4:Q:128:CYS:CB	2.27	0.47
5:R:7:PHE:O	5:R:11:PHE:CD2	2.68	0.47
5:R:12:ILE:HA	5:R:15:PHE:HE1	1.78	0.47
12:B:201:CLA:HAA1	12:B:201:CLA:CGD	2.45	0.47
3:C:136:PRO:HB2	3:C:142:ILE:O	2.15	0.47
14:E:101:BCR:H322	7:G:23:GLN:HE22	1.80	0.47
1:N:148:VAL:CG1	1:N:183:TYR:CE2	2.97	0.47
2:O:151:LEU:HD12	2:O:151:LEU:O	2.15	0.47
3:P:55:ASP:C	3:P:57:LYS:H	2.23	0.47
3:P:90:ILE:HG21	3:P:96:LYS:HG2	1.97	0.47
4:Q:132:GLN:C	4:Q:133:TYR:HD2	2.23	0.47
6:S:11:LEU:HD12	6:S:12:LEU:H	1.79	0.47
1:A:52:PHE:O	1:A:53:ALA:C	2.58	0.47
2:B:108:LEU:C	2:B:110:LEU:N	2.73	0.47
10:B:305:OPC:OAB	10:B:305:OPC:CBN	2.62	0.47
3:C:10:PRO:O	3:C:106:TYR:CE2	2.68	0.47
3:C:34:VAL:HG11	3:C:151:LEU:CB	2.45	0.47
3:C:81:GLY:O	3:C:134:PRO:HG3	2.14	0.47
6:F:18:PHE:O	6:F:19:VAL:C	2.58	0.47
6:F:20:GLY:HA3	7:G:21:TYR:CD1	2.50	0.47
11:O:1309:BNT:CAM	3:P:148:ALA:HB2	2.45	0.47
3:P:216:GLU:C	3:P:217:LEU:HG	2.40	0.47
3:P:251:ASP:O	3:P:254:ARG:CB	2.60	0.47
1:A:105:TYR:C	1:A:105:TYR:CD2	2.93	0.46
2:B:36:LEU:O	2:B:39:VAL:HG22	2.14	0.46
2:B:96:LEU:HD13	2:B:96:LEU:C	2.39	0.46
3:C:92:GLU:HG3	3:C:94:LEU:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:LEU:O	4:D:36:TYR:C	2.58	0.46
2:O:101:MET:C	2:O:103:SER:H	2.24	0.46
3:P:265:VAL:O	3:P:266:MET:C	2.59	0.46
4:Q:43:ILE:O	4:Q:44:PRO:O	2.33	0.46
1:A:19:ASP:O	1:A:20:ASP:CB	2.63	0.46
1:A:19:ASP:O	1:A:20:ASP:CG	2.59	0.46
1:A:57:TYR:CE1	1:A:76:VAL:HG13	2.47	0.46
6:F:8:TYR:CD2	6:F:8:TYR:C	2.94	0.46
1:N:32:ILE:HG12	7:T:26:ARG:NH2	2.30	0.46
10:N:1305:OPC:HAY2	10:N:1305:OPC:HCB2	1.97	0.46
3:P:52:ILE:CG2	3:P:155:ARG:NH2	2.77	0.46
3:P:158:GLY:H	9:P:301:HEC:CAD	2.27	0.46
3:P:269:GLN:NE2	7:T:18:TYR:HD2	2.13	0.46
7:T:20:ALA:C	7:T:24:TYR:CZ	2.93	0.46
7:T:30:LEU:HD22	7:T:30:LEU:N	2.30	0.46
1:A:29:HIS:CD2	1:A:211:ILE:HD12	2.50	0.46
1:A:87:ARG:HH12	3:C:146:LYS:NZ	2.13	0.46
2:B:48:PHE:CE1	2:B:52:VAL:HG22	2.51	0.46
2:B:76:LEU:HD13	2:B:79:TRP:HZ2	1.81	0.46
2:B:81:LEU:O	2:B:85:PHE:HB2	2.15	0.46
6:F:22:GLY:O	6:F:23:LEU:C	2.59	0.46
1:N:15:GLN:C	1:N:15:GLN:NE2	2.67	0.46
1:N:122:VAL:O	1:N:125:ALA:N	2.45	0.46
1:N:185:SER:O	1:N:189:PHE:CB	2.61	0.46
2:O:40:PHE:O	2:O:43:VAL:N	2.48	0.46
2:O:46:GLY:HA3	7:T:19:ALA:HB2	1.97	0.46
2:O:101:MET:CG	2:O:102:ALA:N	2.78	0.46
2:O:136:GLY:HA3	12:O:1201:CLA:C1C	2.45	0.46
3:P:34:VAL:HG11	3:P:151:LEU:HB3	1.97	0.46
3:P:93:GLU:O	3:P:94:LEU:C	2.57	0.46
4:Q:80:LEU:HD23	4:Q:80:LEU:H	1.79	0.46
1:A:22:THR:O	1:A:23:SER:C	2.59	0.46
1:A:34:TYR:O	9:A:303:HEC:HMB2	2.15	0.46
1:A:58:TYR:HD2	1:A:184:TYR:CE1	2.30	0.46
1:A:154:VAL:HB	1:A:155:PRO:CD	2.45	0.46
3:C:90:ILE:O	3:C:91:PRO:C	2.59	0.46
3:C:200:GLN:O	3:C:201:THR:C	2.58	0.46
4:D:80:LEU:CB	4:D:90:TYR:HA	2.45	0.46
5:E:24:PHE:O	5:E:26:ILE:N	2.48	0.46
1:N:61:THR:CG2	1:N:64:GLU:HB3	2.46	0.46
1:N:105:TYR:CD2	1:N:106:LEU:HD23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:110:PHE:CD2	1:N:110:PHE:N	2.81	0.46
3:P:9:TYR:CE1	3:P:21:VAL:HG11	2.51	0.46
3:P:258:MET:SD	3:P:258:MET:C	2.99	0.46
3:P:279:VAL:HG12	3:P:279:VAL:O	2.14	0.46
6:S:12:LEU:O	6:S:16:LEU:HD23	2.15	0.46
2:B:38:TYR:HA	2:B:41:PRO:HG3	1.98	0.46
2:B:57:LEU:HD22	7:G:10:PHE:CE1	2.50	0.46
10:B:305:OPC:HBP2	10:B:305:OPC:CAH	2.46	0.46
11:B:309:BNT:CAM	3:C:148:ALA:HB2	2.46	0.46
3:C:90:ILE:HG21	3:C:96:LYS:HG2	1.96	0.46
3:C:104:GLN:NE2	3:C:104:GLN:N	2.62	0.46
4:D:59:LYS:HB2	4:D:59:LYS:HZ2	1.79	0.46
7:G:4:LEU:N	7:G:6:LEU:HD11	2.30	0.46
1:N:111:LYS:HG3	1:N:112:LYS:N	2.30	0.46
3:P:92:GLU:HG3	3:P:94:LEU:HB2	1.97	0.46
4:Q:90:TYR:O	4:Q:103:GLY:HA3	2.15	0.46
4:Q:177:TRP:CD1	4:Q:177:TRP:H	2.33	0.46
6:S:20:GLY:O	6:S:21:TRP:C	2.58	0.46
1:A:72:ILE:N	1:A:72:ILE:HD12	2.31	0.46
1:A:114:ARG:CD	1:A:208:LYS:HD3	2.46	0.46
3:C:46:PHE:HE2	3:C:133:SER:HB2	1.80	0.46
4:D:90:TYR:HB2	4:D:104:ILE:HD11	1.96	0.46
1:N:44:PHE:C	1:N:46:ILE:H	2.23	0.46
10:N:1305:OPC:HAY2	10:N:1305:OPC:CBZ	2.42	0.46
3:P:251:ASP:HB3	3:P:254:ARG:CB	2.46	0.46
3:P:277:LYS:HZ3	3:P:278:GLN:CD	2.22	0.46
4:Q:82:GLN:HE21	4:Q:82:GLN:CA	2.28	0.46
4:Q:126:CYS:HB3	4:Q:131:SER:H	1.80	0.46
1:A:44:PHE:C	1:A:46:ILE:N	2.73	0.46
1:A:54:MET:C	1:A:56:PHE:H	2.23	0.46
1:A:148:VAL:O	1:A:148:VAL:CG1	2.61	0.46
2:B:144:GLY:O	2:B:145:ILE:CD1	2.63	0.46
3:C:4:TRP:N	3:C:4:TRP:HE3	2.13	0.46
3:C:10:PRO:O	3:C:106:TYR:HE2	1.98	0.46
3:C:158:GLY:HA3	9:C:301:HEC:C2D	2.46	0.46
3:C:265:VAL:O	3:C:266:MET:C	2.58	0.46
4:D:69:PHE:HA	4:D:73:HIS:CE1	2.50	0.46
5:E:3:LEU:HG	5:E:7:PHE:CE2	2.51	0.46
8:H:3:VAL:HA	8:H:6:TRP:HD1	1.80	0.46
1:N:72:ILE:N	1:N:72:ILE:HD12	2.30	0.46
2:O:18:LEU:HG	2:O:30:PRO:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:96:LEU:HD13	2:O:96:LEU:O	2.15	0.46
3:P:54:TYR:HB2	3:P:58:LEU:CD2	2.44	0.46
3:P:101:VAL:CG2	3:P:103:PHE:HE2	2.22	0.46
3:P:272:LEU:HG	4:Q:27:VAL:HG21	1.97	0.46
4:Q:121:GLU:OE2	4:Q:125:LYS:HE3	2.15	0.46
5:R:14:LEU:O	5:R:17:GLY:CA	2.64	0.46
1:A:132:GLY:O	1:A:133:VAL:C	2.58	0.46
1:A:179:THR:O	1:A:183:TYR:CD1	2.68	0.46
2:B:85:PHE:HD1	2:B:86:GLN:N	2.14	0.46
2:B:118:ASN:HB3	2:B:121:GLN:O	2.15	0.46
3:C:171:VAL:HG13	3:C:234:ASN:HD22	1.81	0.46
3:C:237:VAL:O	3:C:238:GLY:C	2.59	0.46
6:F:16:LEU:HA	6:F:19:VAL:CB	2.46	0.46
6:F:21:TRP:O	6:F:25:VAL:HG23	2.16	0.46
1:N:52:PHE:O	1:N:53:ALA:C	2.58	0.46
1:N:52:PHE:HA	1:N:55:THR:CG2	2.45	0.46
1:N:68:SER:O	1:N:72:ILE:HD12	2.16	0.46
1:N:118:TRP:HH2	2:O:108:LEU:O	1.99	0.46
1:N:165:ILE:CD1	1:N:168:LEU:HD12	2.46	0.46
1:N:203:PHE:O	1:N:204:LEU:C	2.58	0.46
2:O:41:PRO:O	2:O:45:MET:HG3	2.15	0.46
2:O:124:PHE:O	5:R:23:ILE:HD13	2.16	0.46
3:P:75:VAL:HG12	3:P:152:GLY:O	2.15	0.46
3:P:280:GLU:O	3:P:280:GLU:CG	2.63	0.46
4:Q:24:PHE:HA	4:Q:27:VAL:HB	1.98	0.46
4:Q:150:LEU:C	4:Q:151:CYS:SG	2.98	0.46
1:A:29:HIS:HB3	1:A:30:VAL:H	1.55	0.46
2:B:26:TYR:HD1	2:B:26:TYR:C	2.24	0.46
10:B:305:OPC:PAJ	10:B:305:OPC:OAN	2.74	0.46
10:B:305:OPC:OBH	10:C:306:OPC:HAU1	2.16	0.46
3:C:28:ALA:HB3	3:C:240:PHE:HB3	1.97	0.46
3:C:266:MET:HA	3:C:269:GLN:HE22	1.80	0.46
3:C:278:GLN:NE2	7:G:25:LYS:HE3	2.31	0.46
4:D:113:CYS:CB	4:D:128:CYS:HG	2.27	0.46
4:D:141:ARG:C	4:D:142:GLY:O	2.57	0.46
1:N:13:GLU:OE2	1:N:14:ILE:HG12	2.15	0.46
2:O:108:LEU:C	2:O:110:LEU:N	2.74	0.46
3:P:54:TYR:HD2	3:P:155:ARG:HH11	1.63	0.46
3:P:269:GLN:O	3:P:273:ILE:HG23	2.16	0.46
3:P:270:LEU:O	3:P:274:LEU:HG	2.15	0.46
4:Q:35:LEU:C	4:Q:37:PRO:HD2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:38:LEU:HD12	4:Q:38:LEU:C	2.40	0.46
1:A:123:ILE:HG21	1:A:198:PHE:CE2	2.50	0.46
2:B:57:LEU:HD13	7:G:10:PHE:CG	2.51	0.46
4:D:121:GLU:OE2	4:D:125:LYS:HE3	2.16	0.46
1:N:15:GLN:C	1:N:17:LEU:N	2.64	0.46
1:N:42:THR:C	1:N:44:PHE:N	2.73	0.46
1:N:148:VAL:HG11	1:N:183:TYR:CE2	2.51	0.46
2:O:45:MET:HE1	3:P:269:GLN:HA	1.98	0.46
3:P:180:ILE:HG13	3:P:199:ILE:HA	1.98	0.46
3:P:277:LYS:NZ	3:P:278:GLN:OE1	2.43	0.46
2:B:65:PRO:HB3	2:B:68:PRO:HG3	1.98	0.45
2:B:73:LEU:HD23	3:C:18:GLY:CA	2.46	0.45
3:C:155:ARG:HG2	3:C:239:GLY:CA	2.45	0.45
3:C:226:LYS:HZ3	3:C:226:LYS:HB3	1.81	0.45
3:C:271:MET:CG	3:C:274:LEU:HD12	2.42	0.45
4:D:82:GLN:HE21	4:D:82:GLN:CA	2.29	0.45
1:N:135:GLY:HA2	1:N:138:LEU:HD12	1.94	0.45
3:P:158:GLY:HA3	9:P:301:HEC:C2D	2.46	0.45
7:T:7:GLY:C	7:T:9:VAL:N	2.74	0.45
1:A:72:ILE:HD12	1:A:72:ILE:H	1.81	0.45
2:B:40:PHE:H	2:B:41:PRO:HD2	1.79	0.45
10:B:305:OPC:HAG1	10:B:305:OPC:CAV	2.46	0.45
4:D:83:GLY:N	4:D:87:ASP:O	2.47	0.45
4:D:104:ILE:HD12	4:D:104:ILE:C	2.41	0.45
1:N:78:PHE:CE1	4:Q:37:PRO:HA	2.51	0.45
5:R:5:ALA:C	5:R:7:PHE:N	2.72	0.45
5:R:14:LEU:O	5:R:18:ILE:N	2.50	0.45
1:A:50:THR:OG1	1:A:51:GLY:N	2.48	0.45
1:A:137:SER:C	1:A:139:PRO:HD2	2.42	0.45
1:A:142:GLN:H	2:B:65:PRO:HG2	1.79	0.45
2:B:26:TYR:C	2:B:26:TYR:CD1	2.94	0.45
2:B:37:LEU:C	2:B:41:PRO:HD2	2.41	0.45
3:C:82:PHE:CE1	3:C:134:PRO:HD2	2.52	0.45
3:C:277:LYS:HA	3:C:280:GLU:HB3	1.97	0.45
8:H:1:ILE:CG2	8:H:2:ASP:H	2.29	0.45
1:N:85:ILE:O	1:N:86:HIS:C	2.60	0.45
2:O:45:MET:CE	3:P:269:GLN:HB3	2.46	0.45
2:O:85:PHE:HD1	2:O:86:GLN:N	2.14	0.45
3:P:54:TYR:CE1	3:P:70:LEU:HD22	2.52	0.45
3:P:199:ILE:HG13	3:P:208:VAL:HA	1.99	0.45
3:P:265:VAL:O	3:P:269:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:278:GLN:C	3:P:279:VAL:HG23	2.41	0.45
4:Q:130:GLY:C	4:Q:131:SER:O	2.60	0.45
14:R:1101:BCR:H361	14:R:1101:BCR:H20C	1.79	0.45
2:B:58:ASP:C	2:B:58:ASP:OD2	2.59	0.45
2:B:79:TRP:HH2	5:E:1:MET:CG	2.30	0.45
3:C:41:LEU:HB3	3:C:42:PRO:HD2	1.99	0.45
3:C:52:ILE:CG2	3:C:155:ARG:NH2	2.77	0.45
3:C:55:ASP:CB	3:C:57:LYS:HD2	2.46	0.45
3:C:93:GLU:O	3:C:94:LEU:C	2.59	0.45
3:C:225:VAL:O	3:C:226:LYS:HB3	2.16	0.45
3:C:256:LYS:O	3:C:259:ILE:N	2.50	0.45
4:D:83:GLY:HA3	4:D:89:THR:OG1	2.16	0.45
6:F:28:LEU:HB3	6:F:33:ALA:CB	2.46	0.45
1:N:83:ARG:NH1	2:O:60:ALA:CB	2.75	0.45
1:N:165:ILE:O	1:N:167:ASP:N	2.50	0.45
3:P:3:PHE:O	3:P:5:ALA:N	2.50	0.45
3:P:28:ALA:CB	3:P:238:GLY:C	2.88	0.45
3:P:226:LYS:NZ	3:P:226:LYS:CB	2.79	0.45
5:R:23:ILE:C	5:R:23:ILE:CD1	2.87	0.45
6:S:20:GLY:HA3	7:T:21:TYR:CD1	2.52	0.45
6:S:27:LEU:CD1	8:U:15:TRP:NE1	2.71	0.45
1:A:51:GLY:HA2	1:A:54:MET:CE	2.46	0.45
1:A:118:TRP:HB2	9:A:302:HEC:HMD3	1.97	0.45
3:C:154:ASN:CG	3:C:155:ARG:N	2.68	0.45
1:N:208:LYS:HG2	2:O:27:TYR:OH	2.16	0.45
2:O:101:MET:HE2	12:O:1201:CLA:H92	1.98	0.45
6:S:27:LEU:HB2	7:T:25:LYS:HZ2	1.81	0.45
7:T:13:LEU:HD13	7:T:13:LEU:C	2.41	0.45
1:A:41:LEU:O	1:A:44:PHE:N	2.45	0.45
1:A:68:SER:O	1:A:72:ILE:HD12	2.15	0.45
2:B:56:VAL:O	2:B:57:LEU:C	2.59	0.45
2:B:124:PHE:CE2	5:E:27:LYS:HB2	2.52	0.45
10:B:305:OPC:OAB	10:B:305:OPC:HBN2	2.17	0.45
3:C:161:TYR:HB2	3:C:165:GLU:O	2.16	0.45
3:C:269:GLN:O	3:C:273:ILE:HG23	2.17	0.45
3:C:273:ILE:O	3:C:278:GLN:CG	2.65	0.45
4:D:122:ASN:HD22	4:D:122:ASN:N	2.14	0.45
4:D:170:PHE:CD1	4:D:170:PHE:N	2.83	0.45
5:E:2:ILE:CG2	5:E:3:LEU:H	2.22	0.45
2:O:123:PRO:HG2	2:O:124:PHE:CZ	2.51	0.45
2:O:151:LEU:C	2:O:152:ASP:CG	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:93:VAL:HA	4:Q:99:ILE:CG2	2.39	0.45
1:A:28:PRO:HG2	1:A:29:HIS:N	2.32	0.45
1:A:103:ARG:HD2	1:A:103:ARG:O	2.17	0.45
1:A:109:GLY:HA3	9:A:302:HEC:HBD2	1.98	0.45
3:C:245:THR:OG1	3:C:246:GLU:N	2.41	0.45
5:E:7:PHE:O	5:E:11:PHE:HD2	2.00	0.45
3:P:273:ILE:HD12	7:T:25:LYS:HD3	1.98	0.45
2:B:76:LEU:O	2:B:77:PRO:C	2.60	0.45
3:C:101:VAL:CG1	3:C:118:PRO:HB2	2.47	0.45
3:C:121:GLY:O	3:C:123:GLN:N	2.49	0.45
3:C:169:ASN:ND2	3:C:236:ASN:HA	2.32	0.45
3:C:199:ILE:HB	3:C:207:VAL:O	2.17	0.45
7:G:10:PHE:O	7:G:11:ALA:C	2.60	0.45
1:N:57:TYR:HE1	1:N:76:VAL:HG21	1.82	0.45
2:O:151:LEU:O	2:O:152:ASP:CB	2.62	0.45
3:P:25:CYS:HB3	3:P:26:HIS:H	1.56	0.45
3:P:34:VAL:HG22	3:P:243:ASP:HB3	1.99	0.45
3:P:55:ASP:CG	3:P:57:LYS:HD2	2.41	0.45
3:P:185:LYS:HD2	3:P:195:TYR:CB	2.42	0.45
4:Q:82:GLN:HE21	4:Q:82:GLN:HA	1.82	0.45
5:R:23:ILE:C	5:R:25:ALA:H	2.24	0.45
1:A:157:ALA:O	1:A:158:ILE:HG13	2.17	0.45
1:A:203:PHE:O	1:A:204:LEU:C	2.60	0.45
4:D:35:LEU:C	4:D:37:PRO:CD	2.90	0.45
4:D:41:TYR:C	4:D:43:ILE:H	2.24	0.45
4:D:88:PRO:HG3	4:D:114:VAL:CG2	2.45	0.45
8:H:10:LEU:O	8:H:13:PHE:HB2	2.17	0.45
1:N:117:THR:HG22	1:N:205:MET:HB3	1.98	0.45
1:N:165:ILE:O	1:N:166:SER:C	2.60	0.45
2:O:82:TYR:N	2:O:83:PRO:HD2	2.32	0.45
4:Q:132:GLN:C	4:Q:133:TYR:CD2	2.94	0.45
6:S:33:ALA:O	6:S:34:GLU:HG3	2.17	0.45
1:A:18:ALA:CB	1:N:208:LYS:HZ1	2.30	0.45
1:A:33:PHE:CE2	14:E:101:BCR:C35	3.00	0.45
1:A:52:PHE:C	1:A:52:PHE:CD1	2.91	0.45
1:A:81:LEU:O	1:A:82:ILE:C	2.57	0.45
1:A:90:ALA:O	1:A:94:VAL:HG23	2.17	0.45
1:A:174:SER:OG	4:Q:86:GLY:HA3	2.17	0.45
2:B:146:GLY:O	2:B:147:ALA:CB	2.64	0.45
3:C:180:ILE:HB	3:C:199:ILE:HA	1.99	0.45
3:C:251:ASP:HB3	3:C:254:ARG:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:4:LEU:O	7:G:6:LEU:HD22	2.16	0.45
1:N:19:ASP:OD1	1:N:22:THR:O	2.35	0.45
1:N:27:PRO:HA	2:O:33:PRO:CG	2.47	0.45
1:N:32:ILE:CD1	7:T:26:ARG:NH2	2.80	0.45
1:N:165:ILE:C	1:N:167:ASP:N	2.75	0.45
2:O:96:LEU:O	2:O:97:GLY:C	2.59	0.45
3:P:28:ALA:CB	3:P:240:PHE:N	2.80	0.45
3:P:44:THR:O	3:P:133:SER:N	2.50	0.45
3:P:101:VAL:CG1	3:P:118:PRO:HB2	2.47	0.45
4:Q:69:PHE:C	4:Q:70:LEU:HG	2.41	0.45
5:R:2:ILE:HG13	5:R:3:LEU:N	2.32	0.45
5:R:23:ILE:C	5:R:25:ALA:N	2.75	0.45
1:A:29:HIS:ND1	2:B:30:PRO:CG	2.80	0.44
1:A:52:PHE:C	1:A:55:THR:HG23	2.40	0.44
1:A:101:VAL:O	1:A:104:VAL:HB	2.17	0.44
1:A:142:GLN:HG2	2:B:65:PRO:HG3	1.98	0.44
2:B:105:PRO:CG	2:B:106:LEU:H	2.21	0.44
3:C:182:LYS:N	3:C:182:LYS:HD2	2.33	0.44
5:E:23:ILE:O	5:E:25:ALA:N	2.50	0.44
8:H:3:VAL:CA	8:H:6:TRP:HD1	2.29	0.44
1:N:154:VAL:HB	1:N:155:PRO:CD	2.46	0.44
1:N:178:ALA:O	1:N:180:LEU:N	2.50	0.44
1:N:179:THR:O	1:N:183:TYR:CD1	2.70	0.44
1:N:191:LEU:HD12	1:N:191:LEU:N	2.14	0.44
2:O:43:VAL:HB	2:O:44:ILE:H	1.58	0.44
2:O:43:VAL:CA	7:T:23:GLN:OE1	2.64	0.44
2:O:73:LEU:N	2:O:73:LEU:CD2	2.80	0.44
3:P:90:ILE:O	3:P:91:PRO:C	2.60	0.44
3:P:93:GLU:C	3:P:95:LYS:H	2.23	0.44
3:P:280:GLU:OE2	7:T:28:ASN:ND2	2.50	0.44
7:T:24:TYR:CD2	7:T:24:TYR:N	2.83	0.44
2:B:81:LEU:CD1	2:B:81:LEU:H	2.30	0.44
2:B:124:PHE:CZ	5:E:27:LYS:HG3	2.52	0.44
2:B:125:ARG:HA	2:B:125:ARG:HD3	1.89	0.44
3:C:60:GLN:HE22	3:C:157:ARG:HG3	1.82	0.44
3:C:78:LEU:HD21	3:C:131:VAL:CG2	2.42	0.44
1:N:62:VAL:HG13	1:N:177:GLN:CD	2.41	0.44
1:N:114:ARG:HD2	1:N:208:LYS:HE2	1.99	0.44
1:N:155:PRO:C	1:N:157:ALA:H	2.23	0.44
1:N:155:PRO:C	1:N:157:ALA:N	2.76	0.44
1:N:158:ILE:O	1:N:160:VAL:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:55:THR:O	4:Q:64:VAL:HB	2.17	0.44
7:T:4:LEU:O	7:T:6:LEU:HD22	2.17	0.44
8:U:6:TRP:O	8:U:7:VAL:C	2.59	0.44
1:A:28:PRO:HG2	2:B:31:ALA:O	2.17	0.44
1:A:82:ILE:CD1	1:A:82:ILE:H	2.30	0.44
1:A:113:PRO:C	1:A:115:GLU:H	2.26	0.44
1:A:165:ILE:O	1:A:166:SER:C	2.57	0.44
10:B:305:OPC:HAV	10:B:305:OPC:CAH	2.47	0.44
3:C:3:PHE:O	3:C:5:ALA:N	2.51	0.44
3:C:61:VAL:HA	3:C:67:LYS:HA	1.98	0.44
3:C:256:LYS:HE2	3:C:257:TRP:CZ3	2.52	0.44
4:D:137:GLY:O	4:D:138:ARG:O	2.35	0.44
6:F:10:ALA:O	6:F:11:LEU:C	2.61	0.44
1:N:101:VAL:O	1:N:104:VAL:HB	2.17	0.44
2:O:40:PHE:H	2:O:41:PRO:HD2	1.81	0.44
2:O:128:VAL:O	2:O:132:ILE:HD11	2.18	0.44
3:P:175:SER:O	3:P:176:ALA:HB2	2.16	0.44
4:Q:67:SER:CA	4:Q:70:LEU:HD21	2.35	0.44
5:R:6:VAL:O	5:R:10:VAL:HG12	2.18	0.44
1:A:33:PHE:CE1	5:E:18:ILE:CD1	2.88	0.44
1:A:50:THR:O	1:A:51:GLY:C	2.58	0.44
1:A:118:TRP:CE2	9:A:302:HEC:HBC1	2.52	0.44
5:E:15:PHE:C	5:E:18:ILE:H	2.23	0.44
6:F:28:LEU:HD22	6:F:31:GLN:HE22	1.83	0.44
9:N:303:HEC:HBC1	10:N:1305:OPC:HAQ1	1.99	0.44
2:O:85:PHE:CD1	2:O:86:GLN:N	2.86	0.44
3:P:161:TYR:HB2	3:P:165:GLU:O	2.18	0.44
3:P:181:THR:OG1	3:P:200:GLN:HG2	2.17	0.44
4:Q:141:ARG:C	4:Q:142:GLY:O	2.59	0.44
4:Q:173:GLY:O	4:Q:174:GLU:OE2	2.35	0.44
5:R:29:ILE:O	5:R:29:ILE:CG2	2.65	0.44
7:T:10:PHE:O	7:T:11:ALA:C	2.60	0.44
1:A:127:ILE:CD1	1:A:194:LEU:HB2	2.47	0.44
1:A:178:ALA:O	1:A:180:LEU:N	2.51	0.44
2:B:99:LEU:O	2:B:100:LEU:C	2.60	0.44
2:B:101:MET:CG	2:B:102:ALA:N	2.80	0.44
2:B:132:ILE:HA	2:B:135:PHE:CD2	2.46	0.44
3:C:3:PHE:O	3:C:4:TRP:C	2.60	0.44
3:C:50:VAL:O	3:C:52:ILE:HG13	2.17	0.44
3:C:172:PHE:CD1	3:C:215:PRO:HG3	2.52	0.44
3:C:274:LEU:O	3:C:275:LYS:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:177:TRP:CD1	4:D:177:TRP:H	2.35	0.44
1:N:14:ILE:CB	1:N:17:LEU:HD11	2.38	0.44
3:P:82:PHE:CE1	3:P:134:PRO:HD2	2.53	0.44
3:P:221:GLU:C	3:P:223:GLN:H	2.25	0.44
3:P:277:LYS:HE3	7:T:27:PRO:CD	2.47	0.44
4:Q:73:HIS:HB2	4:Q:93:VAL:HG21	1.99	0.44
4:Q:88:PRO:HD2	4:Q:107:VAL:HG23	1.99	0.44
4:Q:94:GLU:CG	4:Q:100:ARG:HG2	2.47	0.44
2:B:48:PHE:CD1	2:B:48:PHE:C	2.94	0.44
2:B:51:ILE:H	2:B:51:ILE:CD1	2.20	0.44
3:C:14:ARG:CZ	3:C:150:HIS:ND1	2.80	0.44
3:C:91:PRO:O	3:C:92:GLU:CG	2.61	0.44
4:D:65:LYS:N	4:D:65:LYS:HD2	2.32	0.44
6:F:8:TYR:HD2	6:F:9:ALA:N	2.15	0.44
1:N:33:PHE:O	1:N:35:CYS:N	2.51	0.44
3:P:46:PHE:CD1	3:P:131:VAL:HG13	2.52	0.44
3:P:231:LEU:HD11	3:P:233:ASN:O	2.18	0.44
3:P:259:ILE:HD11	7:T:12:THR:HG21	2.00	0.44
5:R:6:VAL:O	5:R:10:VAL:CG1	2.65	0.44
3:C:93:GLU:C	3:C:95:LYS:H	2.26	0.44
4:D:132:GLN:C	4:D:133:TYR:CD2	2.95	0.44
5:E:23:ILE:C	5:E:25:ALA:N	2.75	0.44
2:O:29:GLU:N	2:O:30:PRO:CD	2.77	0.44
3:P:3:PHE:HD2	3:P:4:TRP:CZ3	2.36	0.44
3:P:60:GLN:HE22	3:P:157:ARG:HG3	1.82	0.44
4:Q:70:LEU:CD1	4:Q:71:GLU:HG2	2.47	0.44
1:A:62:VAL:HG23	1:A:63:THR:HG23	1.99	0.44
2:B:43:VAL:O	2:B:44:ILE:C	2.60	0.44
3:C:15:GLU:HB2	3:C:19:ARG:O	2.17	0.44
3:C:144:PHE:O	3:C:147:TYR:CE1	2.71	0.44
3:C:167:SER:OG	3:C:168:ASN:N	2.49	0.44
1:N:50:THR:O	1:N:51:GLY:C	2.59	0.44
1:N:120:SER:HA	1:N:123:ILE:HD13	2.00	0.44
2:O:72:PRO:O	2:O:74:GLU:N	2.51	0.44
2:O:106:LEU:O	2:O:107:GLY:C	2.60	0.44
3:P:55:ASP:HB2	3:P:57:LYS:CD	2.48	0.44
3:P:277:LYS:HA	3:P:280:GLU:HB3	2.00	0.44
4:Q:94:GLU:HG2	4:Q:99:ILE:C	2.42	0.44
4:Q:117:TRP:CZ3	4:Q:119:ALA:HA	2.53	0.44
5:R:15:PHE:O	5:R:19:ALA:N	2.50	0.44
8:U:3:VAL:CA	8:U:6:TRP:HD1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PRO:O	1:A:140:TRP:CB	2.66	0.44
2:B:42:VAL:HA	2:B:45:MET:CE	2.48	0.44
3:C:46:PHE:CE1	3:C:131:VAL:HG13	2.52	0.44
3:C:184:ALA:HB3	3:C:197:VAL:N	2.33	0.44
3:C:196:GLN:HE22	3:C:210:THR:HB	1.79	0.44
4:D:35:LEU:N	4:D:37:PRO:HD2	2.22	0.44
4:D:173:GLY:O	4:D:174:GLU:OE2	2.36	0.44
5:E:11:PHE:C	5:E:13:ALA:N	2.75	0.44
6:F:4:GLU:HG3	6:F:5:GLU:H	1.82	0.44
8:H:15:TRP:C	8:H:17:ILE:H	2.26	0.44
1:N:78:PHE:HE1	4:Q:37:PRO:HA	1.82	0.44
1:N:105:TYR:HD2	1:N:106:LEU:CD2	2.31	0.44
2:O:57:LEU:HD23	2:O:57:LEU:HA	1.87	0.44
2:O:62:VAL:HG22	11:O:1309:BNT:CAK	2.48	0.44
3:P:120:PRO:HG2	3:P:124:TYR:HB2	1.99	0.44
3:P:144:PHE:O	3:P:147:TYR:CE1	2.70	0.44
3:P:199:ILE:HD12	3:P:208:VAL:HA	2.00	0.44
3:P:271:MET:CE	4:Q:22:LEU:HG	2.44	0.44
6:S:16:LEU:HA	6:S:19:VAL:CB	2.48	0.44
8:U:15:TRP:C	8:U:17:ILE:H	2.26	0.44
1:A:48:PHE:O	1:A:52:PHE:HB3	2.18	0.43
1:A:54:MET:C	1:A:56:PHE:N	2.72	0.43
1:A:160:VAL:HG12	1:A:161:VAL:N	2.30	0.43
4:D:19:MET:O	4:D:21:LEU:N	2.50	0.43
4:D:73:HIS:CG	4:D:93:VAL:HG21	2.53	0.43
5:E:12:ILE:HA	5:E:15:PHE:CE1	2.53	0.43
5:E:15:PHE:O	5:E:19:ALA:N	2.51	0.43
2:O:96:LEU:HD13	2:O:96:LEU:C	2.42	0.43
3:P:6:GLN:HB3	3:P:106:TYR:CE2	2.53	0.43
1:A:183:TYR:O	1:A:184:TYR:C	2.60	0.43
2:B:101:MET:C	2:B:103:SER:H	2.25	0.43
10:B:305:OPC:HAU1	10:B:305:OPC:HAX2	1.67	0.43
10:B:305:OPC:HBZ2	10:B:305:OPC:HAX2	1.99	0.43
3:C:76:LEU:HD23	3:C:77:MET:C	2.43	0.43
3:C:151:LEU:HD23	3:C:151:LEU:O	2.18	0.43
4:D:80:LEU:H	4:D:80:LEU:CD2	2.29	0.43
5:E:5:ALA:C	5:E:7:PHE:N	2.76	0.43
6:F:10:ALA:C	6:F:12:LEU:H	2.25	0.43
1:N:43:CYS:HB2	1:N:93:MET:HB2	2.00	0.43
1:N:82:ILE:H	1:N:82:ILE:HD12	1.84	0.43
1:A:34:TYR:CD1	1:A:103:ARG:CD	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:HG22	1:A:205:MET:HB3	1.98	0.43
2:B:38:TYR:HA	2:B:41:PRO:CG	2.48	0.43
2:B:86:GLN:O	2:B:87:ILE:C	2.59	0.43
4:D:108:CYS:SG	4:D:110:HIS:HB3	2.58	0.43
4:D:115:VAL:HG22	4:D:126:CYS:HB2	1.99	0.43
5:E:9:ILE:CG2	5:E:10:VAL:H	2.31	0.43
5:E:22:ILE:O	5:E:23:ILE:C	2.61	0.43
6:F:26:LEU:C	6:F:26:LEU:CD2	2.91	0.43
1:N:110:PHE:HA	1:N:114:ARG:O	2.18	0.43
1:N:146:TRP:C	1:N:148:VAL:H	2.25	0.43
1:N:183:TYR:O	1:N:184:TYR:C	2.60	0.43
1:N:211:ILE:CG2	1:N:212:SER:N	2.81	0.43
2:O:79:TRP:HA	2:O:82:TYR:CZ	2.53	0.43
2:O:125:ARG:HH11	2:O:126:ARG:N	1.88	0.43
3:P:6:GLN:HB3	3:P:106:TYR:CZ	2.53	0.43
3:P:87:GLU:HA	3:P:90:ILE:HD12	2.00	0.43
3:P:177:THR:HG22	3:P:177:THR:O	2.18	0.43
3:P:199:ILE:N	3:P:208:VAL:HG12	2.33	0.43
3:P:261:PHE:HE2	4:Q:34:ALA:N	2.16	0.43
4:Q:102:TYR:HB2	4:Q:150:LEU:HB3	2.00	0.43
1:A:15:GLN:O	1:A:17:LEU:CD1	2.67	0.43
1:A:119:ILE:O	1:A:122:VAL:N	2.52	0.43
1:A:165:ILE:O	1:A:168:LEU:N	2.49	0.43
1:A:170:ARG:HA	1:A:179:THR:HA	2.00	0.43
1:A:195:ILE:CG2	1:A:196:ALA:N	2.81	0.43
2:B:96:LEU:CD1	2:B:100:LEU:HD12	2.48	0.43
2:B:146:GLY:O	2:B:147:ALA:HB3	2.18	0.43
3:C:9:TYR:CE1	3:C:21:VAL:HG11	2.54	0.43
3:C:83:LYS:HE3	3:C:134:PRO:CA	2.48	0.43
3:C:177:THR:O	3:C:177:THR:HG22	2.19	0.43
3:C:262:ILE:C	3:C:264:LEU:N	2.75	0.43
10:C:306:OPC:CAA	4:D:17:GLN:HG2	2.49	0.43
4:D:147:SER:C	4:D:148:LEU:HG	2.44	0.43
5:E:23:ILE:C	5:E:23:ILE:CD1	2.89	0.43
8:H:22:TRP:C	8:H:24:ARG:N	2.75	0.43
1:N:159:PRO:C	1:N:161:VAL:N	2.64	0.43
1:N:200:LEU:N	1:N:200:LEU:HD22	2.33	0.43
2:O:135:PHE:O	2:O:137:THR:N	2.49	0.43
3:P:91:PRO:O	3:P:92:GLU:CG	2.60	0.43
3:P:110:GLN:HB3	3:P:113:VAL:HG23	2.00	0.43
5:R:14:LEU:HD22	5:R:14:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:22:ILE:HG23	5:R:23:ILE:N	2.33	0.43
1:A:128:THR:O	1:A:129:VAL:C	2.61	0.43
2:B:67:ASN:N	2:B:68:PRO:CD	2.81	0.43
2:B:95:LEU:N	2:B:95:LEU:HD23	2.32	0.43
2:B:122:ASN:HB2	2:B:123:PRO:CD	2.43	0.43
3:C:6:GLN:HB3	3:C:106:TYR:CZ	2.53	0.43
3:C:81:GLY:C	3:C:134:PRO:CG	2.92	0.43
3:C:275:LYS:HZ1	10:C:306:OPC:HBG3	1.77	0.43
4:D:88:PRO:CB	2:O:69:PHE:CD2	2.99	0.43
4:D:117:TRP:CZ3	4:D:119:ALA:HA	2.53	0.43
4:D:163:THR:HB	4:D:164:PRO:HD2	2.00	0.43
6:F:25:VAL:O	6:F:28:LEU:N	2.41	0.43
7:G:13:LEU:HD13	7:G:13:LEU:C	2.44	0.43
1:N:28:PRO:CG	2:O:32:TRP:HB3	2.29	0.43
1:N:117:THR:O	1:N:202:HIS:CE1	2.71	0.43
1:N:167:ASP:OD2	1:N:172:GLY:O	2.36	0.43
2:O:79:TRP:HZ2	5:R:1:MET:HA	1.82	0.43
3:P:76:LEU:HD23	3:P:77:MET:C	2.43	0.43
3:P:81:GLY:O	3:P:134:PRO:HG3	2.19	0.43
3:P:273:ILE:CG2	7:T:22:GLN:HB3	2.34	0.43
4:Q:66:VAL:HG13	4:Q:159:ASN:O	2.18	0.43
4:Q:88:PRO:O	4:Q:106:ALA:HB3	2.18	0.43
3:C:28:ALA:HB3	3:C:240:PHE:CB	2.48	0.43
3:C:278:GLN:C	3:C:279:VAL:HG23	2.43	0.43
4:D:71:GLU:HG3	4:D:72:SER:N	2.33	0.43
1:N:15:GLN:H	1:N:17:LEU:HD12	1.83	0.43
1:N:142:GLN:HG2	2:O:64:GLU:CG	2.49	0.43
2:O:42:VAL:HA	2:O:45:MET:CE	2.47	0.43
3:P:140:LYS:HD2	3:P:140:LYS:N	2.33	0.43
3:P:180:ILE:HB	3:P:199:ILE:HA	2.00	0.43
3:P:271:MET:HA	3:P:274:LEU:HG	1.98	0.43
4:Q:51:GLY:O	4:Q:52:GLY:C	2.61	0.43
5:R:18:ILE:O	5:R:23:ILE:HG23	2.19	0.43
5:R:25:ALA:O	5:R:29:ILE:HD12	2.18	0.43
7:T:16:LEU:O	7:T:16:LEU:CD2	2.61	0.43
1:A:112:LYS:HG3	1:A:113:PRO:HD3	2.00	0.43
2:B:57:LEU:HD21	7:G:9:VAL:C	2.43	0.43
2:B:106:LEU:O	2:B:107:GLY:C	2.61	0.43
2:B:124:PHE:CE1	5:E:23:ILE:HD11	2.53	0.43
11:B:309:BNT:CAM	3:C:148:ALA:N	2.81	0.43
3:C:180:ILE:HG13	3:C:199:ILE:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:65:LYS:HB2	4:D:68:LYS:HZ3	1.83	0.43
1:N:25:TYR:HB2	1:N:26:VAL:H	1.73	0.43
1:N:114:ARG:HG2	1:N:114:ARG:HH11	1.83	0.43
2:O:86:GLN:O	2:O:87:ILE:C	2.61	0.43
2:O:147:ALA:O	2:O:149:LEU:CD2	2.64	0.43
3:P:225:VAL:O	3:P:226:LYS:HB3	2.18	0.43
4:Q:163:THR:HB	4:Q:164:PRO:CD	2.48	0.43
14:R:1101:BCR:H322	7:T:23:GLN:HE22	1.83	0.43
6:S:8:TYR:HD2	6:S:9:ALA:H	1.67	0.43
1:A:26:VAL:HB	2:B:29:GLU:CG	2.27	0.43
1:A:30:VAL:C	1:A:211:ILE:CD1	2.91	0.43
1:A:51:GLY:O	1:A:52:PHE:C	2.59	0.43
1:A:87:ARG:NH1	2:B:60:ALA:HA	2.33	0.43
1:A:108:GLY:O	1:A:110:PHE:CD2	2.72	0.43
2:B:127:PRO:O	2:B:130:THR:N	2.51	0.43
3:C:34:VAL:HG11	3:C:151:LEU:HD22	2.00	0.43
3:C:161:TYR:HE1	3:C:167:SER:HA	1.82	0.43
4:D:41:TYR:CD2	4:D:42:PHE:N	2.86	0.43
4:D:63:ASN:O	4:D:65:LYS:HD2	2.19	0.43
4:D:110:HIS:CD2	4:D:143:PRO:HB2	2.53	0.43
1:N:82:ILE:O	1:N:83:ARG:C	2.59	0.43
1:N:111:LYS:CB	1:N:113:PRO:HD2	2.44	0.43
1:N:205:MET:O	1:N:207:ARG:HG3	2.18	0.43
2:O:23:GLY:C	2:O:25:ASN:H	2.27	0.43
3:P:117:GLY:O	3:P:119:LEU:CD2	2.66	0.43
4:Q:33:GLY:O	4:Q:37:PRO:CD	2.67	0.43
4:Q:35:LEU:O	4:Q:36:TYR:C	2.58	0.43
7:T:16:LEU:C	7:T:16:LEU:CD1	2.88	0.43
1:A:65:ALA:O	1:A:69:VAL:HG23	2.18	0.43
1:A:99:LEU:HA	1:A:102:PHE:CD1	2.54	0.43
1:A:101:VAL:HG11	12:B:201:CLA:HMA2	2.01	0.43
1:A:184:TYR:O	1:A:185:SER:C	2.60	0.43
2:B:141:ILE:O	2:B:144:GLY:N	2.42	0.43
3:C:83:LYS:HE3	3:C:134:PRO:HA	2.01	0.43
4:D:69:PHE:HA	4:D:73:HIS:ND1	2.34	0.43
4:D:94:GLU:HG2	4:D:99:ILE:C	2.43	0.43
5:E:5:ALA:HB1	6:F:10:ALA:N	2.34	0.43
1:N:43:CYS:O	1:N:46:ILE:HB	2.18	0.43
1:N:163:VAL:C	1:N:165:ILE:N	2.77	0.43
1:N:165:ILE:HD13	1:N:165:ILE:C	2.43	0.43
2:O:130:THR:O	2:O:131:THR:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:34:VAL:HG11	3:P:151:LEU:CB	2.49	0.43
3:P:76:LEU:HD21	3:P:78:LEU:HD12	2.01	0.43
3:P:205:LYS:HZ1	3:P:207:VAL:HA	1.82	0.43
4:Q:19:MET:O	4:Q:21:LEU:N	2.51	0.43
4:Q:35:LEU:C	4:Q:37:PRO:N	2.75	0.43
4:Q:41:TYR:HD2	4:Q:42:PHE:N	2.16	0.43
4:Q:157:ASP:O	4:Q:158:ASP:CB	2.67	0.43
1:A:48:PHE:HA	9:A:301:HEC:CMC	2.49	0.43
1:A:210:GLY:O	1:A:211:ILE:HB	2.18	0.43
3:C:54:TYR:CE1	3:C:70:LEU:HD22	2.54	0.43
3:C:169:ASN:CG	3:C:236:ASN:HA	2.44	0.43
1:N:116:LEU:HD13	1:N:205:MET:SD	2.59	0.43
1:N:165:ILE:HG22	1:N:166:SER:H	1.84	0.43
1:N:209:GLN:CD	2:O:27:TYR:C	2.87	0.43
3:P:3:PHE:O	3:P:4:TRP:C	2.61	0.43
3:P:6:GLN:HA	3:P:106:TYR:OH	2.19	0.43
3:P:83:LYS:HZ2	3:P:83:LYS:H	1.66	0.43
3:P:216:GLU:O	3:P:217:LEU:HD23	2.19	0.43
5:R:3:LEU:HD12	5:R:3:LEU:O	2.19	0.43
1:A:103:ARG:C	1:A:103:ARG:HD2	2.44	0.42
1:A:191:LEU:C	1:A:193:TRP:N	2.74	0.42
2:B:79:TRP:HA	2:B:82:TYR:HE2	1.80	0.42
10:C:306:OPC:HAA1	4:D:17:GLN:HG2	2.00	0.42
4:D:102:TYR:HB2	4:D:150:LEU:HB3	2.00	0.42
1:N:15:GLN:HE21	1:N:16:ALA:N	2.16	0.42
1:N:36:LEU:HB3	1:N:100:HIS:HB2	2.00	0.42
1:N:57:TYR:CE1	1:N:76:VAL:HG21	2.53	0.42
1:N:110:PHE:CB	1:N:115:GLU:HA	2.48	0.42
1:N:165:ILE:O	1:N:168:LEU:N	2.48	0.42
1:N:191:LEU:C	1:N:193:TRP:N	2.76	0.42
2:O:81:LEU:HD23	2:O:81:LEU:O	2.19	0.42
2:O:150:PRO:O	2:O:151:LEU:CB	2.67	0.42
3:P:78:LEU:HD21	3:P:131:VAL:CG2	2.43	0.42
3:P:226:LYS:HB3	3:P:226:LYS:HZ3	1.83	0.42
4:Q:14:GLY:O	4:Q:15:ARG:HB2	2.19	0.42
6:S:22:GLY:O	6:S:23:LEU:C	2.62	0.42
1:A:47:GLN:NE2	1:A:89:SER:C	2.77	0.42
1:A:171:GLY:HA3	1:A:178:ALA:CB	2.46	0.42
1:A:176:GLY:C	1:A:178:ALA:N	2.74	0.42
2:B:32:TRP:CE2	7:G:28:ASN:HB3	2.54	0.42
11:B:309:BNT:CAM	3:C:148:ALA:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:PRO:O	3:C:87:GLU:C	2.61	0.42
3:C:110:GLN:HB3	3:C:113:VAL:HG23	2.01	0.42
3:C:280:GLU:O	3:C:282:VAL:N	2.52	0.42
4:D:128:CYS:HB2	4:D:129:HIS:ND1	2.34	0.42
5:E:6:VAL:O	5:E:10:VAL:CG1	2.67	0.42
14:E:101:BCR:H20C	14:E:101:BCR:H361	1.76	0.42
1:N:80:TRP:CD2	3:P:254:ARG:NH2	2.86	0.42
1:N:114:ARG:NH2	9:N:302:HEC:O1D	2.52	0.42
10:O:1306:OPC:HBR	10:O:1306:OPC:HBF2	2.01	0.42
3:P:136:PRO:HB2	3:P:142:ILE:O	2.19	0.42
3:P:161:TYR:HE1	3:P:167:SER:HA	1.82	0.42
7:T:6:LEU:H	7:T:6:LEU:CD2	2.23	0.42
1:A:43:CYS:O	1:A:46:ILE:HB	2.18	0.42
1:A:165:ILE:HD11	1:A:168:LEU:HD12	2.00	0.42
6:F:28:LEU:HD23	6:F:31:GLN:NE2	2.34	0.42
1:N:47:GLN:CB	9:N:301:HEC:HBB2	2.49	0.42
1:N:204:LEU:O	1:N:207:ARG:HG3	2.19	0.42
2:O:62:VAL:HG23	2:O:63:GLY:N	2.35	0.42
2:O:64:GLU:H	2:O:65:PRO:HD2	1.83	0.42
2:O:122:ASN:HD22	5:R:27:LYS:CA	2.31	0.42
2:O:149:LEU:HA	2:O:150:PRO:HD3	1.74	0.42
3:P:13:PRO:HB2	3:P:20:ILE:HG22	2.00	0.42
6:S:20:GLY:HA3	7:T:21:TYR:CE1	2.54	0.42
1:A:123:ILE:O	1:A:124:LEU:C	2.62	0.42
1:A:142:GLN:NE2	2:B:68:PRO:CB	2.75	0.42
1:A:146:TRP:HB3	2:B:75:ILE:CD1	2.50	0.42
2:B:130:THR:O	2:B:131:THR:C	2.60	0.42
3:C:86:PRO:HG2	3:C:89:ARG:HB2	2.00	0.42
3:C:216:GLU:O	3:C:217:LEU:HD23	2.18	0.42
4:D:132:GLN:C	4:D:133:TYR:HD2	2.27	0.42
5:E:14:LEU:HD22	5:E:14:LEU:N	2.34	0.42
1:N:33:PHE:CD1	1:N:34:TYR:CE1	3.08	0.42
3:P:225:VAL:HB	3:P:226:LYS:H	1.49	0.42
3:P:275:LYS:O	3:P:276:LYS:C	2.61	0.42
1:A:55:THR:OG1	1:N:185:SER:CB	2.68	0.42
1:A:82:ILE:O	1:A:83:ARG:C	2.63	0.42
2:B:72:PRO:HG2	2:B:75:ILE:CG1	2.40	0.42
2:B:116:ASN:O	2:B:116:ASN:ND2	2.52	0.42
3:C:34:VAL:HG13	3:C:151:LEU:HD22	2.00	0.42
3:C:270:LEU:C	3:C:274:LEU:HG	2.45	0.42
5:E:14:LEU:O	5:E:18:ILE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:6:TRP:O	8:H:9:LEU:N	2.53	0.42
1:N:24:LYS:H	1:N:24:LYS:HG2	1.49	0.42
1:N:84:SER:HB2	2:O:55:SER:HB3	2.02	0.42
1:N:170:ARG:O	1:N:179:THR:N	2.53	0.42
3:P:21:VAL:O	3:P:22:CYS:C	2.62	0.42
3:P:81:GLY:C	3:P:134:PRO:CG	2.92	0.42
3:P:83:LYS:O	3:P:131:VAL:HG23	2.20	0.42
3:P:277:LYS:C	3:P:279:VAL:N	2.77	0.42
4:Q:105:ASN:ND2	4:Q:107:VAL:HB	2.33	0.42
4:Q:115:VAL:CG2	4:Q:126:CYS:HB2	2.50	0.42
1:A:40:THR:O	1:A:93:MET:HG3	2.20	0.42
1:A:177:GLN:C	1:A:177:GLN:OE1	2.62	0.42
1:A:191:LEU:O	1:A:193:TRP:N	2.53	0.42
2:B:85:PHE:CD1	2:B:86:GLN:N	2.87	0.42
2:B:124:PHE:CZ	5:E:27:LYS:CB	2.98	0.42
4:D:69:PHE:C	4:D:70:LEU:HG	2.45	0.42
4:D:110:HIS:HB2	4:D:144:ALA:CA	2.34	0.42
1:N:18:ALA:C	1:N:20:ASP:H	2.27	0.42
1:N:127:ILE:CD1	1:N:194:LEU:HB2	2.45	0.42
2:O:48:PHE:O	2:O:50:CYS:N	2.53	0.42
3:P:54:TYR:HD2	3:P:155:ARG:NH1	2.17	0.42
5:R:5:ALA:CB	6:S:6:MET:O	2.67	0.42
1:A:95:LEU:HD23	1:A:99:LEU:HD21	2.00	0.42
2:B:126:ARG:HA	2:B:127:PRO:HD2	1.73	0.42
2:B:126:ARG:HG2	2:B:128:VAL:HG23	2.00	0.42
10:B:305:OPC:HBV2	10:C:306:OPC:HBT1	2.01	0.42
3:C:263:CYS:HA	3:C:266:MET:CB	2.50	0.42
4:D:82:GLN:HA	4:D:82:GLN:NE2	2.35	0.42
6:F:8:TYR:O	6:F:11:LEU:CD1	2.68	0.42
7:G:26:ARG:CD	7:G:27:PRO:HD3	2.27	0.42
2:O:68:PRO:HG2	2:O:69:PHE:N	2.32	0.42
3:P:199:ILE:C	3:P:208:VAL:HG12	2.44	0.42
4:Q:81:VAL:CG1	4:Q:82:GLN:H	2.16	0.42
4:Q:178:TRP:O	4:Q:179:VAL:C	2.61	0.42
1:A:44:PHE:C	1:A:46:ILE:H	2.26	0.42
1:A:73:MET:O	1:A:74:ASN:C	2.63	0.42
1:A:120:SER:OG	1:A:121:GLY:N	2.53	0.42
1:A:174:SER:HB3	4:Q:86:GLY:HA3	2.02	0.42
5:E:7:PHE:O	5:E:11:PHE:CD2	2.72	0.42
1:N:66:TYR:HB2	2:O:65:PRO:HG2	2.01	0.42
1:N:74:ASN:HB3	3:P:143:HIS:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:184:TYR:C	1:N:184:TYR:CD2	2.98	0.42
1:N:186:ALA:HA	1:N:190:VAL:HB	2.02	0.42
2:O:28:GLY:C	2:O:30:PRO:HD3	2.44	0.42
2:O:70:ALA:O	2:O:71:THR:OG1	2.36	0.42
3:P:86:PRO:O	3:P:87:GLU:C	2.63	0.42
3:P:121:GLY:C	3:P:123:GLN:N	2.71	0.42
3:P:205:LYS:HE2	3:P:206:THR:C	2.45	0.42
3:P:271:MET:HE3	4:Q:22:LEU:CG	2.43	0.42
4:Q:82:GLN:HA	4:Q:82:GLN:NE2	2.35	0.42
4:Q:104:ILE:HD12	4:Q:104:ILE:C	2.44	0.42
4:Q:110:HIS:ND1	4:Q:111:LEU:HB2	2.34	0.42
2:B:96:LEU:O	2:B:97:GLY:C	2.62	0.42
2:B:100:LEU:O	2:B:103:SER:HB2	2.20	0.42
2:B:108:LEU:O	2:B:110:LEU:N	2.53	0.42
4:D:63:ASN:O	4:D:159:ASN:ND2	2.52	0.42
4:D:69:PHE:O	4:D:99:ILE:HD13	2.20	0.42
1:N:41:LEU:O	1:N:44:PHE:CB	2.66	0.42
1:N:72:ILE:HD12	1:N:72:ILE:H	1.85	0.42
3:P:2:PRO:O	3:P:3:PHE:C	2.63	0.42
3:P:52:ILE:HA	3:P:53:PRO:HD2	1.66	0.42
5:R:3:LEU:HG	5:R:7:PHE:CE2	2.55	0.42
6:S:16:LEU:HD22	6:S:16:LEU:N	2.34	0.42
1:A:22:THR:O	1:A:22:THR:HG23	2.19	0.42
1:A:39:ILE:CD1	2:B:43:VAL:HG12	2.49	0.42
1:A:53:ALA:CA	4:D:42:PHE:CZ	2.97	0.42
2:B:57:LEU:HD22	7:G:10:PHE:CD1	2.55	0.42
2:B:149:LEU:HB3	2:B:150:PRO:HD2	2.02	0.42
3:C:19:ARG:NH1	3:C:23:ALA:HB3	2.35	0.42
3:C:20:ILE:HG13	3:C:152:GLY:HA3	2.02	0.42
3:C:95:LYS:O	3:C:96:LYS:C	2.63	0.42
3:C:169:ASN:C	3:C:236:ASN:HB2	2.44	0.42
3:C:185:LYS:NZ	3:C:195:TYR:HB3	2.35	0.42
4:D:163:THR:HB	4:D:164:PRO:CD	2.50	0.42
5:E:22:ILE:HG23	5:E:23:ILE:N	2.30	0.42
7:G:17:PHE:HB3	7:G:21:TYR:HE1	1.82	0.42
1:N:38:GLY:CA	15:N:1306:HOH:O	2.67	0.42
1:N:58:TYR:CD2	1:N:184:TYR:CE1	3.05	0.42
2:O:18:LEU:HD23	2:O:18:LEU:N	2.34	0.42
3:P:193:VAL:O	3:P:213:ALA:HB2	2.20	0.42
3:P:272:LEU:HD23	3:P:272:LEU:HA	1.82	0.42
6:S:6:MET:O	6:S:9:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:10:ALA:C	6:S:12:LEU:H	2.27	0.42
1:A:31:ASN:ND2	1:A:34:TYR:CE2	2.87	0.41
1:A:36:LEU:HD13	1:A:36:LEU:N	2.35	0.41
1:A:85:ILE:O	1:A:86:HIS:C	2.63	0.41
1:A:116:LEU:O	1:A:118:TRP:N	2.53	0.41
3:C:181:THR:HG22	3:C:181:THR:O	2.20	0.41
3:C:272:LEU:HD23	3:C:272:LEU:HA	1.83	0.41
3:C:281:LYS:HD3	3:C:281:LYS:H	1.85	0.41
4:D:35:LEU:C	4:D:37:PRO:N	2.75	0.41
5:E:7:PHE:CA	5:E:10:VAL:HG12	2.38	0.41
6:F:5:GLU:O	6:F:8:TYR:CD2	2.73	0.41
6:F:8:TYR:O	6:F:11:LEU:HD12	2.20	0.41
1:N:64:GLU:OE1	1:N:64:GLU:HA	2.20	0.41
1:N:167:ASP:N	1:N:167:ASP:OD1	2.53	0.41
1:N:206:ILE:HB	9:N:303:HEC:O1D	2.20	0.41
9:N:303:HEC:HBD2	9:N:303:HEC:CHA	2.50	0.41
2:O:36:LEU:O	2:O:39:VAL:HG22	2.19	0.41
10:O:1306:OPC:HBX2	10:O:1306:OPC:CBS	2.49	0.41
4:Q:63:ASN:O	4:Q:159:ASN:ND2	2.53	0.41
5:R:9:ILE:HG12	6:S:11:LEU:HA	2.01	0.41
5:R:15:PHE:C	5:R:18:ILE:H	2.28	0.41
6:S:10:ALA:O	6:S:11:LEU:C	2.61	0.41
8:U:7:VAL:O	8:U:11:VAL:HB	2.20	0.41
3:C:120:PRO:HG2	3:C:124:TYR:HB2	2.01	0.41
4:D:110:HIS:ND1	4:D:111:LEU:HB2	2.35	0.41
5:E:2:ILE:HG13	5:E:3:LEU:N	2.34	0.41
5:E:11:PHE:C	5:E:14:LEU:HD23	2.45	0.41
6:F:24:GLY:HA2	6:F:27:LEU:CD2	2.50	0.41
1:N:62:VAL:H	1:N:177:GLN:HE22	1.68	0.41
1:N:105:TYR:CD1	12:O:1201:CLA:HMB2	2.55	0.41
1:N:110:PHE:HB2	1:N:115:GLU:HA	2.02	0.41
1:N:116:LEU:O	1:N:118:TRP:N	2.53	0.41
2:O:101:MET:C	2:O:103:SER:N	2.77	0.41
2:O:133:PHE:HB2	12:O:1201:CLA:HAB	2.02	0.41
10:O:1306:OPC:OBH	10:O:1306:OPC:HAU1	2.19	0.41
1:A:165:ILE:CD1	1:A:168:LEU:HD12	2.50	0.41
1:A:190:VAL:HB	1:A:191:LEU:HD12	2.02	0.41
1:A:203:PHE:O	1:A:206:ILE:HB	2.19	0.41
2:B:42:VAL:CG2	3:C:272:LEU:HD13	2.50	0.41
2:B:86:GLN:HE21	2:B:86:GLN:HB2	1.61	0.41
2:B:102:ALA:O	2:B:105:PRO:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:ASP:CG	3:C:57:LYS:HD2	2.45	0.41
3:C:78:LEU:HB2	3:C:112:ASN:O	2.20	0.41
4:D:110:HIS:CE1	4:D:111:LEU:HB2	2.55	0.41
5:E:6:VAL:O	5:E:6:VAL:CG1	2.68	0.41
1:N:74:ASN:O	1:N:75:GLU:CB	2.45	0.41
1:N:135:GLY:CA	1:N:138:LEU:HG	2.50	0.41
2:O:86:GLN:HE21	2:O:86:GLN:HB2	1.60	0.41
3:P:41:LEU:CD2	7:T:6:LEU:HD12	2.50	0.41
3:P:50:VAL:O	3:P:52:ILE:HG13	2.20	0.41
3:P:78:LEU:HB2	3:P:112:ASN:O	2.20	0.41
5:R:22:ILE:O	5:R:23:ILE:C	2.63	0.41
1:A:32:ILE:O	1:A:33:PHE:C	2.62	0.41
1:A:36:LEU:H	1:A:36:LEU:CD2	2.07	0.41
1:A:82:ILE:HG12	4:D:41:TYR:CE1	2.55	0.41
1:A:128:THR:OG1	9:A:302:HEC:HBB1	2.21	0.41
3:C:3:PHE:HD2	3:C:4:TRP:CZ3	2.39	0.41
3:C:9:TYR:CD1	3:C:9:TYR:N	2.88	0.41
3:C:38:GLN:O	3:C:247:ILE:HG13	2.21	0.41
3:C:84:ILE:O	3:C:84:ILE:HG23	2.21	0.41
3:C:92:GLU:HG3	3:C:94:LEU:HB2	2.02	0.41
3:C:170:ASN:HA	3:C:236:ASN:HB2	2.02	0.41
3:C:216:GLU:HB2	3:C:233:ASN:OD1	2.20	0.41
1:N:40:THR:O	1:N:93:MET:HG3	2.20	0.41
1:N:52:PHE:C	1:N:55:THR:HG23	2.42	0.41
1:N:82:ILE:CD1	1:N:82:ILE:N	2.84	0.41
1:N:123:ILE:CD1	1:N:123:ILE:N	2.72	0.41
2:O:45:MET:HE3	2:O:45:MET:HB2	1.84	0.41
2:O:79:TRP:CZ2	5:R:1:MET:HA	2.55	0.41
2:O:80:TYR:N	2:O:80:TYR:CD2	2.80	0.41
3:P:75:VAL:HG22	3:P:76:LEU:N	2.36	0.41
3:P:271:MET:HG2	4:Q:23:ALA:HA	2.03	0.41
4:Q:88:PRO:HG3	4:Q:114:VAL:CG2	2.47	0.41
1:A:165:ILE:HD13	1:A:165:ILE:C	2.46	0.41
6:F:28:LEU:CD2	6:F:31:GLN:HE22	2.34	0.41
7:G:18:TYR:O	7:G:21:TYR:CB	2.68	0.41
1:N:17:LEU:HG	1:N:20:ASP:CG	2.45	0.41
1:N:64:GLU:O	1:N:68:SER:HB3	2.19	0.41
1:N:195:ILE:HG23	1:N:196:ALA:H	1.84	0.41
3:P:53:PRO:O	3:P:54:TYR:O	2.38	0.41
3:P:176:ALA:N	3:P:228:GLY:HA3	2.35	0.41
4:Q:147:SER:C	4:Q:148:LEU:HG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:23:ILE:O	5:R:25:ALA:N	2.54	0.41
1:A:76:VAL:O	1:A:77:SER:C	2.63	0.41
1:A:174:SER:CB	4:Q:86:GLY:HA3	2.50	0.41
2:B:45:MET:HE3	2:B:45:MET:HB2	1.83	0.41
2:B:80:TYR:C	2:B:82:TYR:H	2.26	0.41
3:C:95:LYS:O	3:C:98:VAL:HG23	2.21	0.41
3:C:277:LYS:C	3:C:279:VAL:N	2.77	0.41
3:C:283:GLN:C	3:C:285:ALA:N	2.76	0.41
8:H:1:ILE:CG2	8:H:2:ASP:N	2.83	0.41
1:N:33:PHE:CG	1:N:34:TYR:N	2.89	0.41
2:O:43:VAL:O	2:O:46:GLY:N	2.53	0.41
3:P:83:LYS:NZ	3:P:132:LEU:C	2.78	0.41
3:P:83:LYS:HE3	3:P:134:PRO:CA	2.50	0.41
3:P:281:LYS:HD3	3:P:281:LYS:H	1.85	0.41
4:Q:121:GLU:O	4:Q:122:ASN:HB2	2.19	0.41
5:R:9:ILE:HG12	6:S:10:ALA:C	2.45	0.41
1:A:111:LYS:HB2	1:A:114:ARG:HH22	1.78	0.41
2:B:108:LEU:C	2:B:110:LEU:H	2.27	0.41
2:B:129:ALA:O	2:B:130:THR:C	2.64	0.41
3:C:199:ILE:C	3:C:208:VAL:HG12	2.46	0.41
4:D:41:TYR:C	4:D:43:ILE:N	2.76	0.41
1:N:103:ARG:HD2	1:N:103:ARG:C	2.45	0.41
1:N:118:TRP:CH2	2:O:109:ILE:HA	2.55	0.41
3:P:26:HIS:CE1	3:P:154:ASN:ND2	2.88	0.41
3:P:155:ARG:HG2	3:P:239:GLY:N	2.36	0.41
4:Q:178:TRP:HB2	4:Q:179:VAL:H	1.58	0.41
2:B:18:LEU:C	2:B:18:LEU:CD1	2.94	0.41
2:B:55:SER:O	2:B:59:PRO:N	2.54	0.41
2:B:135:PHE:O	2:B:137:THR:N	2.52	0.41
12:B:201:CLA:H41	12:B:201:CLA:H61	1.91	0.41
3:C:87:GLU:O	3:C:88:GLU:C	2.63	0.41
3:C:272:LEU:O	3:C:276:LYS:HG2	2.21	0.41
14:E:101:BCR:H322	7:G:23:GLN:NE2	2.35	0.41
2:O:31:ALA:HB1	7:T:30:LEU:CB	2.40	0.41
2:O:144:GLY:O	2:O:145:ILE:HD12	2.21	0.41
3:P:277:LYS:NZ	3:P:278:GLN:HE22	2.19	0.41
4:Q:20:ASN:O	4:Q:23:ALA:HB3	2.21	0.41
4:Q:106:ALA:CB	4:Q:114:VAL:HG13	2.50	0.41
5:R:9:ILE:HG21	6:S:10:ALA:CA	2.51	0.41
2:B:43:VAL:O	2:B:46:GLY:N	2.54	0.41
2:B:48:PHE:O	2:B:50:CYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:VAL:H	2:B:105:PRO:CD	2.32	0.41
3:C:21:VAL:O	3:C:22:CYS:C	2.64	0.41
3:C:194:LYS:HE3	3:C:212:PRO:HB3	2.03	0.41
4:D:66:VAL:HG13	4:D:159:ASN:O	2.21	0.41
4:D:105:ASN:ND2	4:D:107:VAL:HB	2.36	0.41
4:D:139:VAL:HG11	4:D:144:ALA:O	2.20	0.41
4:D:157:ASP:O	4:D:158:ASP:CB	2.69	0.41
5:E:3:LEU:HG	5:E:7:PHE:HE2	1.86	0.41
1:N:19:ASP:O	1:N:19:ASP:OD1	2.38	0.41
1:N:69:VAL:HA	1:N:72:ILE:CD1	2.42	0.41
1:N:199:MET:HE3	9:N:302:HEC:HMB1	2.02	0.41
1:N:200:LEU:N	1:N:200:LEU:CD2	2.84	0.41
2:O:43:VAL:HG13	14:R:1101:BCR:HC22	2.03	0.41
2:O:61:MET:SD	2:O:61:MET:N	2.93	0.41
2:O:68:PRO:CG	2:O:69:PHE:H	2.32	0.41
2:O:76:LEU:HD13	2:O:76:LEU:HA	1.89	0.41
2:O:87:ILE:HA	2:O:90:SER:HB2	2.01	0.41
2:O:101:MET:HE2	12:O:1201:CLA:C9	2.51	0.41
10:O:1306:OPC:HBR	10:O:1306:OPC:CBF	2.51	0.41
3:P:92:GLU:CD	3:P:94:LEU:HB2	2.46	0.41
3:P:95:LYS:O	3:P:96:LYS:C	2.63	0.41
3:P:181:THR:O	3:P:181:THR:HG22	2.21	0.41
3:P:262:ILE:O	3:P:264:LEU:N	2.54	0.41
3:P:281:LYS:N	3:P:281:LYS:CD	2.81	0.41
4:Q:35:LEU:C	4:Q:37:PRO:CD	2.93	0.41
4:Q:70:LEU:HD12	4:Q:71:GLU:N	2.34	0.41
4:Q:118:ASN:O	4:Q:119:ALA:C	2.64	0.41
4:Q:137:GLY:O	4:Q:138:ARG:O	2.39	0.41
6:S:27:LEU:CB	7:T:25:LYS:HZ2	2.34	0.41
1:A:81:LEU:HD11	1:A:85:ILE:HD11	2.02	0.41
1:A:82:ILE:N	1:A:82:ILE:CD1	2.84	0.41
1:A:165:ILE:HG22	1:A:166:SER:H	1.86	0.41
1:A:200:LEU:O	1:A:204:LEU:HG	2.21	0.41
2:B:96:LEU:C	2:B:96:LEU:CD1	2.94	0.41
3:C:25:CYS:HB3	3:C:26:HIS:H	1.56	0.41
3:C:125:GLN:C	3:C:127:ILE:HD12	2.46	0.41
6:F:9:ALA:O	6:F:12:LEU:HB3	2.21	0.41
1:N:115:GLU:OE1	1:N:115:GLU:N	2.54	0.41
1:N:184:TYR:C	1:N:186:ALA:N	2.77	0.41
2:O:81:LEU:HA	2:O:84:VAL:HG22	2.03	0.41
10:O:1306:OPC:HBB2	10:O:1306:OPC:CCA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:101:VAL:CB	3:P:118:PRO:HB2	2.51	0.41
3:P:160:ILE:O	9:P:301:HEC:HMD2	2.21	0.41
3:P:213:ALA:O	3:P:215:PRO:HD2	2.21	0.41
4:Q:65:LYS:HB2	4:Q:68:LYS:HZ3	1.83	0.41
4:Q:69:PHE:HA	4:Q:73:HIS:ND1	2.36	0.41
5:R:11:PHE:O	5:R:14:LEU:HD23	2.20	0.41
6:S:26:LEU:C	6:S:26:LEU:CD2	2.93	0.41
3:C:218:ILE:HD11	3:C:232:THR:HA	2.03	0.40
10:C:306:OPC:HAL2	10:C:306:OPC:HAP1	1.97	0.40
4:D:35:LEU:O	4:D:38:LEU:N	2.54	0.40
1:N:36:LEU:H	1:N:36:LEU:HD22	1.85	0.40
1:N:58:TYR:HD2	1:N:184:TYR:CE1	2.27	0.40
3:P:25:CYS:CA	3:P:160:ILE:HD12	2.46	0.40
3:P:73:GLY:O	3:P:74:ALA:HB2	2.21	0.40
3:P:171:VAL:HG13	3:P:234:ASN:HD22	1.85	0.40
3:P:172:PHE:CD1	3:P:215:PRO:HG3	2.56	0.40
4:Q:35:LEU:HD21	4:Q:39:VAL:HG21	2.03	0.40
1:A:110:PHE:HB3	1:A:118:TRP:CG	2.56	0.40
1:A:120:SER:HA	1:A:123:ILE:HD13	2.04	0.40
1:A:184:TYR:C	1:A:186:ALA:N	2.77	0.40
2:B:52:VAL:O	2:B:53:ALA:C	2.64	0.40
3:C:28:ALA:CB	3:C:240:PHE:N	2.83	0.40
3:C:58:LEU:HD12	3:C:58:LEU:N	2.36	0.40
4:D:44:PRO:HA	4:D:45:PRO:HD3	1.77	0.40
4:D:73:HIS:ND1	4:D:93:VAL:CG2	2.84	0.40
4:D:113:CYS:HG	4:D:128:CYS:CB	2.27	0.40
4:D:131:SER:OG	4:D:143:PRO:HD2	2.21	0.40
7:G:16:LEU:O	7:G:16:LEU:CD2	2.63	0.40
1:N:51:GLY:O	1:N:52:PHE:C	2.64	0.40
1:N:157:ALA:O	1:N:158:ILE:HG13	2.21	0.40
1:N:174:SER:O	1:N:175:VAL:CG2	2.68	0.40
2:O:146:GLY:O	2:O:147:ALA:HB3	2.21	0.40
3:P:60:GLN:O	3:P:68:VAL:N	2.51	0.40
3:P:184:ALA:HB3	3:P:197:VAL:N	2.36	0.40
3:P:202:ASP:O	3:P:204:GLY:N	2.53	0.40
3:P:235:PRO:O	3:P:236:ASN:C	2.64	0.40
3:P:261:PHE:CZ	4:Q:34:ALA:HB2	2.57	0.40
1:A:81:LEU:CD1	1:A:85:ILE:HD11	2.51	0.40
1:A:82:ILE:CD1	4:D:41:TYR:CD1	3.03	0.40
2:B:61:MET:CG	3:C:146:LYS:O	2.60	0.40
2:B:78:GLU:O	2:B:82:TYR:HE2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:PHE:CD2	2:B:137:THR:HG21	2.56	0.40
2:B:149:LEU:HD11	6:F:2:MET:CB	2.50	0.40
3:C:188:ASP:N	3:C:193:VAL:HG22	2.20	0.40
6:F:21:TRP:HA	7:G:24:TYR:CD1	2.57	0.40
6:F:35:LYS:H	6:F:35:LYS:CD	2.35	0.40
7:G:17:PHE:O	7:G:20:ALA:HB3	2.20	0.40
1:N:66:TYR:CE1	2:O:63:GLY:HA3	2.57	0.40
1:N:157:ALA:C	1:N:158:ILE:HG13	2.47	0.40
2:O:69:PHE:O	2:O:69:PHE:HD1	2.04	0.40
2:O:96:LEU:CD1	2:O:100:LEU:HD12	2.51	0.40
2:O:129:ALA:O	2:O:130:THR:C	2.64	0.40
3:P:194:LYS:HE3	3:P:212:PRO:HB3	2.03	0.40
3:P:231:LEU:HD13	3:P:232:THR:N	2.36	0.40
4:Q:65:LYS:H	4:Q:68:LYS:HZ3	1.69	0.40
4:Q:80:LEU:H	4:Q:80:LEU:CD2	2.34	0.40
4:Q:92:VAL:CG1	4:Q:93:VAL:N	2.84	0.40
4:Q:134:ASP:HB2	4:Q:135:GLU:H	1.60	0.40
4:Q:139:VAL:CG2	4:Q:144:ALA:O	2.63	0.40
4:Q:147:SER:O	4:Q:148:LEU:HG	2.22	0.40
1:A:33:PHE:CZ	5:E:14:LEU:HD13	2.57	0.40
1:A:117:THR:HG22	1:A:205:MET:SD	2.61	0.40
1:A:127:ILE:O	1:A:128:THR:C	2.64	0.40
1:A:134:THR:O	1:A:135:GLY:C	2.64	0.40
1:A:184:TYR:C	1:A:184:TYR:CD2	2.99	0.40
2:B:80:TYR:C	2:B:82:TYR:N	2.79	0.40
3:C:44:THR:O	3:C:133:SER:N	2.54	0.40
3:C:135:ASN:CG	3:C:138:THR:HG23	2.46	0.40
3:C:271:MET:HA	3:C:274:LEU:HB2	2.04	0.40
3:C:277:LYS:HD3	3:C:278:GLN:CD	2.46	0.40
5:E:9:ILE:HG21	6:F:10:ALA:CA	2.50	0.40
5:E:12:ILE:HA	5:E:15:PHE:HE1	1.86	0.40
14:E:101:BCR:H362	6:F:18:PHE:CZ	2.57	0.40
3:P:34:VAL:HG13	3:P:151:LEU:HD22	2.02	0.40
3:P:54:TYR:CZ	3:P:70:LEU:HD22	2.57	0.40
3:P:83:LYS:HE3	3:P:134:PRO:HG3	2.04	0.40
3:P:155:ARG:HG2	3:P:239:GLY:H	1.85	0.40
1:A:118:TRP:HA	9:A:302:HEC:HHD	2.04	0.40
1:A:162:GLY:O	1:A:165:ILE:CG2	2.69	0.40
2:B:29:GLU:HA	2:B:30:PRO:HD2	1.98	0.40
2:B:40:PHE:O	2:B:44:ILE:N	2.54	0.40
3:C:144:PHE:HB3	3:C:145:GLY:H	1.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:LEU:HD23	3:C:151:LEU:C	2.46	0.40
3:C:265:VAL:HG12	3:C:269:GLN:CG	2.51	0.40
4:D:156:GLN:C	4:D:158:ASP:N	2.79	0.40
1:N:32:ILE:O	1:N:34:TYR:CD2	2.75	0.40
1:N:165:ILE:HG22	1:N:166:SER:N	2.33	0.40
1:N:200:LEU:O	1:N:204:LEU:N	2.45	0.40
11:O:1309:BNT:HAM3	3:P:148:ALA:CB	2.51	0.40
3:P:2:PRO:CB	3:P:115:LEU:HD22	2.47	0.40
3:P:93:GLU:HA	3:P:96:LYS:HD2	2.03	0.40
5:R:4:GLY:HA2	5:R:7:PHE:CE2	2.57	0.40
5:R:9:ILE:CG2	5:R:10:VAL:H	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/215 (93%)	90 (45%)	64 (32%)	46 (23%)	0	0
1	N	200/215 (93%)	92 (46%)	58 (29%)	50 (25%)	0	0
2	B	135/160 (84%)	56 (42%)	45 (33%)	34 (25%)	0	0
2	O	135/160 (84%)	52 (38%)	39 (29%)	44 (33%)	0	0
3	C	284/289 (98%)	153 (54%)	83 (29%)	48 (17%)	0	2
3	P	284/289 (98%)	153 (54%)	81 (28%)	50 (18%)	0	2
4	D	166/179 (93%)	85 (51%)	50 (30%)	31 (19%)	0	1
4	Q	166/179 (93%)	86 (52%)	49 (30%)	31 (19%)	0	1
5	E	30/32 (94%)	13 (43%)	6 (20%)	11 (37%)	0	0
5	R	30/32 (94%)	13 (43%)	6 (20%)	11 (37%)	0	0
6	F	33/35 (94%)	15 (46%)	11 (33%)	7 (21%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	33/35 (94%)	15 (46%)	12 (36%)	6 (18%)	0	2
7	G	25/37 (68%)	11 (44%)	10 (40%)	4 (16%)	0	2
7	T	25/37 (68%)	11 (44%)	10 (40%)	4 (16%)	0	2
8	H	25/29 (86%)	12 (48%)	6 (24%)	7 (28%)	0	0
8	U	25/29 (86%)	12 (48%)	6 (24%)	7 (28%)	0	0
All	All	1796/1952 (92%)	869 (48%)	536 (30%)	391 (22%)	0	1

All (391) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	20	ASP
1	A	21	VAL
1	A	22	THR
1	A	26	VAL
1	A	28	PRO
1	A	29	HIS
1	A	53	ALA
1	A	65	ALA
1	A	77	SER
1	A	115	GLU
1	A	133	VAL
1	A	176	GLY
1	A	190	VAL
1	A	206	ILE
2	B	32	TRP
2	B	33	PRO
2	B	35	ASP
2	B	44	ILE
2	B	49	ALA
2	B	56	VAL
2	B	67	ASN
2	B	76	LEU
2	B	78	GLU
2	B	90	SER
2	B	93	ASN
2	B	98	VAL
2	B	126	ARG
2	B	147	ALA
3	C	53	PRO

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Mol	Chain	Res	Type
3	C	61	VAL
3	C	89	ARG
3	C	92	GLU
3	C	193	VAL
3	C	218	ILE
3	C	225	VAL
3	C	227	ALA
3	C	242	GLN
3	C	275	LYS
3	C	276	LYS
3	C	279	VAL
4	D	49	ALA
4	D	70	LEU
4	D	98	ALA
4	D	107	VAL
4	D	124	PHE
4	D	146	LEU
4	D	161	VAL
4	D	164	PRO
4	D	166	THR
5	E	3	LEU
5	E	18	ILE
5	E	19	ALA
5	E	22	ILE
5	E	23	ILE
6	F	35	LYS
8	H	3	VAL
8	H	10	LEU
1	N	16	ALA
1	N	17	LEU
1	N	20	ASP
1	N	21	VAL
1	N	30	VAL
1	N	32	ILE
1	N	33	PHE
1	N	34	TYR
1	N	53	ALA
1	N	62	VAL
1	N	75	GLU
1	N	77	SER
1	N	133	VAL
1	N	160	VAL

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Mol	Chain	Res	Type
1	N	163	VAL
1	N	174	SER
1	N	190	VAL
1	N	206	ILE
1	N	209	GLN
1	N	211	ILE
2	O	26	TYR
2	O	30	PRO
2	O	33	PRO
2	O	35	ASP
2	O	44	ILE
2	O	49	ALA
2	O	64	GLU
2	O	65	PRO
2	O	71	THR
2	O	75	ILE
2	O	77	PRO
2	O	79	TRP
2	O	90	SER
2	O	93	ASN
2	O	98	VAL
2	O	117	VAL
2	O	118	ASN
2	O	125	ARG
2	O	127	PRO
2	O	153	LYS
3	P	53	PRO
3	P	61	VAL
3	P	89	ARG
3	P	193	VAL
3	P	218	ILE
3	P	225	VAL
3	P	227	ALA
3	P	242	GLN
3	P	275	LYS
3	P	276	LYS
3	P	279	VAL
4	Q	44	PRO
4	Q	70	LEU
4	Q	98	ALA
4	Q	107	VAL
4	Q	124	PHE

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Mol	Chain	Res	Type
4	Q	138	ARG
4	Q	146	LEU
4	Q	161	VAL
4	Q	164	PRO
4	Q	166	THR
5	R	3	LEU
5	R	18	ILE
5	R	19	ALA
5	R	22	ILE
5	R	23	ILE
8	U	3	VAL
8	U	10	LEU
1	A	17	LEU
1	A	35	CYS
1	A	43	CYS
1	A	64	GLU
1	A	90	ALA
1	A	104	VAL
1	A	145	TYR
1	A	160	VAL
1	A	168	LEU
2	B	30	PRO
2	B	39	VAL
2	B	43	VAL
2	B	62	VAL
2	B	75	ILE
2	B	105	PRO
2	B	128	VAL
2	B	135	PHE
3	C	4	TRP
3	C	26	HIS
3	C	54	TYR
3	C	62	ALA
3	C	91	PRO
3	C	97	GLU
3	C	110	GLN
3	C	122	GLU
3	C	155	ARG
3	C	169	ASN
3	C	184	ALA
3	C	216	GLU
3	C	263	CYS

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Mol	Chain	Res	Type
4	D	20	ASN
4	D	35	LEU
4	D	45	PRO
4	D	46	SER
4	D	138	ARG
4	D	159	ASN
4	D	176	PRO
5	E	11	PHE
6	F	10	ALA
6	F	29	LYS
7	G	11	ALA
8	H	9	LEU
1	N	15	GLN
1	N	28	PRO
1	N	36	LEU
1	N	43	CYS
1	N	64	GLU
1	N	73	MET
1	N	90	ALA
1	N	91	SER
1	N	104	VAL
1	N	112	LYS
1	N	145	TYR
1	N	159	PRO
1	N	168	LEU
2	O	19	ALA
2	O	23	GLY
2	O	39	VAL
2	O	43	VAL
2	O	105	PRO
2	O	121	GLN
2	O	128	VAL
2	O	135	PHE
2	O	146	GLY
2	O	151	LEU
3	P	4	TRP
3	P	26	HIS
3	P	54	TYR
3	P	66	SER
3	P	91	PRO
3	P	92	GLU
3	P	97	GLU

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Mol	Chain	Res	Type
3	P	110	GLN
3	P	155	ARG
3	P	184	ALA
3	P	190	TYR
3	P	196	GLN
3	P	216	GLU
4	Q	20	ASN
4	Q	35	LEU
4	Q	52	GLY
4	Q	159	ASN
4	Q	176	PRO
5	R	11	PHE
5	R	25	ALA
6	S	10	ALA
6	S	29	LYS
7	T	11	ALA
7	T	27	PRO
7	T	29	GLU
8	U	9	LEU
8	U	11	VAL
1	A	74	ASN
1	A	78	PHE
1	A	91	SER
1	A	166	SER
2	B	69	PHE
2	B	81	LEU
2	B	99	LEU
3	C	29	ALA
3	C	32	ALA
3	C	48	ALA
3	C	66	SER
3	C	170	ASN
3	C	190	TYR
3	C	223	GLN
3	C	269	GLN
4	D	85	LYS
4	D	145	PRO
4	D	147	SER
5	E	24	PHE
5	E	25	ALA
6	F	4	GLU
6	F	11	LEU

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Mol	Chain	Res	Type
6	F	12	LEU
7	G	28	ASN
8	H	5	GLY
8	H	11	VAL
1	N	25	TYR
1	N	83	ARG
1	N	111	LYS
1	N	158	ILE
2	O	20	LYS
2	O	73	LEU
2	O	99	LEU
2	O	152	ASP
3	P	29	ALA
3	P	32	ALA
3	P	48	ALA
3	P	62	ALA
3	P	69	GLY
3	P	122	GLU
3	P	127	ILE
3	P	169	ASN
3	P	176	ALA
3	P	192	ASN
3	P	223	GLN
3	P	263	CYS
3	P	269	GLN
4	Q	19	MET
4	Q	57	LYS
4	Q	64	VAL
4	Q	106	ALA
4	Q	145	PRO
4	Q	147	SER
5	R	24	PHE
6	S	4	GLU
6	S	12	LEU
8	U	2	ASP
8	U	5	GLY
1	A	34	TYR
1	A	42	THR
1	A	49	ALA
1	A	76	VAL
1	A	83	ARG
1	A	177	GLN

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Mol	Chain	Res	Type
1	A	211	ILE
2	B	52	VAL
2	B	86	GLN
3	C	69	GLY
3	C	127	ILE
3	C	173	THR
3	C	176	ALA
3	C	186	GLU
3	C	192	ASN
3	C	196	GLN
4	D	19	MET
4	D	51	GLY
4	D	57	LYS
4	D	64	VAL
4	D	97	GLU
4	D	106	ALA
4	D	119	ALA
5	E	7	PHE
7	G	27	PRO
8	H	2	ASP
1	N	42	THR
1	N	49	ALA
1	N	105	TYR
1	N	166	SER
1	N	173	SER
1	N	179	THR
2	O	86	GLN
2	O	149	LEU
3	P	94	LEU
3	P	173	THR
3	P	186	GLU
3	P	199	ILE
4	Q	85	LYS
5	R	7	PHE
6	S	11	LEU
1	A	19	ASP
1	A	80	TRP
1	A	178	ALA
1	A	179	THR
2	B	64	GLU
2	B	68	PRO
2	B	87	ILE

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Mol	Chain	Res	Type
2	B	114	ILE
3	C	68	VAL
3	C	199	ILE
4	D	87	ASP
4	D	112	GLY
1	N	18	ALA
1	N	23	SER
1	N	147	ALA
2	O	32	TRP
2	O	76	LEU
2	O	114	ILE
3	P	34	VAL
4	Q	15	ARG
4	Q	45	PRO
4	Q	87	ASP
4	Q	112	GLY
4	Q	131	SER
4	Q	158	ASP
6	S	19	VAL
8	U	16	SER
1	A	30	VAL
1	A	147	ALA
2	B	71	THR
3	C	18	GLY
3	C	34	VAL
3	C	144	PHE
4	D	158	ASP
4	D	173	GLY
6	F	19	VAL
8	H	16	SER
1	N	26	VAL
2	O	68	PRO
2	O	87	ILE
2	O	134	LEU
3	P	25	CYS
3	P	68	VAL
3	P	144	PHE
3	P	226	LYS
3	P	266	MET
4	Q	28	THR
4	Q	173	GLY
1	A	112	LYS

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Mol	Chain	Res	Type
2	B	122	ASN
1	N	14	ILE
3	P	18	GLY
3	P	238	GLY
2	B	149	LEU
2	O	21	GLY
1	A	122	VAL
5	E	4	GLY
7	G	9	VAL
1	N	122	VAL
2	O	123	PRO
5	R	4	GLY
1	A	132	GLY
1	A	197	VAL
3	C	120	PRO
3	C	238	GLY
4	D	29	GLY
1	N	197	VAL
4	Q	29	GLY
5	R	20	VAL
7	T	9	VAL
1	A	161	VAL
3	C	191	GLY
5	E	20	VAL
3	P	21	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/184 (94%)	146 (85%)	26 (15%)	3	16
1	N	172/184 (94%)	145 (84%)	27 (16%)	2	15
2	B	116/136 (85%)	98 (84%)	18 (16%)	2	15
2	O	116/136 (85%)	90 (78%)	26 (22%)	1	5
3	C	240/243 (99%)	194 (81%)	46 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	240/243 (99%)	195 (81%)	45 (19%)	1	10
4	D	136/146 (93%)	111 (82%)	25 (18%)	1	11
4	Q	136/146 (93%)	110 (81%)	26 (19%)	1	9
5	E	25/25 (100%)	19 (76%)	6 (24%)	1	4
5	R	25/25 (100%)	18 (72%)	7 (28%)	0	2
6	F	27/27 (100%)	23 (85%)	4 (15%)	3	16
6	S	27/27 (100%)	22 (82%)	5 (18%)	1	11
7	G	21/28 (75%)	15 (71%)	6 (29%)	0	2
7	T	21/28 (75%)	15 (71%)	6 (29%)	0	2
8	H	22/24 (92%)	20 (91%)	2 (9%)	9	32
8	U	22/24 (92%)	20 (91%)	2 (9%)	9	32
All	All	1518/1626 (93%)	1241 (82%)	277 (18%)	2	12

All (277) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	21	VAL
1	A	24	LYS
1	A	26	VAL
1	A	29	HIS
1	A	33	PHE
1	A	35	CYS
1	A	36	LEU
1	A	47	GLN
1	A	75	GLU
1	A	83	ARG
1	A	95	LEU
1	A	99	LEU
1	A	112	LYS
1	A	114	ARG
1	A	116	LEU
1	A	123	ILE
1	A	134	THR
1	A	140	TRP
1	A	150	ILE
1	A	160	VAL
1	A	165	ILE

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Mol	Chain	Res	Type
1	A	175	VAL
1	A	177	GLN
1	A	185	SER
1	A	193	TRP
2	B	27	TYR
2	B	32	TRP
2	B	33	PRO
2	B	39	VAL
2	B	47	THR
2	B	48	PHE
2	B	61	MET
2	B	76	LEU
2	B	81	LEU
2	B	86	GLN
2	B	96	LEU
2	B	106	LEU
2	B	115	GLU
2	B	120	PHE
2	B	124	PHE
2	B	125	ARG
2	B	132	ILE
2	B	135	PHE
3	C	3	PHE
3	C	4	TRP
3	C	6	GLN
3	C	9	TYR
3	C	20	ILE
3	C	25	CYS
3	C	35	GLU
3	C	51	LYS
3	C	54	TYR
3	C	55	ASP
3	C	70	LEU
3	C	78	LEU
3	C	80	GLU
3	C	83	LYS
3	C	88	GLU
3	C	91	PRO
3	C	93	GLU
3	C	97	GLU
3	C	104	GLN
3	C	119	LEU

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Mol	Chain	Res	Type
3	C	123	GLN
3	C	126	GLU
3	C	127	ILE
3	C	131	VAL
3	C	151	LEU
3	C	169	ASN
3	C	171	VAL
3	C	180	ILE
3	C	182	LYS
3	C	205	LYS
3	C	206	THR
3	C	216	GLU
3	C	218	ILE
3	C	221	GLU
3	C	226	LYS
3	C	231	LEU
3	C	249	LEU
3	C	253	ASN
3	C	254	ARG
3	C	257	TRP
3	C	258	MET
3	C	266	MET
3	C	269	GLN
3	C	271	MET
3	C	280	GLU
3	C	283	GLN
4	D	12	ASP
4	D	13	MET
4	D	15	ARG
4	D	17	GLN
4	D	41	TYR
4	D	59	LYS
4	D	63	ASN
4	D	69	PHE
4	D	70	LEU
4	D	72	SER
4	D	78	ARG
4	D	81	VAL
4	D	82	GLN
4	D	84	LEU
4	D	90	TYR
4	D	99	ILE

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Mol	Chain	Res	Type
4	D	101	ASP
4	D	134	ASP
4	D	152	HIS
4	D	165	TRP
4	D	166	THR
4	D	170	PHE
4	D	171	ARG
4	D	172	THR
4	D	178	TRP
5	E	2	ILE
5	E	11	PHE
5	E	22	ILE
5	E	23	ILE
5	E	27	LYS
5	E	29	ILE
6	F	6	MET
6	F	8	TYR
6	F	11	LEU
6	F	27	LEU
7	G	6	LEU
7	G	16	LEU
7	G	17	PHE
7	G	21	TYR
7	G	26	ARG
7	G	29	GLU
8	H	19	MET
8	H	25	ASN
1	N	15	GLN
1	N	17	LEU
1	N	21	VAL
1	N	24	LYS
1	N	25	TYR
1	N	29	HIS
1	N	34	TYR
1	N	47	GLN
1	N	62	VAL
1	N	75	GLU
1	N	83	ARG
1	N	95	LEU
1	N	99	LEU
1	N	110	PHE
1	N	114	ARG

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Mol	Chain	Res	Type
1	N	116	LEU
1	N	123	ILE
1	N	134	THR
1	N	141	ASP
1	N	150	ILE
1	N	161	VAL
1	N	165	ILE
1	N	170	ARG
1	N	185	SER
1	N	193	TRP
1	N	208	LYS
1	N	211	ILE
2	O	20	LYS
2	O	24	HIS
2	O	32	TRP
2	O	33	PRO
2	O	39	VAL
2	O	47	THR
2	O	48	PHE
2	O	51	ILE
2	O	61	MET
2	O	62	VAL
2	O	65	PRO
2	O	69	PHE
2	O	77	PRO
2	O	86	GLN
2	O	95	LEU
2	O	96	LEU
2	O	106	LEU
2	O	115	GLU
2	O	120	PHE
2	O	125	ARG
2	O	127	PRO
2	O	132	ILE
2	O	135	PHE
2	O	145	ILE
2	O	152	ASP
2	O	154	THR
3	P	3	PHE
3	P	4	TRP
3	P	6	GLN
3	P	9	TYR

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Mol	Chain	Res	Type
3	P	20	ILE
3	P	25	CYS
3	P	35	GLU
3	P	51	LYS
3	P	55	ASP
3	P	70	LEU
3	P	78	LEU
3	P	80	GLU
3	P	83	LYS
3	P	88	GLU
3	P	91	PRO
3	P	93	GLU
3	P	97	GLU
3	P	104	GLN
3	P	119	LEU
3	P	123	GLN
3	P	126	GLU
3	P	127	ILE
3	P	131	VAL
3	P	151	LEU
3	P	169	ASN
3	P	171	VAL
3	P	180	ILE
3	P	202	ASP
3	P	205	LYS
3	P	206	THR
3	P	216	GLU
3	P	218	ILE
3	P	221	GLU
3	P	226	LYS
3	P	231	LEU
3	P	249	LEU
3	P	253	ASN
3	P	254	ARG
3	P	257	TRP
3	P	258	MET
3	P	266	MET
3	P	269	GLN
3	P	271	MET
3	P	280	GLU
3	P	283	GLN
4	Q	12	ASP

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Mol	Chain	Res	Type
4	Q	13	MET
4	Q	15	ARG
4	Q	17	GLN
4	Q	41	TYR
4	Q	50	VAL
4	Q	59	LYS
4	Q	63	ASN
4	Q	69	PHE
4	Q	70	LEU
4	Q	72	SER
4	Q	78	ARG
4	Q	81	VAL
4	Q	82	GLN
4	Q	84	LEU
4	Q	90	TYR
4	Q	99	ILE
4	Q	101	ASP
4	Q	134	ASP
4	Q	152	HIS
4	Q	165	TRP
4	Q	166	THR
4	Q	170	PHE
4	Q	171	ARG
4	Q	172	THR
4	Q	178	TRP
5	R	2	ILE
5	R	11	PHE
5	R	18	ILE
5	R	22	ILE
5	R	23	ILE
5	R	27	LYS
5	R	29	ILE
6	S	6	MET
6	S	8	TYR
6	S	11	LEU
6	S	27	LEU
6	S	36	GLU
7	T	6	LEU
7	T	16	LEU
7	T	17	PHE
7	T	21	TYR
7	T	26	ARG

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Mol	Chain	Res	Type
7	T	30	LEU
8	U	19	MET
8	U	25	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	29	HIS
1	A	31	ASN
1	A	47	GLN
1	A	74	ASN
1	A	142	GLN
2	B	25	ASN
2	B	34	ASN
2	B	86	GLN
2	B	116	ASN
3	C	6	GLN
3	C	7	GLN
3	C	104	GLN
3	C	112	ASN
3	C	123	GLN
3	C	125	GLN
3	C	154	ASN
3	C	168	ASN
3	C	169	ASN
3	C	196	GLN
3	C	233	ASN
3	C	234	ASN
3	C	242	GLN
3	C	283	GLN
4	D	17	GLN
4	D	63	ASN
4	D	82	GLN
4	D	105	ASN
4	D	118	ASN
4	D	122	ASN
4	D	132	GLN
4	D	159	ASN
6	F	31	GLN
7	G	23	GLN
1	N	15	GLN

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Mol	Chain	Res	Type
1	N	31	ASN
1	N	47	GLN
1	N	209	GLN
2	O	34	ASN
2	O	116	ASN
2	O	122	ASN
3	P	6	GLN
3	P	7	GLN
3	P	104	GLN
3	P	123	GLN
3	P	125	GLN
3	P	154	ASN
3	P	168	ASN
3	P	169	ASN
3	P	196	GLN
3	P	233	ASN
3	P	234	ASN
3	P	242	GLN
3	P	283	GLN
4	Q	17	GLN
4	Q	63	ASN
4	Q	82	GLN
4	Q	105	ASN
4	Q	118	ASN
4	Q	122	ASN
4	Q	132	GLN
4	Q	159	ASN
6	S	31	GLN
7	T	28	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
9	HEC	A	302	1	50,50,50	1.93	15 (30%)	68,82,82	2.26	14 (20%)
9	HEC	N	303	1,15	50,50,50	1.53	8 (16%)	68,82,82	1.66	12 (17%)
9	HEC	P	301	3	50,50,50	2.08	15 (30%)	68,82,82	2.05	13 (19%)
12	CLA	B	201	-	69,73,73	2.05	16 (23%)	82,113,113	1.93	15 (18%)
12	CLA	O	1201	-	69,73,73	2.01	17 (24%)	82,113,113	1.86	13 (15%)
14	BCR	R	1101	-	41,41,41	2.58	13 (31%)	56,56,56	2.42	21 (37%)
9	HEC	C	301	3	50,50,50	2.05	14 (28%)	68,82,82	2.02	12 (17%)
11	BNT	O	1309	-	12,14,14	3.33	5 (41%)	13,21,21	1.53	2 (15%)
9	HEC	A	303	1,15	50,50,50	1.56	10 (20%)	68,82,82	1.17	5 (7%)
14	BCR	E	101	-	41,41,41	2.48	13 (31%)	56,56,56	2.43	20 (35%)
10	OPC	B	305	-	53,53,54	1.36	8 (15%)	59,61,64	1.09	3 (5%)
9	HEC	A	301	1	50,50,50	2.03	15 (30%)	68,82,82	2.06	11 (16%)
10	OPC	O	1306	-	53,53,54	1.36	8 (15%)	59,61,64	1.12	4 (6%)
13	FES	D	201	4	0,4,4	-	-	-	-	-
9	HEC	N	301	1	50,50,50	2.08	17 (34%)	68,82,82	2.06	14 (20%)
10	OPC	N	1305	-	53,53,54	1.36	8 (15%)	59,61,64	1.17	4 (6%)
9	HEC	N	302	1	50,50,50	1.96	16 (32%)	68,82,82	2.34	14 (20%)
13	FES	Q	201	4	0,4,4	-	-	-	-	-
10	OPC	C	306	-	53,53,54	1.36	8 (15%)	59,61,64	1.20	4 (6%)
11	BNT	B	309	-	12,14,14	3.18	5 (41%)	13,21,21	1.57	2 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEC	A	302	1	1/1/3/7	5/14/54/54	-
9	HEC	N	303	1,15	1/1/3/7	4/14/54/54	-
9	HEC	P	301	3	1/1/3/7	6/14/54/54	-
12	CLA	B	201	-	3/3/15/20	10/39/115/115	-
12	CLA	O	1201	-	3/3/15/20	14/39/115/115	-
14	BCR	R	1101	-	-	7/29/63/63	0/2/2/2
9	HEC	C	301	3	1/1/3/7	6/14/54/54	-
11	BNT	O	1309	-	-	0/4/28/28	0/1/1/1
9	HEC	A	303	1,15	1/1/3/7	4/14/54/54	-
14	BCR	E	101	-	-	7/29/63/63	0/2/2/2
10	OPC	B	305	-	-	11/57/57/60	-
9	HEC	A	301	1	1/1/3/7	4/14/54/54	-
10	OPC	O	1306	-	-	16/57/57/60	-
13	FES	D	201	4	-	-	0/1/1/1
9	HEC	N	301	1	1/1/3/7	2/14/54/54	-
10	OPC	N	1305	-	-	17/57/57/60	-
9	HEC	N	302	1	1/1/3/7	4/14/54/54	-
13	FES	Q	201	4	-	-	0/1/1/1
10	OPC	C	306	-	-	11/57/57/60	-
11	BNT	B	309	-	-	0/4/28/28	0/1/1/1

All (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	1309	BNT	CAD-CAE	-9.09	1.39	1.52
11	B	309	BNT	CAD-CAE	-8.38	1.40	1.52
14	R	1101	BCR	C30-C25	8.24	1.64	1.53
12	O	1201	CLA	C3A-C2A	-7.17	1.35	1.54
14	E	101	BCR	C30-C25	6.86	1.62	1.53
12	B	201	CLA	C3A-C2A	-6.72	1.36	1.54
14	R	1101	BCR	C1-C6	6.52	1.62	1.53
14	E	101	BCR	C26-C25	6.36	1.45	1.34
14	E	101	BCR	C1-C6	6.25	1.61	1.53
12	B	201	CLA	C4C-C3C	6.17	1.55	1.45
12	B	201	CLA	C1C-C2C	6.07	1.56	1.44
14	R	1101	BCR	C26-C25	5.96	1.44	1.34
12	O	1201	CLA	C1C-C2C	5.67	1.56	1.44
9	A	301	HEC	C1C-C2C	5.63	1.56	1.43
11	O	1309	BNT	CAM-CAL	-5.50	1.39	1.50
9	C	301	HEC	C4C-C3C	5.49	1.55	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	309	BNT	CAM-CAL	-5.46	1.39	1.50
12	O	1201	CLA	O2D-CGD	5.08	1.45	1.33
12	B	201	CLA	O2D-CGD	5.08	1.45	1.33
12	O	1201	CLA	C4C-C3C	5.07	1.53	1.45
9	N	302	HEC	C1C-C2C	5.04	1.55	1.43
9	N	301	HEC	C1C-C2C	5.03	1.54	1.43
9	C	301	HEC	C1C-C2C	5.00	1.54	1.43
9	N	301	HEC	C4C-C3C	4.88	1.54	1.44
9	A	301	HEC	C4C-C3C	4.87	1.54	1.44
9	P	301	HEC	C4C-C3C	4.77	1.54	1.44
9	P	301	HEC	C1C-C2C	4.65	1.54	1.43
9	C	301	HEC	FE-NC	4.54	2.10	1.95
9	P	301	HEC	C1A-C2A	4.46	1.53	1.45
9	A	302	HEC	C1C-C2C	4.37	1.53	1.43
9	P	301	HEC	CBC-CAC	-4.36	1.32	1.51
9	N	301	HEC	CBC-CAC	-4.33	1.33	1.51
9	A	301	HEC	CBC-CAC	-4.33	1.33	1.51
14	R	1101	BCR	C2-C1	4.26	1.63	1.54
9	A	302	HEC	C4C-C3C	4.22	1.53	1.44
9	N	302	HEC	C4C-C3C	4.18	1.53	1.44
9	C	301	HEC	CBC-CAC	-4.16	1.33	1.51
9	N	302	HEC	CBC-CAC	-4.13	1.33	1.51
9	A	302	HEC	CBC-CAC	-4.09	1.34	1.51
12	O	1201	CLA	MG-NA	-4.08	1.96	2.06
14	E	101	BCR	C29-C30	4.03	1.63	1.54
9	P	301	HEC	FE-NB	4.00	2.07	1.94
14	R	1101	BCR	C29-C30	4.00	1.63	1.54
14	R	1101	BCR	C5-C6	3.95	1.41	1.34
9	N	303	HEC	C1D-C2D	3.93	1.52	1.44
9	P	301	HEC	FE-NA	3.91	2.08	1.95
10	N	1305	OPC	CAV-CAW	3.88	1.53	1.31
10	C	306	OPC	CAV-CAW	3.86	1.53	1.31
10	O	1306	OPC	CAV-CAW	3.84	1.53	1.31
10	B	305	OPC	CAV-CAW	3.83	1.53	1.31
9	A	303	HEC	CMD-C2D	3.81	1.58	1.50
12	B	201	CLA	O2A-CGA	3.78	1.44	1.33
14	E	101	BCR	C38-C26	3.74	1.56	1.50
14	E	101	BCR	C2-C1	3.73	1.62	1.54
12	B	201	CLA	CBC-CAC	-3.71	1.35	1.51
9	C	301	HEC	FE-NB	3.64	2.06	1.94
12	O	1201	CLA	CBC-CAC	-3.62	1.36	1.51
10	O	1306	OPC	CAL-CAM	-3.60	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	305	OPC	CAL-CAM	-3.60	1.39	1.50
9	A	302	HEC	CBB-CAB	-3.60	1.36	1.51
12	O	1201	CLA	C1D-ND	-3.58	1.33	1.37
9	N	301	HEC	CBB-CAB	-3.57	1.36	1.51
9	A	303	HEC	FE-ND	3.56	2.05	1.94
10	C	306	OPC	CAL-CAM	-3.53	1.39	1.50
9	A	301	HEC	CBB-CAB	-3.53	1.36	1.51
9	N	302	HEC	FE-NB	3.52	2.05	1.94
10	N	1305	OPC	CAL-CAM	-3.52	1.39	1.50
10	N	1305	OPC	CAQ-CAP	-3.51	1.39	1.52
9	A	302	HEC	FE-NB	3.51	2.05	1.94
9	N	302	HEC	C1D-ND	-3.51	1.34	1.40
14	E	101	BCR	C5-C6	3.49	1.40	1.34
9	N	301	HEC	C4A-C3A	3.46	1.52	1.45
9	A	302	HEC	FE-NC	3.45	2.06	1.95
9	P	301	HEC	CBB-CAB	-3.45	1.36	1.51
10	B	305	OPC	CAQ-CAP	-3.44	1.39	1.52
12	B	201	CLA	C2-C3	3.43	1.41	1.33
10	C	306	OPC	CAQ-CAP	-3.43	1.39	1.52
10	O	1306	OPC	CAQ-CAP	-3.42	1.39	1.52
9	N	302	HEC	CBB-CAB	-3.41	1.37	1.51
14	R	1101	BCR	C38-C26	3.41	1.56	1.50
9	C	301	HEC	CBB-CAB	-3.35	1.37	1.51
9	C	301	HEC	C1A-C2A	3.32	1.51	1.45
9	A	302	HEC	C1D-ND	-3.30	1.34	1.40
12	B	201	CLA	O1D-CGD	3.29	1.29	1.21
9	P	301	HEC	C4A-C3A	3.22	1.51	1.45
9	N	303	HEC	FE-ND	3.19	2.04	1.94
9	A	301	HEC	FE-NC	3.18	2.05	1.95
9	N	301	HEC	FE-NC	3.18	2.05	1.95
9	N	301	HEC	O2A-CGA	3.16	1.41	1.30
9	N	303	HEC	CMD-C2D	3.16	1.57	1.50
9	N	301	HEC	C1A-C2A	3.13	1.50	1.45
9	C	301	HEC	C4A-C3A	3.11	1.51	1.45
9	N	301	HEC	FE-ND	3.10	2.04	1.94
9	A	301	HEC	FE-NB	3.08	2.04	1.94
9	C	301	HEC	O2A-CGA	3.08	1.41	1.30
9	A	303	HEC	FE-NC	3.06	2.05	1.95
12	B	201	CLA	MG-NC	3.06	2.13	2.06
10	O	1306	OPC	CAY-CAX	-3.04	1.39	1.52
10	N	1305	OPC	CAY-CAX	-3.04	1.39	1.52
10	B	305	OPC	CAY-CAX	-3.04	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	306	OPC	CAY-CAX	-3.03	1.39	1.52
9	C	301	HEC	FE-ND	3.02	2.04	1.94
9	A	301	HEC	C4D-ND	-3.01	1.32	1.38
9	A	301	HEC	C1A-C2A	2.98	1.50	1.45
9	N	301	HEC	C1D-ND	-2.97	1.35	1.40
9	P	301	HEC	O2A-CGA	2.95	1.40	1.30
9	N	302	HEC	FE-ND	2.94	2.04	1.94
12	O	1201	CLA	C2-C3	2.93	1.39	1.33
9	P	301	HEC	FE-NC	2.90	2.04	1.95
9	A	301	HEC	C1D-ND	-2.90	1.35	1.40
12	O	1201	CLA	O2A-CGA	2.87	1.41	1.33
9	N	301	HEC	FE-NA	2.83	2.04	1.95
9	N	302	HEC	C4D-C3D	2.80	1.49	1.45
12	B	201	CLA	CAC-C3C	2.80	1.58	1.51
9	A	301	HEC	FE-NA	2.80	2.04	1.95
9	N	301	HEC	CMA-C3A	2.77	1.56	1.50
14	E	101	BCR	C8-C9	2.76	1.51	1.46
11	B	309	BNT	CAE-CAF	-2.71	1.39	1.47
9	P	301	HEC	C1D-ND	-2.69	1.35	1.40
9	P	301	HEC	FE-ND	2.69	2.03	1.94
9	A	303	HEC	C4A-C3A	2.68	1.50	1.45
9	N	301	HEC	CHA-C1A	-2.67	1.33	1.38
14	R	1101	BCR	C8-C9	2.65	1.51	1.46
12	O	1201	CLA	MG-NB	2.64	2.11	2.05
9	A	303	HEC	C4D-C3D	2.64	1.49	1.45
9	A	303	HEC	C1D-C2D	2.63	1.49	1.44
12	B	201	CLA	CHB-C4A	2.63	1.44	1.37
14	R	1101	BCR	C7-C6	2.61	1.54	1.45
9	N	303	HEC	C4B-C3B	2.60	1.49	1.45
12	B	201	CLA	CBA-CGA	2.60	1.58	1.50
9	N	302	HEC	FE-NC	2.58	2.03	1.95
9	A	302	HEC	CMA-C3A	2.58	1.56	1.50
12	O	1201	CLA	MG-NC	2.57	2.12	2.06
9	N	303	HEC	FE-NC	2.56	2.03	1.95
9	A	302	HEC	FE-ND	2.55	2.02	1.94
14	R	1101	BCR	C24-C23	2.55	1.40	1.33
12	O	1201	CLA	O1D-CGD	2.53	1.27	1.21
9	A	301	HEC	C4A-C3A	2.51	1.50	1.45
9	C	301	HEC	C1D-ND	-2.50	1.35	1.40
10	N	1305	OPC	CAQ-CAR	-2.50	1.39	1.51
9	N	303	HEC	C1C-NC	-2.50	1.34	1.39
14	E	101	BCR	C7-C6	2.49	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	302	HEC	CHB-C1B	-2.49	1.33	1.39
11	O	1309	BNT	CAE-CAF	-2.49	1.40	1.47
10	B	305	OPC	CBP-CBO	-2.48	1.39	1.51
10	B	305	OPC	CBO-CBN	-2.47	1.39	1.51
10	O	1306	OPC	CBP-CBO	-2.47	1.39	1.51
10	C	306	OPC	CBO-CBN	-2.47	1.39	1.51
9	A	301	HEC	CMA-C3A	2.46	1.55	1.50
10	O	1306	OPC	CBO-CBN	-2.46	1.39	1.51
14	E	101	BCR	C24-C23	2.45	1.40	1.33
10	N	1305	OPC	CBO-CBN	-2.45	1.39	1.51
9	C	301	HEC	CAC-C3C	2.45	1.57	1.51
10	C	306	OPC	CBP-CBO	-2.45	1.39	1.51
10	O	1306	OPC	CAQ-CAR	-2.44	1.39	1.51
10	N	1305	OPC	CBP-CBO	-2.44	1.39	1.51
10	B	305	OPC	CAQ-CAR	-2.44	1.39	1.51
10	C	306	OPC	CAQ-CAR	-2.43	1.39	1.51
9	A	301	HEC	CAD-C3D	-2.42	1.45	1.51
14	R	1101	BCR	C33-C5	2.41	1.54	1.50
14	E	101	BCR	C10-C9	2.40	1.41	1.35
9	A	302	HEC	C1A-C2A	2.40	1.49	1.45
9	N	301	HEC	FE-NB	2.37	2.02	1.94
11	B	309	BNT	CAK-CAJ	2.37	1.54	1.46
9	A	301	HEC	O2A-CGA	2.35	1.38	1.30
9	A	303	HEC	C4B-C3B	2.35	1.49	1.45
9	N	302	HEC	C1A-C2A	2.34	1.49	1.45
9	N	301	HEC	C4D-ND	-2.34	1.34	1.38
9	N	303	HEC	C4A-C3A	2.34	1.50	1.45
9	A	302	HEC	CHB-C1B	-2.33	1.33	1.39
12	O	1201	CLA	C4-C3	2.32	1.56	1.50
9	N	302	HEC	C2A-C3A	-2.31	1.31	1.36
9	A	303	HEC	CAA-C2A	2.31	1.57	1.51
12	B	201	CLA	C5-C3	2.31	1.56	1.51
14	R	1101	BCR	C10-C9	2.30	1.41	1.35
9	A	302	HEC	O2A-CGA	2.26	1.38	1.30
12	B	201	CLA	MG-NA	2.24	2.11	2.06
9	P	301	HEC	CMA-C3A	2.24	1.55	1.50
14	R	1101	BCR	C8-C7	2.23	1.39	1.33
9	C	301	HEC	FE-NA	2.23	2.02	1.95
11	O	1309	BNT	CAK-CAJ	2.22	1.53	1.46
9	N	301	HEC	CAD-C3D	-2.22	1.45	1.51
9	A	301	HEC	CHA-C1A	-2.21	1.34	1.38
12	O	1201	CLA	C5-C3	2.18	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	201	CLA	C1D-ND	-2.18	1.35	1.37
9	A	303	HEC	CHB-C4A	2.18	1.42	1.38
11	O	1309	BNT	CAL-CAK	-2.17	1.39	1.47
12	O	1201	CLA	MG-ND	-2.17	2.01	2.05
9	N	303	HEC	C4D-C3D	2.17	1.48	1.45
9	A	302	HEC	C4D-C3D	2.16	1.48	1.45
10	O	1306	OPC	OAK-CAL	-2.16	1.36	1.44
9	P	301	HEC	CBA-CGA	2.15	1.55	1.50
9	P	301	HEC	CBD-CGD	2.14	1.55	1.50
12	O	1201	CLA	CAC-C3C	2.14	1.56	1.51
9	N	302	HEC	C4D-ND	-2.14	1.34	1.38
9	N	302	HEC	O2A-CGA	2.13	1.37	1.30
11	B	309	BNT	CAL-CAK	-2.12	1.40	1.47
9	N	301	HEC	CBA-CGA	2.12	1.55	1.50
10	C	306	OPC	OAK-CAL	-2.12	1.36	1.44
10	B	305	OPC	OAK-CAL	-2.11	1.36	1.44
9	C	301	HEC	CMA-C3A	2.10	1.55	1.50
12	O	1201	CLA	CBD-CHA	2.10	1.62	1.51
14	E	101	BCR	C8-C7	2.09	1.39	1.33
9	N	302	HEC	CBA-CAA	2.09	1.59	1.51
14	E	101	BCR	C33-C5	2.07	1.54	1.50
9	N	302	HEC	FE-NA	2.07	2.02	1.95
10	N	1305	OPC	OAK-CAL	-2.05	1.36	1.44
9	A	303	HEC	CHA-C1A	2.05	1.42	1.38
9	A	302	HEC	C4D-ND	-2.04	1.34	1.38
12	B	201	CLA	MG-ND	-2.03	2.01	2.05
9	A	302	HEC	C2A-C3A	-2.03	1.32	1.36

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	302	HEC	CBA-CAA-C2A	-8.54	88.92	112.53
9	A	302	HEC	CBA-CAA-C2A	-8.03	90.33	112.53
9	P	301	HEC	CAB-C3B-C4B	7.65	134.74	124.79
9	N	302	HEC	CAB-C3B-C4B	7.63	134.72	124.79
9	C	301	HEC	CAB-C3B-C4B	7.60	134.69	124.79
9	A	302	HEC	CAB-C3B-C4B	7.53	134.59	124.79
12	B	201	CLA	C4A-NA-C1A	7.37	110.04	106.68
9	A	301	HEC	CAB-C3B-C4B	7.34	134.34	124.79
12	B	201	CLA	CAA-C2A-C3A	7.24	132.57	113.00
14	R	1101	BCR	C38-C26-C25	7.22	132.36	124.48
14	E	101	BCR	C38-C26-C25	7.16	132.29	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	301	HEC	CAB-C3B-C4B	7.01	133.91	124.79
12	O	1201	CLA	CAA-C2A-C3A	6.61	130.87	113.00
9	N	302	HEC	CAA-CBA-CGA	6.35	130.51	113.67
10	C	306	OPC	OAN-CAO-CAP	5.93	124.31	111.48
12	O	1201	CLA	C4A-NA-C1A	5.84	109.34	106.68
10	O	1306	OPC	OAN-CAO-CAP	5.67	123.76	111.48
10	N	1305	OPC	OAN-CAO-CAP	5.67	123.75	111.48
9	N	301	HEC	CAD-C3D-C2D	5.64	138.43	127.87
9	A	302	HEC	CBB-CAB-C3B	5.62	127.65	112.42
9	P	301	HEC	CBC-CAC-C3C	5.53	127.40	112.42
9	N	301	HEC	CBB-CAB-C3B	5.51	127.35	112.42
12	O	1201	CLA	CMA-C3A-C2A	5.44	135.01	113.98
9	A	301	HEC	CBB-CAB-C3B	5.43	127.14	112.42
9	C	301	HEC	CBC-CAC-C3C	5.38	127.00	112.42
12	B	201	CLA	CBC-CAC-C3C	5.38	127.00	112.42
9	N	302	HEC	CBB-CAB-C3B	5.35	126.93	112.42
9	C	301	HEC	CBB-CAB-C3B	5.28	126.74	112.42
9	P	301	HEC	CBB-CAB-C3B	5.24	126.62	112.42
10	B	305	OPC	OAN-CAO-CAP	5.24	122.81	111.48
9	A	301	HEC	CAD-C3D-C2D	5.18	137.56	127.87
12	B	201	CLA	CMA-C3A-C2A	5.15	133.88	113.98
9	P	301	HEC	CAB-C3B-C2B	-5.14	118.12	127.56
12	O	1201	CLA	CBC-CAC-C3C	5.10	126.24	112.42
9	A	301	HEC	CBC-CAC-C3C	5.09	126.22	112.42
9	N	303	HEC	CAA-CBA-CGA	5.08	127.15	113.67
14	E	101	BCR	C33-C5-C6	5.03	129.97	124.48
9	C	301	HEC	CAB-C3B-C2B	-5.03	118.33	127.56
9	N	302	HEC	CBC-CAC-C3C	5.01	126.01	112.42
9	N	302	HEC	CAB-C3B-C2B	-5.01	118.36	127.56
9	A	302	HEC	CAA-CBA-CGA	4.98	126.88	113.67
9	P	301	HEC	CAD-C3D-C2D	4.98	137.20	127.87
9	A	301	HEC	CAB-C3B-C2B	-4.97	118.43	127.56
14	E	101	BCR	C30-C25-C26	-4.94	115.89	122.64
9	A	302	HEC	CAB-C3B-C2B	-4.93	118.49	127.56
14	R	1101	BCR	C33-C5-C6	4.88	129.81	124.48
9	C	301	HEC	CAD-C3D-C2D	4.88	137.01	127.87
9	A	301	HEC	CMA-C3A-C4A	-4.80	116.28	124.73
9	N	303	HEC	C2A-C1A-NA	4.72	114.88	110.32
12	O	1201	CLA	C2A-C3A-C4A	4.72	109.49	101.87
14	R	1101	BCR	C30-C25-C26	-4.68	116.25	122.64
9	N	301	HEC	CAD-C3D-C4D	-4.63	116.62	124.70
9	N	301	HEC	CAB-C3B-C2B	-4.61	119.10	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	302	HEC	CMA-C3A-C4A	-4.53	116.75	124.73
9	P	301	HEC	CMA-C3A-C4A	-4.49	116.82	124.73
9	N	302	HEC	CMA-C3A-C4A	-4.49	116.83	124.73
12	B	201	CLA	C2A-C3A-C4A	4.47	109.09	101.87
9	C	301	HEC	CMA-C3A-C4A	-4.41	116.96	124.73
9	N	301	HEC	CMA-C3A-C4A	-4.38	117.02	124.73
9	N	301	HEC	CBC-CAC-C3C	4.35	124.21	112.42
14	E	101	BCR	C29-C30-C25	4.25	116.61	110.44
9	A	302	HEC	CBC-CAC-C3C	4.19	123.77	112.42
9	A	301	HEC	CAD-C3D-C4D	-4.17	117.42	124.70
9	N	303	HEC	C3D-C4D-ND	4.09	114.31	110.35
9	A	302	HEC	C2A-C1A-NA	-4.01	106.45	110.32
14	E	101	BCR	C2-C1-C6	4.01	116.26	110.44
14	R	1101	BCR	C21-C20-C19	3.98	134.75	123.20
14	R	1101	BCR	C29-C30-C25	3.98	116.23	110.44
14	E	101	BCR	C38-C26-C27	-3.97	105.12	113.60
14	E	101	BCR	C21-C20-C19	3.91	134.53	123.20
14	R	1101	BCR	C38-C26-C27	-3.90	105.28	113.60
14	R	1101	BCR	C11-C10-C9	3.88	132.72	127.28
14	E	101	BCR	C11-C10-C9	3.85	132.68	127.28
14	R	1101	BCR	C7-C8-C9	3.82	131.88	126.23
14	R	1101	BCR	C2-C1-C6	3.79	115.94	110.44
9	N	302	HEC	CAD-C3D-C2D	3.78	134.96	127.87
12	O	1201	CLA	C2A-C1A-CHA	3.76	130.39	123.87
12	O	1201	CLA	C4D-C3D-CAD	3.75	112.18	108.11
14	E	101	BCR	C1-C6-C5	-3.72	117.55	122.64
14	R	1101	BCR	C24-C23-C22	3.69	131.69	126.23
9	A	302	HEC	CAD-C3D-C2D	3.60	134.60	127.87
14	R	1101	BCR	C1-C6-C5	-3.57	117.75	122.64
14	E	101	BCR	C7-C8-C9	3.54	131.47	126.23
9	C	301	HEC	CAD-C3D-C4D	-3.47	118.66	124.70
9	P	301	HEC	CAD-C3D-C4D	-3.45	118.68	124.70
9	N	302	HEC	CMA-C3A-C2A	3.45	135.47	126.15
12	B	201	CLA	C2A-C1A-CHA	3.44	129.84	123.87
9	A	301	HEC	CMA-C3A-C2A	3.43	135.44	126.15
9	A	302	HEC	CMA-C3A-C2A	3.40	135.34	126.15
9	N	303	HEC	C1D-C2D-C3D	3.38	110.54	106.98
9	A	303	HEC	CAA-CBA-CGA	3.37	122.60	113.67
14	E	101	BCR	C24-C23-C22	3.34	131.17	126.23
14	R	1101	BCR	C23-C24-C25	3.30	135.81	127.00
14	E	101	BCR	C33-C5-C4	-3.29	106.59	113.60
9	A	301	HEC	CHA-C4D-ND	3.27	127.95	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	1201	CLA	CED-O2D-CGD	3.23	123.25	115.92
9	N	302	HEC	C2A-C1A-NA	-3.22	107.22	110.32
14	E	101	BCR	C23-C24-C25	3.21	135.58	127.00
14	R	1101	BCR	C33-C5-C4	-3.21	106.75	113.60
9	N	301	HEC	CHA-C4D-ND	3.21	127.87	124.42
9	N	303	HEC	C2D-C1D-ND	-3.20	106.16	109.84
9	C	301	HEC	CMA-C3A-C2A	3.20	134.81	126.15
12	O	1201	CLA	C3A-C2A-C1A	3.20	106.13	101.34
9	C	301	HEC	CAA-C2A-C3A	3.18	133.82	127.87
9	P	301	HEC	CMA-C3A-C2A	3.17	134.72	126.15
9	P	301	HEC	CAA-C2A-C3A	3.17	133.80	127.87
9	N	301	HEC	CMA-C3A-C2A	3.15	134.66	126.15
9	A	303	HEC	C2A-C1A-NA	3.14	113.36	110.32
11	B	309	BNT	CAC-CAD-CAE	3.12	119.57	112.74
12	B	201	CLA	C1-C2-C3	3.12	131.31	126.20
12	B	201	CLA	CED-O2D-CGD	3.12	122.99	115.92
10	C	306	OPC	CAM-OAN-CAO	3.10	125.21	117.80
9	A	302	HEC	C1D-ND-C4D	3.07	108.84	105.21
14	E	101	BCR	C8-C7-C6	3.05	135.14	127.00
9	N	301	HEC	CAA-CBA-CGA	3.04	121.72	113.67
9	A	301	HEC	CAA-C2A-C3A	3.01	133.50	127.87
9	P	301	HEC	CHA-C4D-ND	2.98	127.63	124.42
12	B	201	CLA	C4D-CHA-C1A	2.97	124.78	121.24
9	A	301	HEC	C1D-ND-C4D	2.96	108.71	105.21
14	E	101	BCR	C1-C6-C7	2.95	123.66	115.65
11	O	1309	BNT	CAC-CAD-CAE	2.95	119.19	112.74
12	B	201	CLA	C4D-C3D-CAD	2.92	111.28	108.11
9	P	301	HEC	C1D-ND-C4D	2.91	108.66	105.21
14	R	1101	BCR	C8-C7-C6	2.90	134.76	127.00
12	O	1201	CLA	CAA-C2A-C1A	2.90	121.49	111.97
9	C	301	HEC	CHA-C4D-ND	2.86	127.50	124.42
9	A	303	HEC	CMD-C2D-C1D	-2.86	120.57	125.03
12	B	201	CLA	CAA-C2A-C1A	2.85	121.33	111.97
9	C	301	HEC	C1D-ND-C4D	2.84	108.57	105.21
14	R	1101	BCR	C1-C6-C7	2.84	123.36	115.65
9	N	301	HEC	CAA-C2A-C3A	2.84	133.18	127.87
12	B	201	CLA	C3A-C2A-C1A	2.82	105.56	101.34
9	N	302	HEC	CAA-C2A-C1A	-2.79	119.18	124.85
10	O	1306	OPC	OAN-CAO-OAD	-2.79	117.19	123.70
9	N	303	HEC	C4D-C3D-C2D	-2.68	103.00	106.89
10	N	1305	OPC	OAN-CAO-OAD	-2.66	117.48	123.70
10	C	306	OPC	OAN-CAO-OAD	-2.64	117.54	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	303	HEC	CHB-C1B-NB	-2.63	121.59	124.42
9	N	303	HEC	CMC-C2C-C3C	2.60	131.14	125.62
9	N	302	HEC	C1D-ND-C4D	2.57	108.25	105.21
12	O	1201	CLA	O2A-CGA-CBA	2.53	119.56	111.83
10	B	305	OPC	OAN-CAO-OAD	-2.49	117.89	123.70
9	N	303	HEC	CHA-C4D-C3D	-2.48	121.16	124.77
14	E	101	BCR	C15-C16-C17	2.47	128.58	123.52
14	R	1101	BCR	C32-C1-C6	2.46	114.10	110.24
9	N	302	HEC	CAA-C2A-C3A	2.45	132.46	127.87
11	O	1309	BNT	BRAI-CAJ-CAK	2.45	120.55	116.16
14	E	101	BCR	C32-C1-C6	2.45	114.09	110.24
10	N	1305	OPC	OBJ-CBK-CBL	2.43	119.25	111.83
10	O	1306	OPC	OBJ-CBK-CBL	2.39	119.13	111.83
9	C	301	HEC	CAA-C2A-C1A	-2.39	120.00	124.85
9	A	303	HEC	CAC-C3C-C2C	2.39	130.66	126.89
10	B	305	OPC	OBJ-CBK-CBL	2.36	119.05	111.83
9	A	302	HEC	CHB-C4A-NA	2.34	127.00	124.45
9	N	301	HEC	CHA-C4D-C3D	-2.34	121.36	124.77
14	R	1101	BCR	C15-C16-C17	2.32	128.26	123.52
14	R	1101	BCR	C30-C25-C24	2.29	121.86	115.65
10	O	1306	OPC	CAM-OAN-CAO	2.29	123.27	117.80
11	B	309	BNT	OAB-CAF-CAG	-2.27	118.60	123.10
12	O	1201	CLA	CBA-CAA-C2A	-2.26	107.06	113.79
14	E	101	BCR	C30-C25-C24	2.25	121.76	115.65
9	N	303	HEC	CAD-CBD-CGD	2.24	119.60	113.67
9	N	301	HEC	CAD-CBD-CGD	-2.24	107.73	113.67
9	N	303	HEC	C2B-C1B-NB	2.23	112.48	109.90
10	N	1305	OPC	OBJ-CBI-CAM	2.22	114.81	108.40
12	B	201	CLA	O2D-CGD-CBD	2.22	115.11	111.23
10	C	306	OPC	OBJ-CBK-CBL	2.21	118.58	111.83
9	P	301	HEC	CAA-C2A-C1A	-2.21	120.36	124.85
12	B	201	CLA	O2A-CGA-CBA	2.21	118.56	111.83
9	N	301	HEC	C1D-ND-C4D	2.19	107.81	105.21
9	N	303	HEC	C3C-C4C-NC	-2.18	107.73	110.15
14	R	1101	BCR	C36-C18-C17	-2.16	119.32	122.82
14	R	1101	BCR	C40-C30-C29	-2.16	100.66	108.95
9	A	302	HEC	CHA-C1A-C2A	2.14	128.24	124.86
9	A	302	HEC	CAD-C3D-C4D	-2.11	121.01	124.70
14	E	101	BCR	C40-C30-C29	-2.11	100.85	108.95
9	N	302	HEC	CAD-C3D-C4D	-2.09	121.06	124.70
14	E	101	BCR	C34-C9-C10	-2.08	119.45	122.82
9	N	303	HEC	CBA-CAA-C2A	-2.04	106.89	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	1201	CLA	C7-C6-C5	-2.04	107.84	113.26
14	R	1101	BCR	C20-C21-C22	-2.01	124.45	127.28
9	P	301	HEC	CMC-C2C-C3C	2.01	129.88	125.62
12	B	201	CLA	CHA-C1A-NA	-2.00	121.86	126.39

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	301	HEC	NA
9	A	302	HEC	NA
9	A	303	HEC	NA
9	C	301	HEC	NA
9	N	301	HEC	NA
9	N	302	HEC	NA
9	N	303	HEC	NA
9	P	301	HEC	NA
12	B	201	CLA	C3A
12	B	201	CLA	C2A
12	B	201	CLA	C8
12	O	1201	CLA	C3A
12	O	1201	CLA	C2A
12	O	1201	CLA	C8

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	303	HEC	C3A-C2A-CAA-CBA
9	N	302	HEC	C2D-C3D-CAD-CBD
9	N	302	HEC	C4D-C3D-CAD-CBD
10	B	305	OPC	CAP-CAO-OAN-CAM
10	B	305	OPC	OAD-CAO-OAN-CAM
10	B	305	OPC	CAL-OAK-PAJ-OBH
10	B	305	OPC	CAL-OAK-PAJ-OAB
10	B	305	OPC	CAL-OAK-PAJ-OAI
10	B	305	OPC	CAH-OAI-PAJ-OAK
10	B	305	OPC	CAH-OAI-PAJ-OBH
10	C	306	OPC	CAP-CAO-OAN-CAM
10	C	306	OPC	OAD-CAO-OAN-CAM
10	C	306	OPC	CAL-OAK-PAJ-OAI
10	C	306	OPC	CAH-OAI-PAJ-OBH
10	N	1305	OPC	CAP-CAO-OAN-CAM
10	N	1305	OPC	OAD-CAO-OAN-CAM

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Mol	Chain	Res	Type	Atoms
10	N	1305	OPC	CAL-OAK-PAJ-OBH
10	N	1305	OPC	CAL-OAK-PAJ-OAB
10	N	1305	OPC	CAL-OAK-PAJ-OAI
10	N	1305	OPC	CAH-OAI-PAJ-OAK
10	N	1305	OPC	CAH-OAI-PAJ-OAB
10	O	1306	OPC	CAP-CAO-OAN-CAM
10	O	1306	OPC	OAD-CAO-OAN-CAM
10	O	1306	OPC	CAL-OAK-PAJ-OBH
10	O	1306	OPC	CAL-OAK-PAJ-OAB
10	O	1306	OPC	CAH-OAI-PAJ-OBH
10	O	1306	OPC	CAG-CAH-OAI-PAJ
12	B	201	CLA	C1A-C2A-CAA-CBA
12	O	1201	CLA	C1A-C2A-CAA-CBA
14	E	101	BCR	C1-C6-C7-C8
14	E	101	BCR	C5-C6-C7-C8
14	E	101	BCR	C11-C10-C9-C8
14	E	101	BCR	C11-C10-C9-C34
14	R	1101	BCR	C5-C6-C7-C8
14	R	1101	BCR	C11-C10-C9-C8
14	R	1101	BCR	C11-C10-C9-C34
12	O	1201	CLA	C2A-CAA-CBA-CGA
9	A	303	HEC	C1A-C2A-CAA-CBA
9	A	302	HEC	C2D-C3D-CAD-CBD
12	B	201	CLA	C2A-CAA-CBA-CGA
14	E	101	BCR	C22-C23-C24-C25
14	R	1101	BCR	C22-C23-C24-C25
14	E	101	BCR	C35-C13-C14-C15
14	R	1101	BCR	C35-C13-C14-C15
9	A	302	HEC	C4D-C3D-CAD-CBD
14	E	101	BCR	C12-C13-C14-C15
14	R	1101	BCR	C12-C13-C14-C15
12	O	1201	CLA	C13-C15-C16-C17
14	R	1101	BCR	C1-C6-C7-C8
9	N	303	HEC	C2B-C3B-CAB-CBB
12	B	201	CLA	CBA-CGA-O2A-C1
9	P	301	HEC	C2C-C3C-CAC-CBC
12	B	201	CLA	O1A-CGA-O2A-C1
12	B	201	CLA	C11-C12-C13-C15
12	B	201	CLA	C14-C13-C15-C16
10	B	305	OPC	CAM-CAL-OAK-PAJ
12	O	1201	CLA	CBA-CGA-O2A-C1
12	O	1201	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
10	O	1306	OPC	CBS-CBT-CBU-CBV
9	A	303	HEC	C4D-C3D-CAD-CBD
12	B	201	CLA	C11-C12-C13-C14
12	O	1201	CLA	C6-C7-C8-C9
12	B	201	CLA	C12-C13-C15-C16
12	O	1201	CLA	C6-C7-C8-C10
10	N	1305	OPC	CAT-CAU-CAV-CAW
12	O	1201	CLA	C2C-C3C-CAC-CBC
12	O	1201	CLA	O1A-CGA-O2A-C1
9	N	303	HEC	C4D-C3D-CAD-CBD
9	P	301	HEC	C4C-C3C-CAC-CBC
10	C	306	OPC	CAL-CAM-OAN-CAO
9	A	303	HEC	C2D-C3D-CAD-CBD
9	N	303	HEC	C4B-C3B-CAB-CBB
10	B	305	OPC	NAF-CAG-CAH-OAI
10	C	306	OPC	NAF-CAG-CAH-OAI
10	N	1305	OPC	NAF-CAG-CAH-OAI
10	O	1306	OPC	NAF-CAG-CAH-OAI
9	C	301	HEC	C2C-C3C-CAC-CBC
10	N	1305	OPC	CBP-CBQ-CBR-CBS
10	C	306	OPC	CAL-OAK-PAJ-OAB
10	C	306	OPC	CAH-OAI-PAJ-OAK
10	C	306	OPC	CAH-OAI-PAJ-OAB
10	N	1305	OPC	CAH-OAI-PAJ-OBH
10	O	1306	OPC	CAL-OAK-PAJ-OAI
10	O	1306	OPC	CAH-OAI-PAJ-OAK
10	O	1306	OPC	CAH-OAI-PAJ-OAB
9	A	302	HEC	C2B-C3B-CAB-CBB
10	O	1306	OPC	CAL-CAM-OAN-CAO
9	N	303	HEC	C2D-C3D-CAD-CBD
9	C	301	HEC	C4C-C3C-CAC-CBC
9	C	301	HEC	CAD-CBD-CGD-O1D
9	P	301	HEC	CAD-CBD-CGD-O1D
9	P	301	HEC	CAD-CBD-CGD-O2D
10	N	1305	OPC	CAL-CAM-OAN-CAO
9	C	301	HEC	CAD-CBD-CGD-O2D
9	A	301	HEC	CAA-CBA-CGA-O1A
9	N	301	HEC	CAD-CBD-CGD-O1D
10	C	306	OPC	CAM-CAL-OAK-PAJ
9	A	302	HEC	CAA-CBA-CGA-O1A
12	O	1201	CLA	C11-C12-C13-C15
10	N	1305	OPC	CAV-CAW-CAX-CAY

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Mol	Chain	Res	Type	Atoms
9	A	301	HEC	CAA-CBA-CGA-O2A
9	N	301	HEC	CAD-CBD-CGD-O2D
9	A	302	HEC	CAA-CBA-CGA-O2A
9	N	302	HEC	CAA-CBA-CGA-O1A
9	C	301	HEC	CAA-CBA-CGA-O1A
9	P	301	HEC	CAA-CBA-CGA-O1A
10	B	305	OPC	OAK-CAL-CAM-OAN
12	B	201	CLA	C4-C3-C5-C6
9	N	302	HEC	CAA-CBA-CGA-O2A
10	N	1305	OPC	CBI-CAM-OAN-CAO
10	O	1306	OPC	CBR-CBS-CBT-CBU
10	O	1306	OPC	OAK-CAL-CAM-OAN
10	B	305	OPC	CBP-CBQ-CBR-CBS
9	C	301	HEC	CAA-CBA-CGA-O2A
9	P	301	HEC	CAA-CBA-CGA-O2A
12	O	1201	CLA	C4-C3-C5-C6
10	N	1305	OPC	OBJ-CBK-CBL-CBM
10	O	1306	OPC	CBU-CBV-CBW-CBX
12	O	1201	CLA	C4B-C3B-CAB-CBB
9	A	301	HEC	CAD-CBD-CGD-O1D
9	A	301	HEC	CAD-CBD-CGD-O2D
12	O	1201	CLA	C11-C12-C13-C14
12	B	201	CLA	C13-C15-C16-C17
12	O	1201	CLA	C4C-C3C-CAC-CBC
10	C	306	OPC	OBJ-CBK-CBL-CBM
10	N	1305	OPC	OCC-CBK-CBL-CBM
10	N	1305	OPC	OAN-CAO-CAP-CAQ
10	O	1306	OPC	CBT-CBU-CBV-CBW

There are no ring outliers.

20 monomers are involved in 177 short contacts:

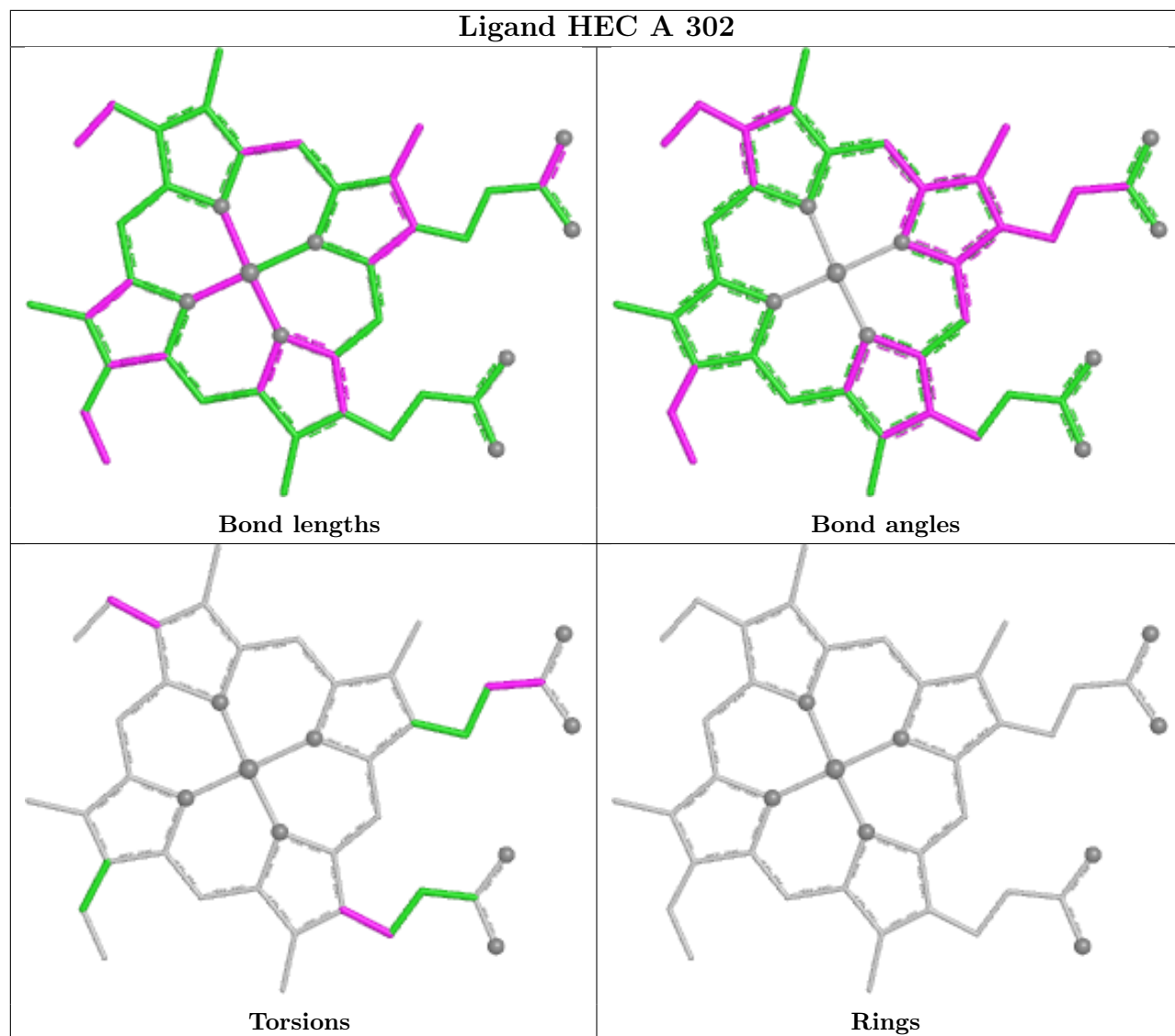
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	302	HEC	11	0
9	N	303	HEC	8	0
9	P	301	HEC	4	0
12	B	201	CLA	8	0
12	O	1201	CLA	9	0
14	R	1101	BCR	8	0
9	C	301	HEC	3	0
11	O	1309	BNT	12	0
9	A	303	HEC	3	0

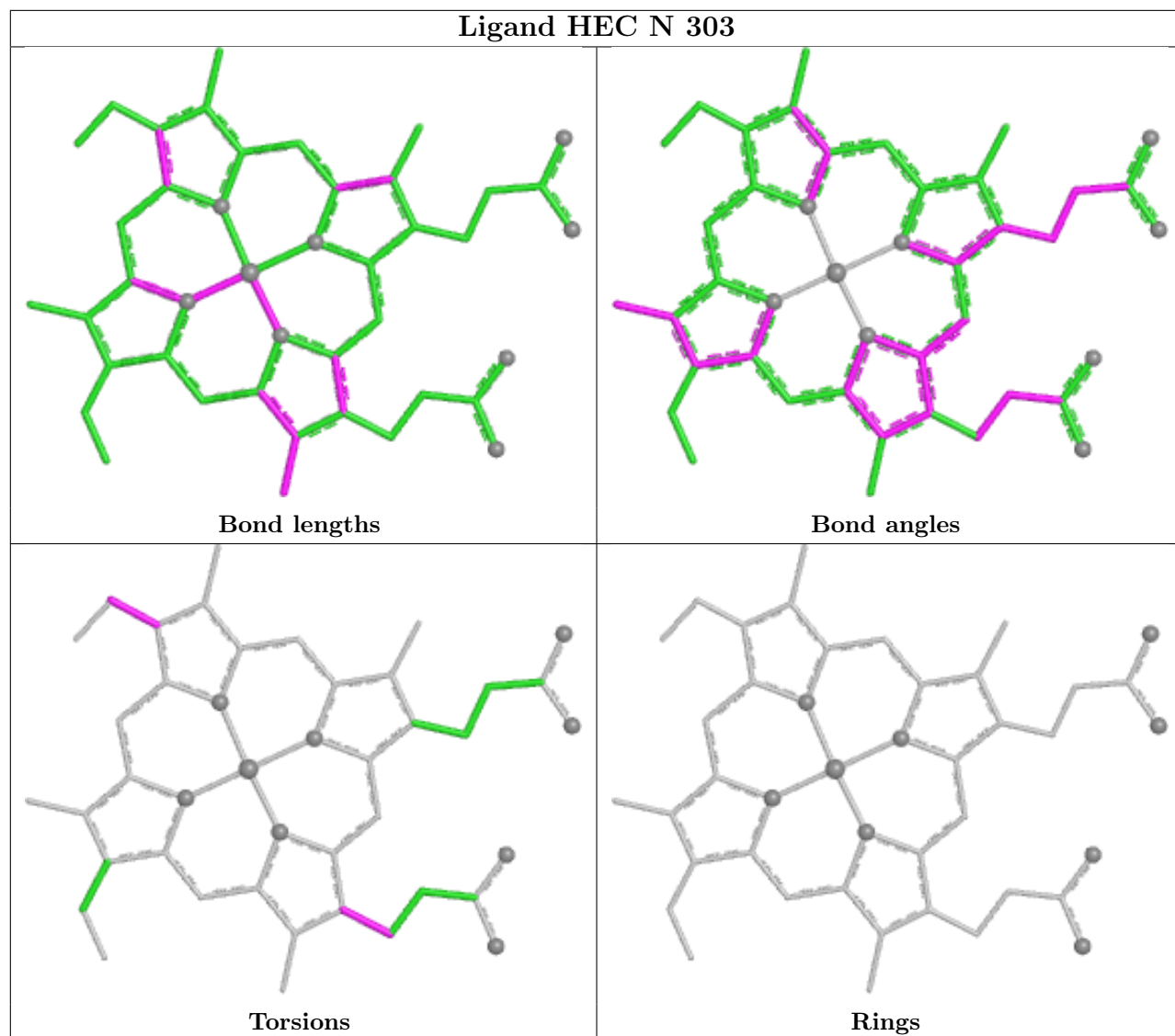
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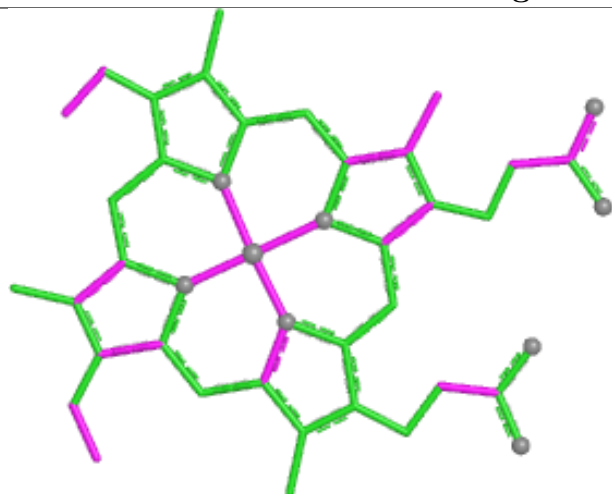
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	E	101	BCR	11	0
10	B	305	OPC	34	0
9	A	301	HEC	3	0
10	O	1306	OPC	17	0
13	D	201	FES	3	0
9	N	301	HEC	6	0
10	N	1305	OPC	14	0
9	N	302	HEC	5	0
13	Q	201	FES	2	0
10	C	306	OPC	20	0
11	B	309	BNT	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

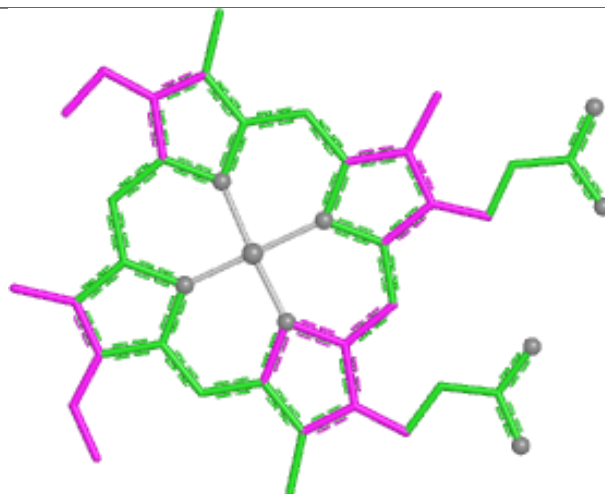




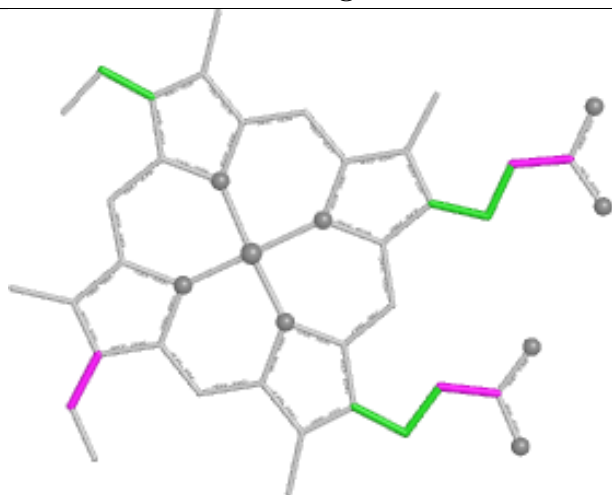
Ligand HEC P 301



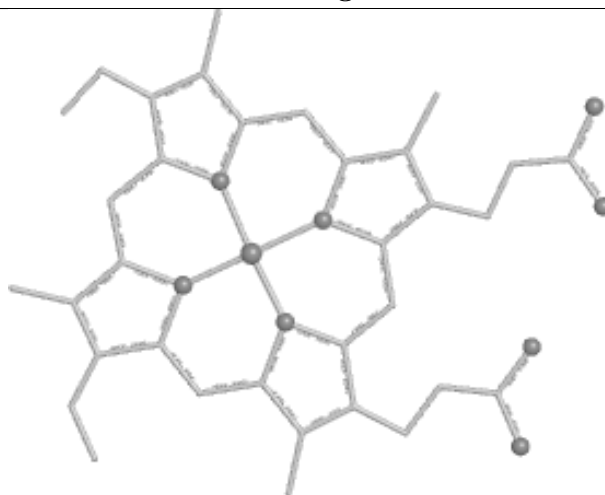
Bond lengths



Bond angles

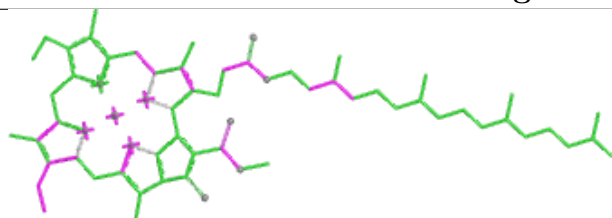


Torsions

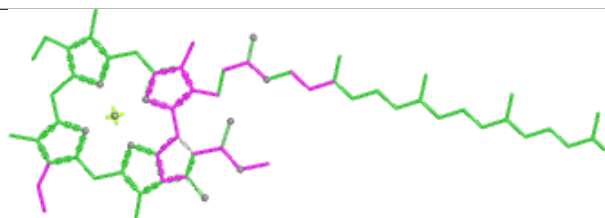


Rings

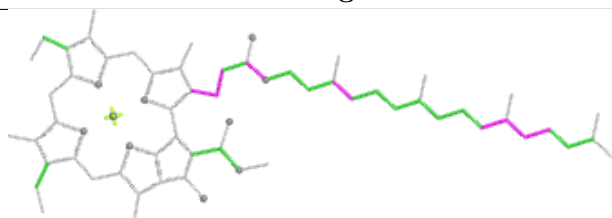
Ligand CLA B 201



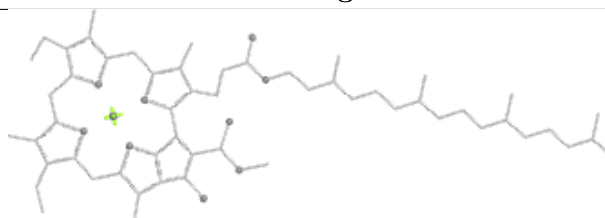
Bond lengths



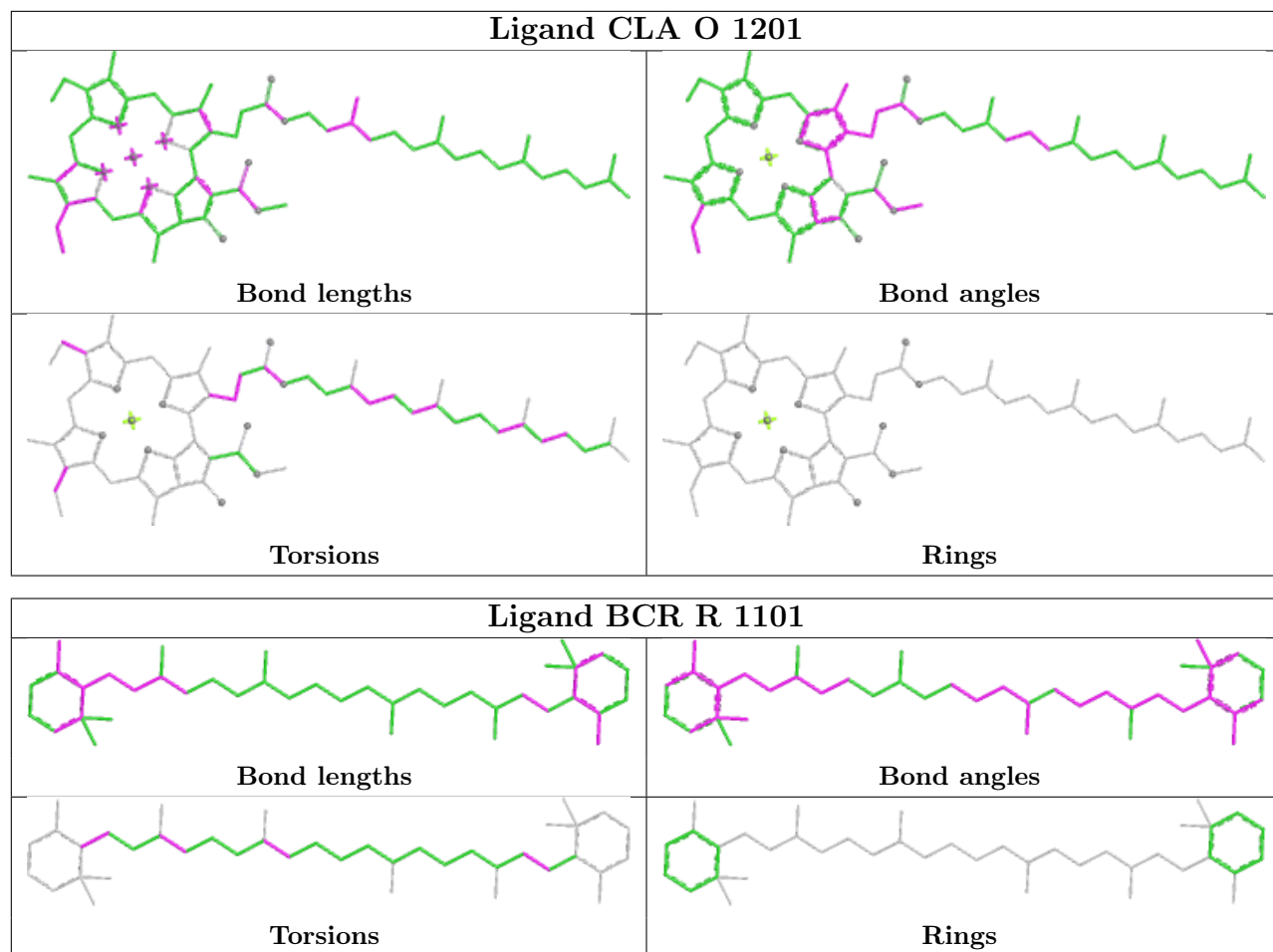
Bond angles



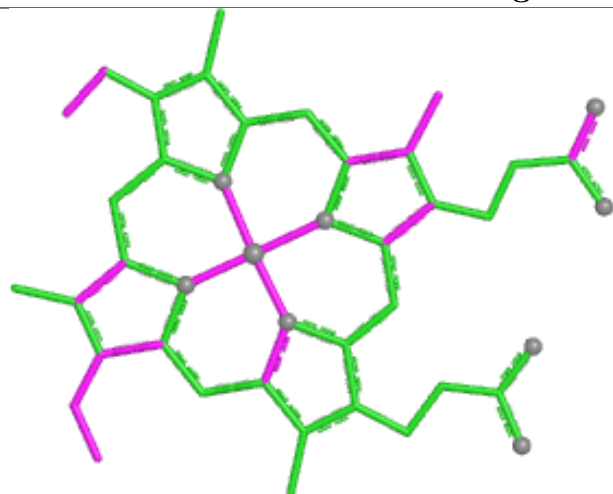
Torsions



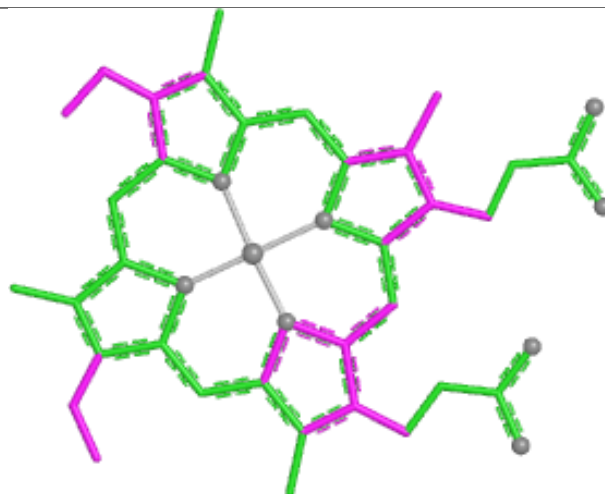
Rings



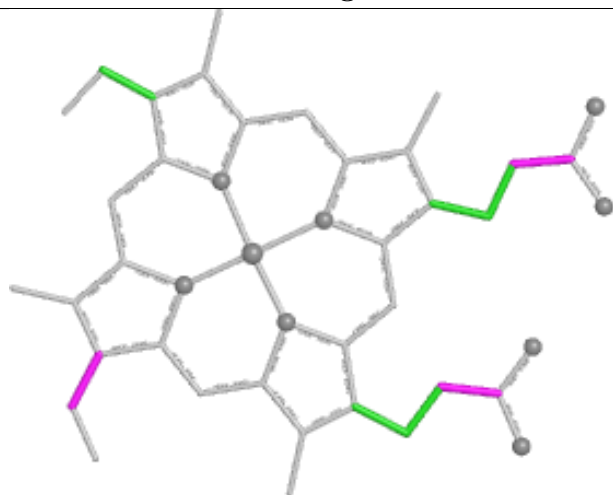
Ligand HEC C 301



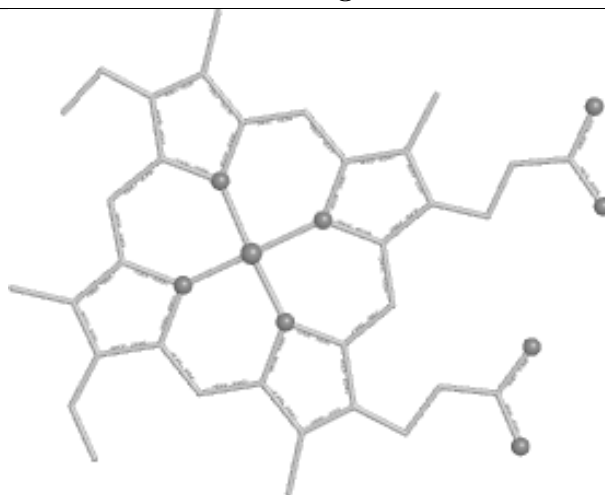
Bond lengths



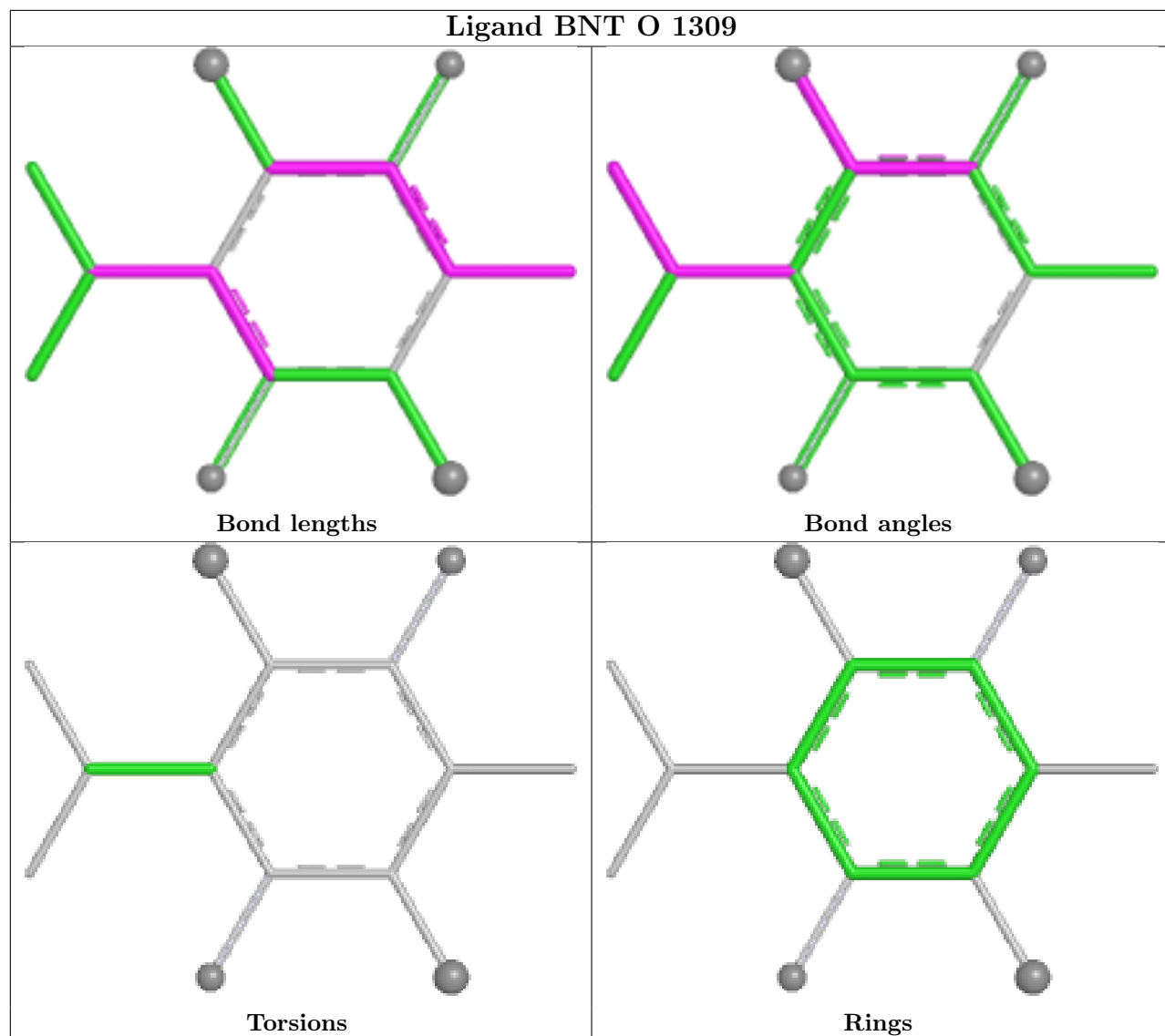
Bond angles



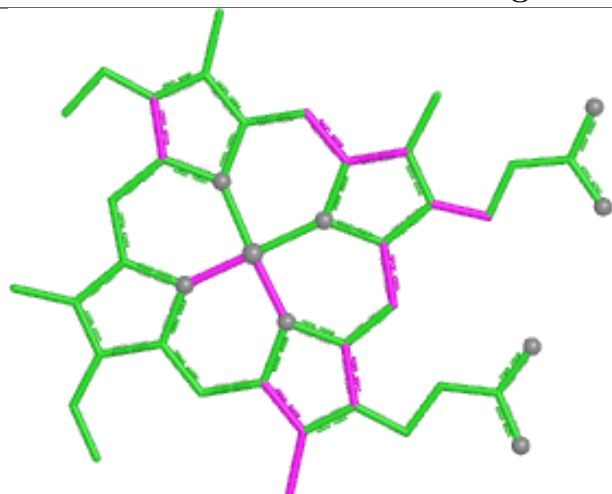
Torsions



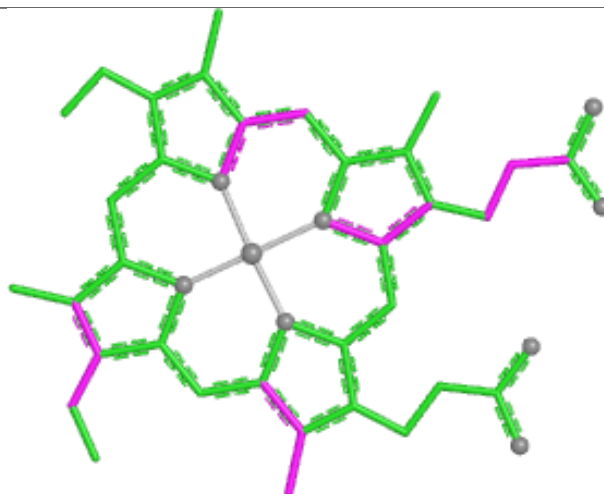
Rings



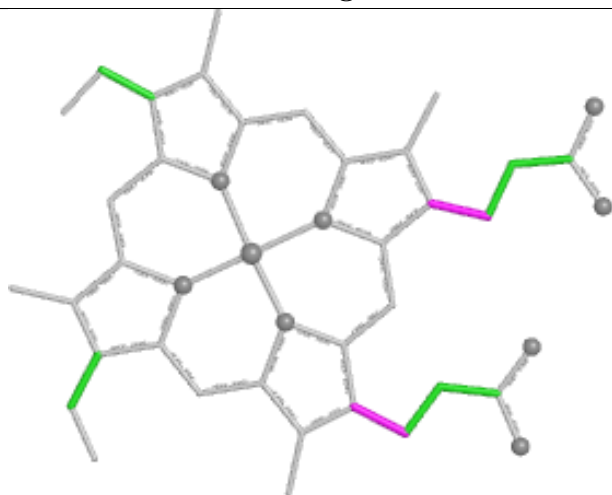
Ligand HEC A 303



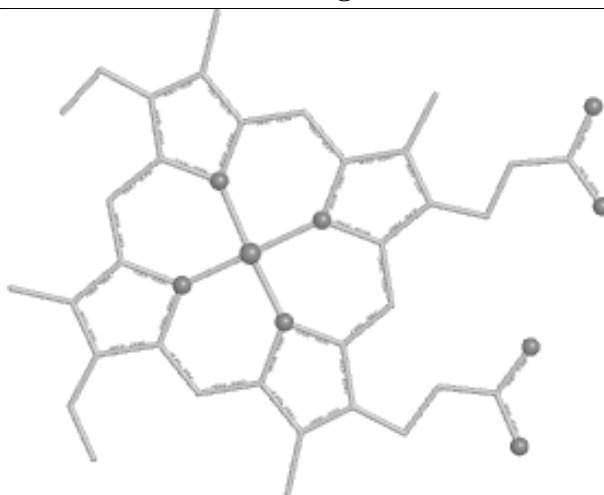
Bond lengths



Bond angles

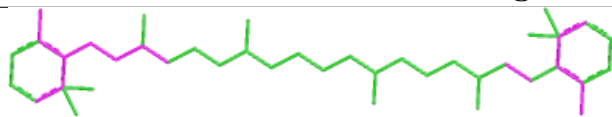


Torsions

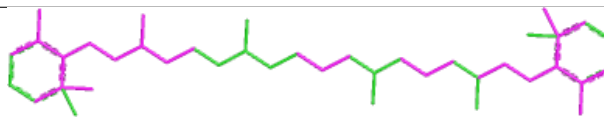


Rings

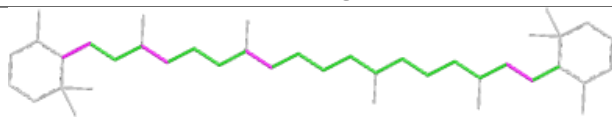
Ligand BCR E 101



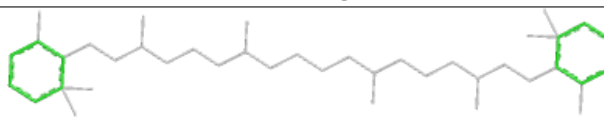
Bond lengths



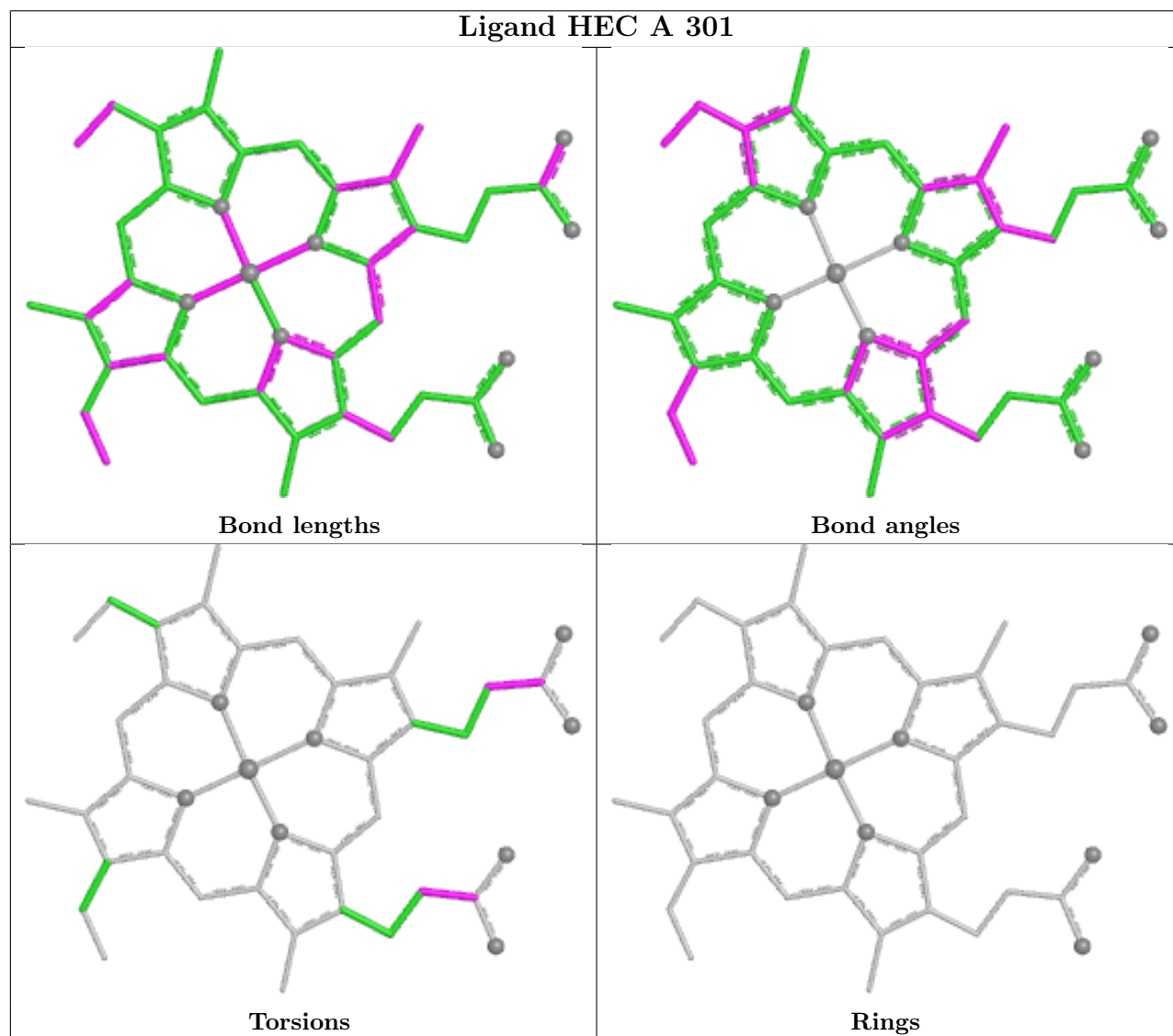
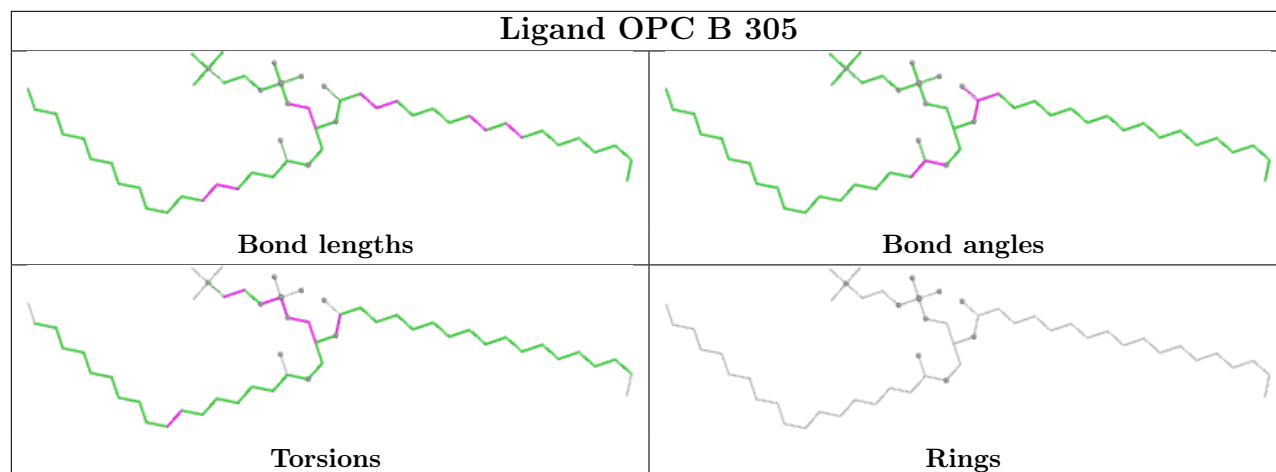
Bond angles

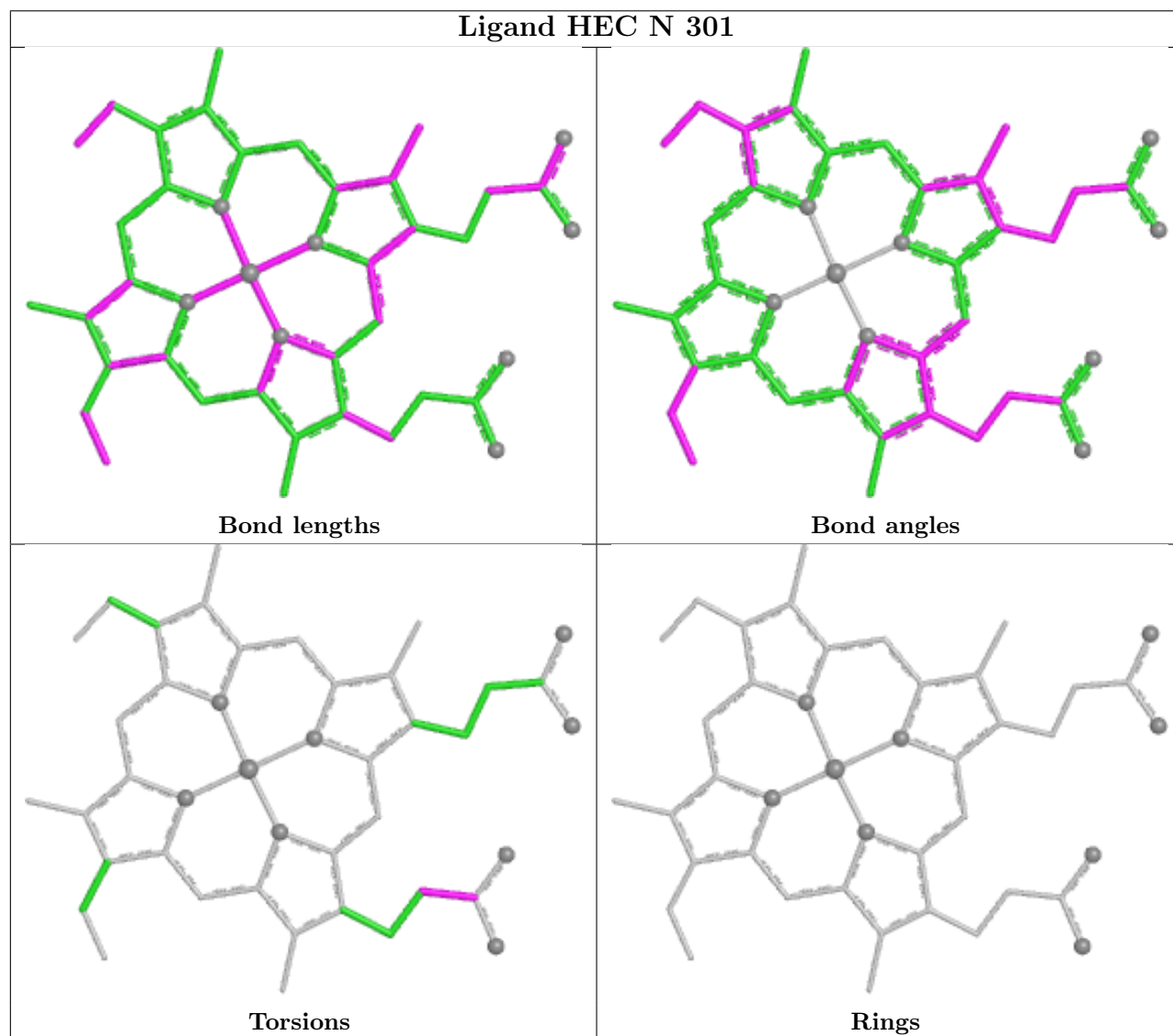
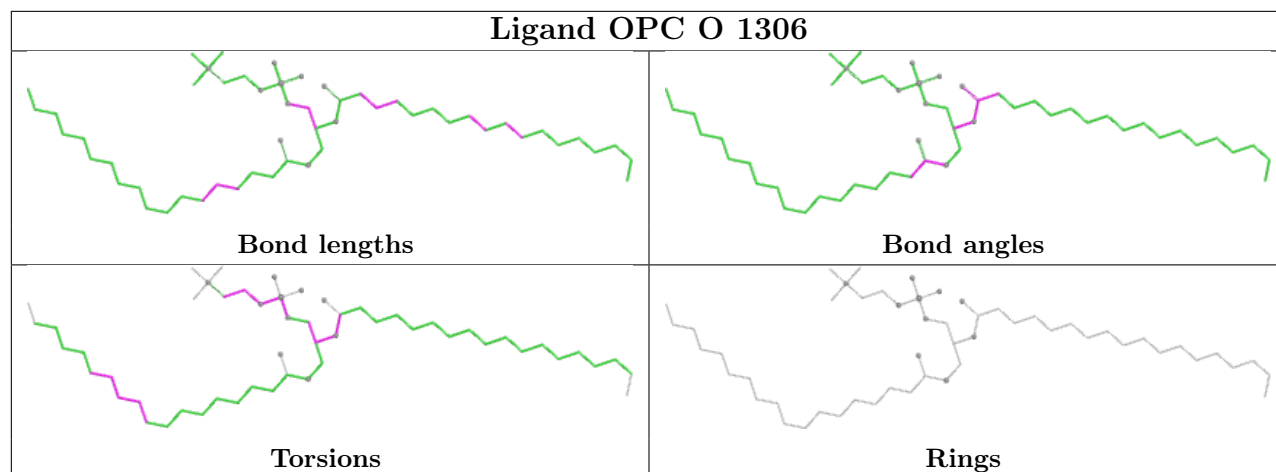


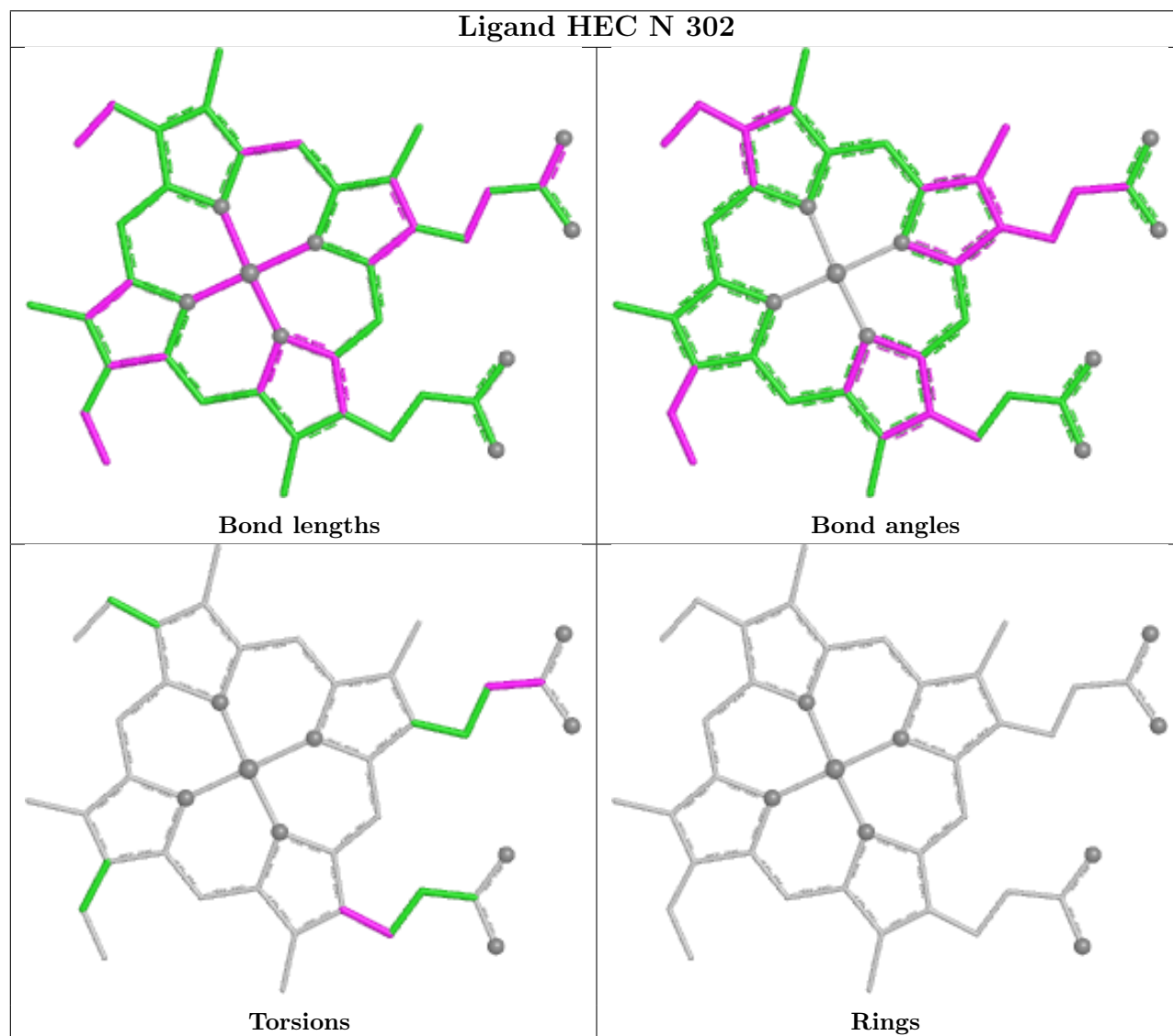
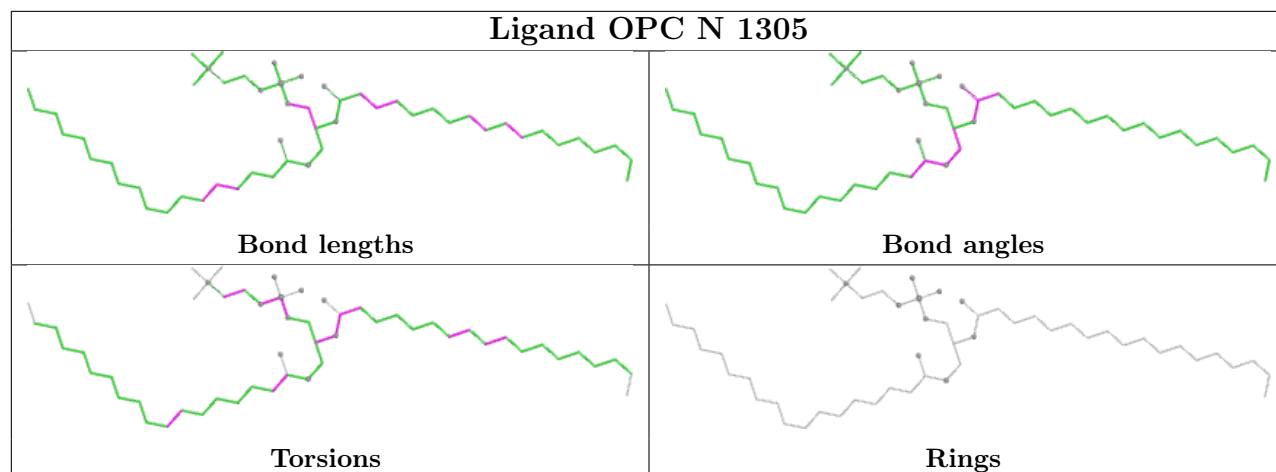
Torsions

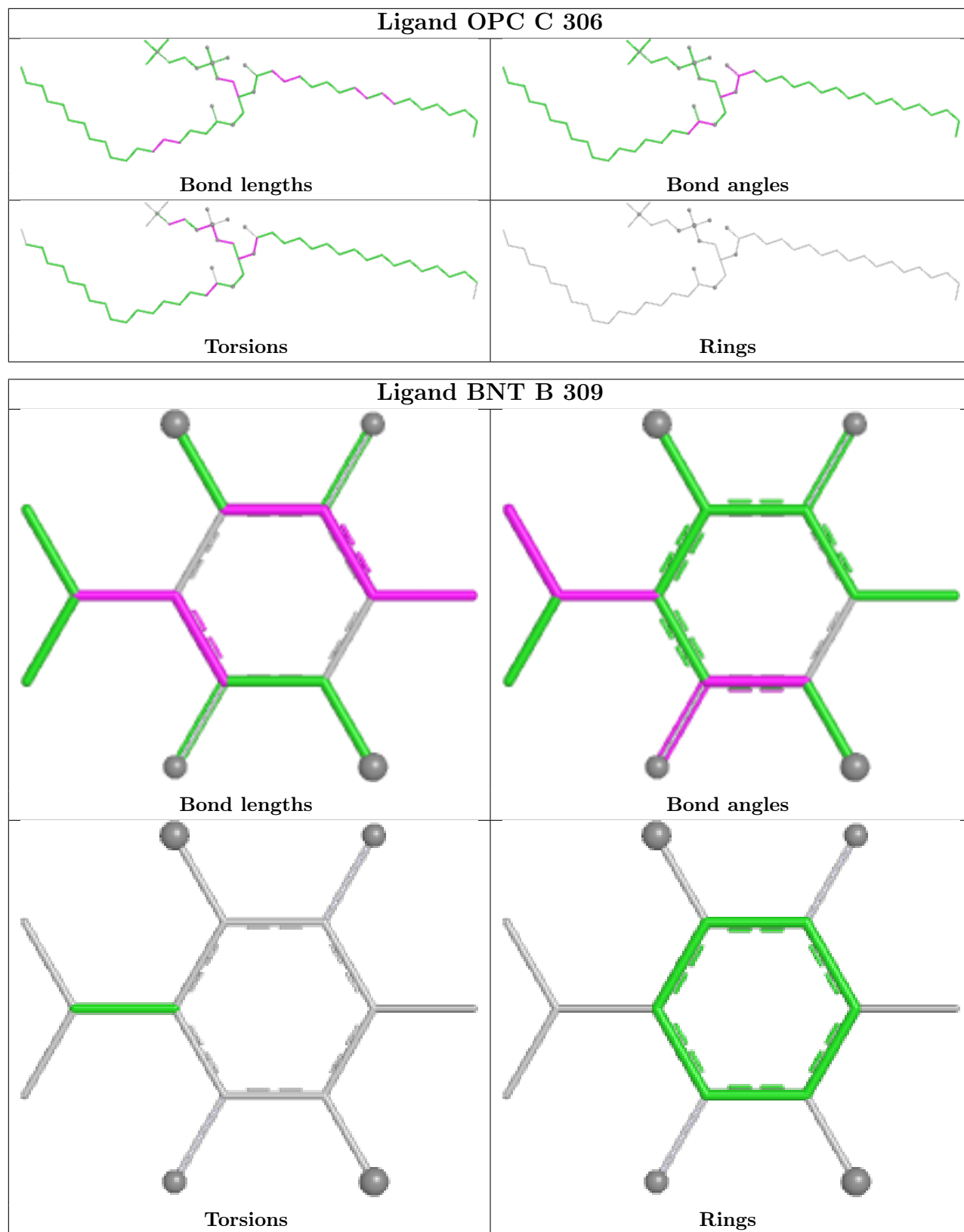


Rings









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	202/215 (93%)	-1.34	0	100	100	12, 58, 120, 164	0
1	N	202/215 (93%)	-1.38	0	100	100	11, 53, 104, 158	0
2	B	137/160 (85%)	-1.34	0	100	100	16, 67, 137, 177	0
2	O	137/160 (85%)	-1.23	1 (0%)	84	65	13, 63, 130, 183	0
3	C	286/289 (98%)	-1.12	2 (0%)	84	65	5, 85, 150, 200	1 (0%)
3	P	286/289 (98%)	-1.13	0	100	100	0, 85, 160, 200	1 (0%)
4	D	168/179 (93%)	-0.98	1 (0%)	85	68	18, 93, 169, 200	0
4	Q	168/179 (93%)	-1.03	0	100	100	26, 94, 158, 195	0
5	E	32/32 (100%)	-1.14	0	100	100	20, 67, 163, 195	0
5	R	32/32 (100%)	-1.23	0	100	100	21, 59, 111, 162	0
6	F	35/35 (100%)	-1.21	0	100	100	8, 69, 133, 144	0
6	S	35/35 (100%)	-1.35	0	100	100	16, 71, 113, 153	0
7	G	27/37 (72%)	-1.33	0	100	100	34, 66, 133, 147	0
7	T	27/37 (72%)	-1.32	0	100	100	30, 76, 136, 178	0
8	H	27/29 (93%)	-1.33	0	100	100	25, 68, 119, 156	0
8	U	27/29 (93%)	-1.30	0	100	100	29, 69, 128, 180	0
All	All	1828/1952 (93%)	-1.20	4 (0%)	91	81	0, 73, 149, 200	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	221	GLU	3.9
4	D	152	HIS	3.0
3	C	222	GLY	2.8
2	O	66	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

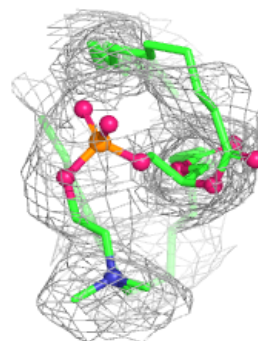
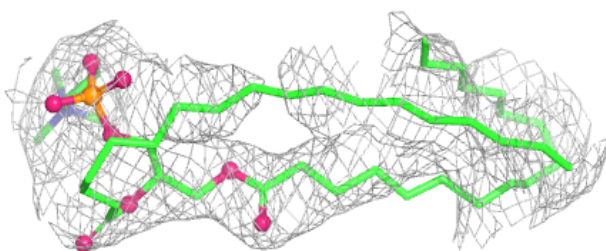
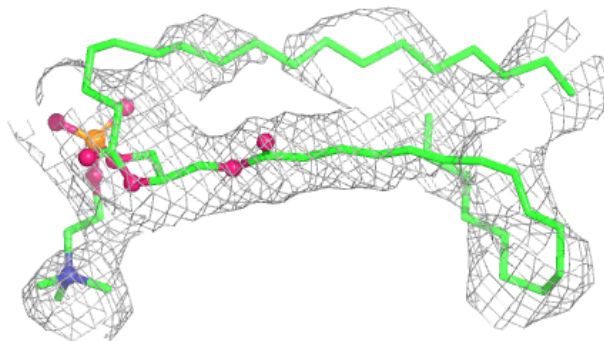
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	OPC	O	1306	54/55	0.98	0.05	73,73,73,73	0
9	HEC	N	303	43/43	0.99	0.05	67,74,74,74	0
10	OPC	B	305	54/55	0.99	0.05	66,66,66,66	0
10	OPC	C	306	54/55	0.99	0.05	84,84,84,84	0
10	OPC	N	1305	54/55	0.99	0.07	107,107,107,107	0
9	HEC	A	303	43/43	0.99	0.06	57,104,104,104	0
11	BNT	B	309	14/14	0.99	0.08	64,64,64,64	0
11	BNT	O	1309	14/14	0.99	0.10	64,64,64,64	0
12	CLA	B	201	65/65	0.99	0.06	20,112,112,112	0
12	CLA	O	1201	65/65	0.99	0.06	29,72,72,72	0
14	BCR	E	101	40/40	0.99	0.07	84,84,84,84	0
14	BCR	R	1101	40/40	0.99	0.09	181,181,181,181	0
9	HEC	A	302	43/43	1.00	0.03	41,58,58,58	0
9	HEC	P	301	43/43	1.00	0.03	54,76,76,76	0
9	HEC	A	301	43/43	1.00	0.02	31,48,48,48	0
9	HEC	C	301	43/43	1.00	0.02	36,59,59,59	0
13	FES	D	201	4/4	1.00	0.01	70,70,97,97	0
13	FES	Q	201	4/4	1.00	0.01	28,28,53,53	0
9	HEC	N	301	43/43	1.00	0.03	26,64,64,64	0
9	HEC	N	302	43/43	1.00	0.03	30,61,61,61	0

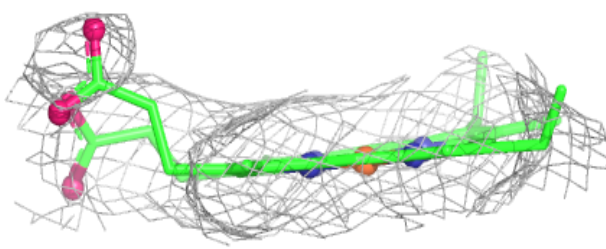
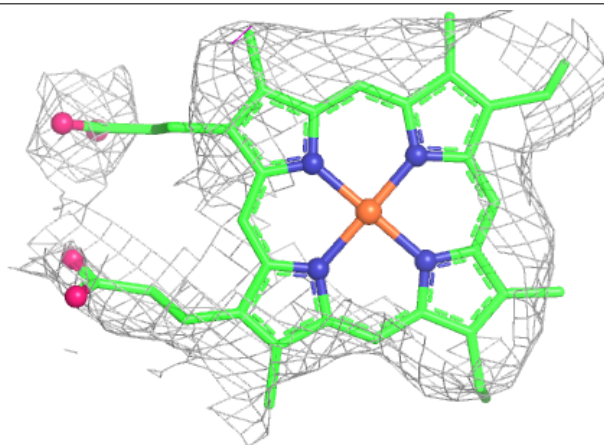
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around OPC O 1306:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

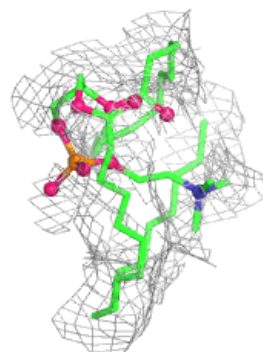
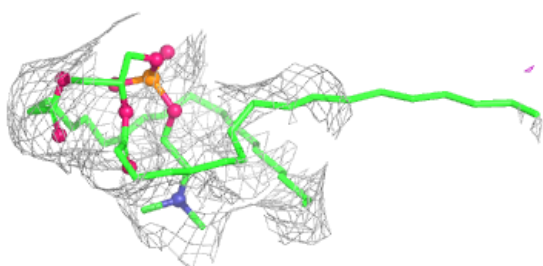
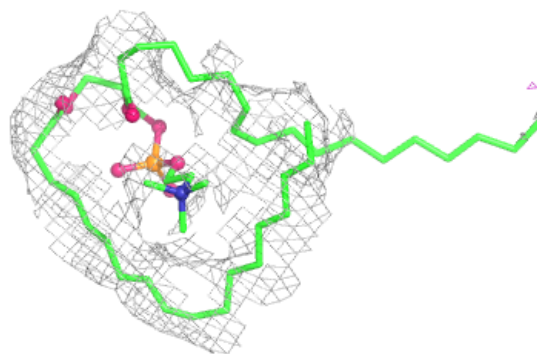
**Electron density around HEC N 303:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

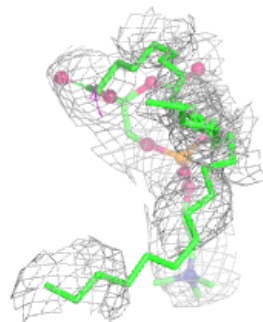
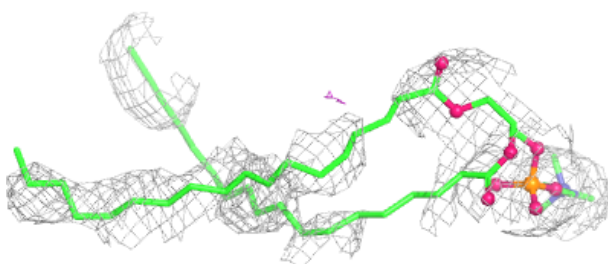
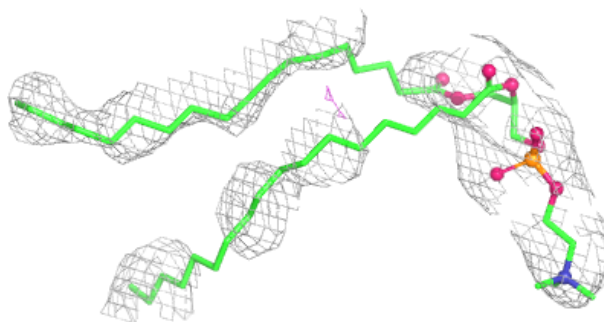


Electron density around OPC B 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

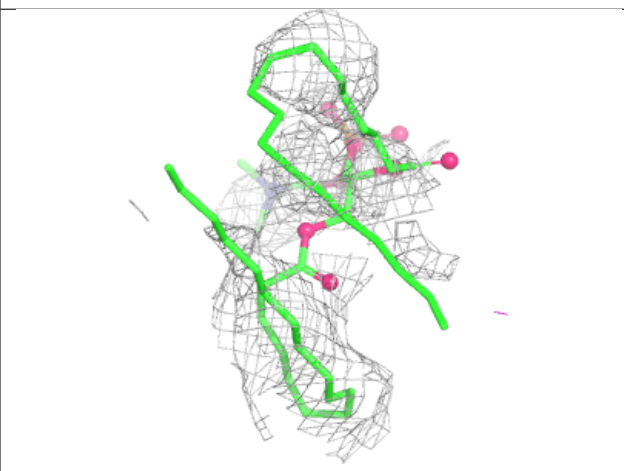
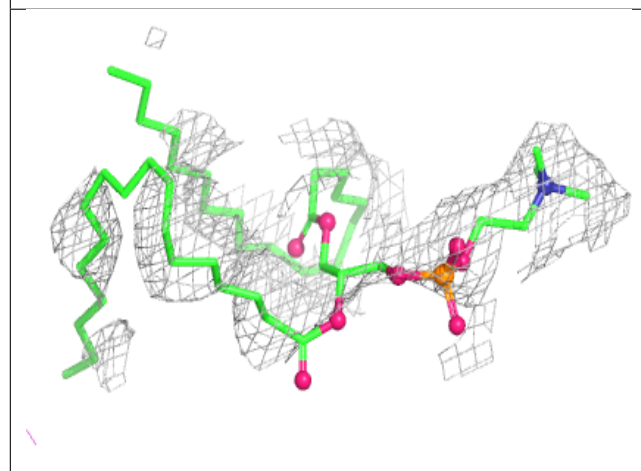
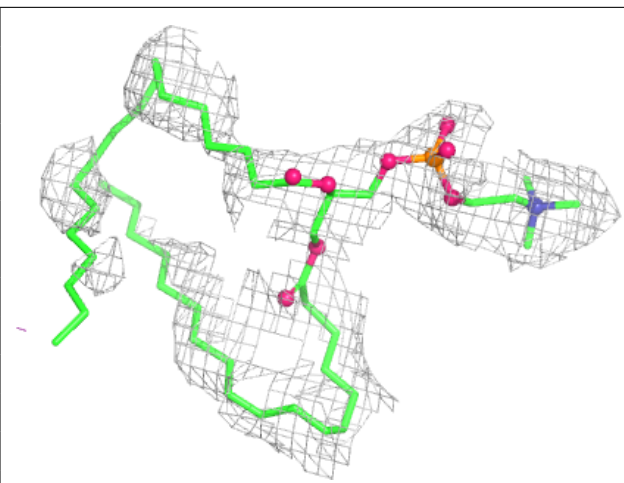
**Electron density around OPC C 306:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



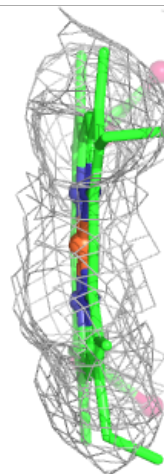
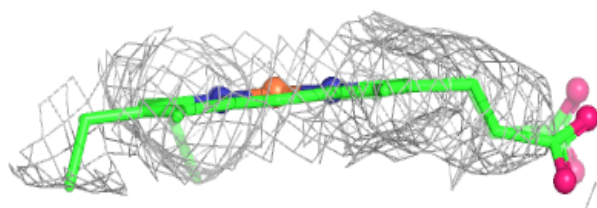
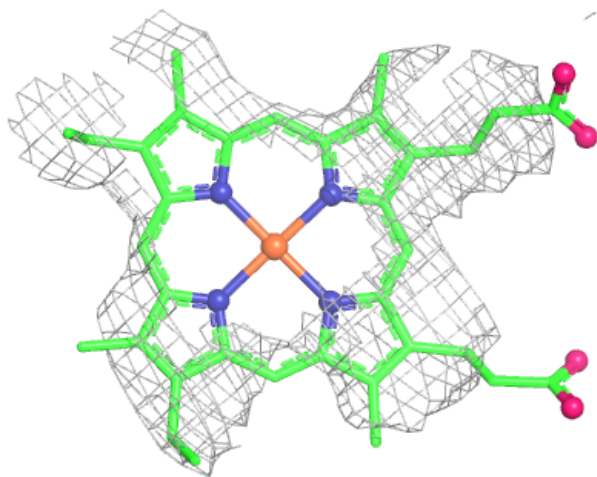
Electron density around OPC N 1305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



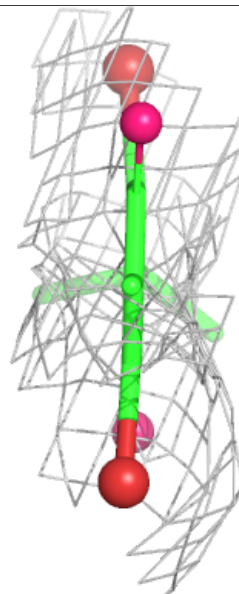
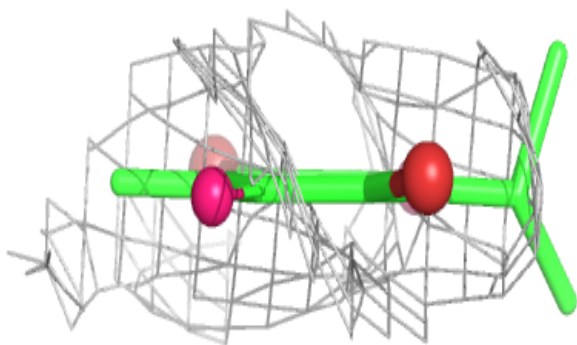
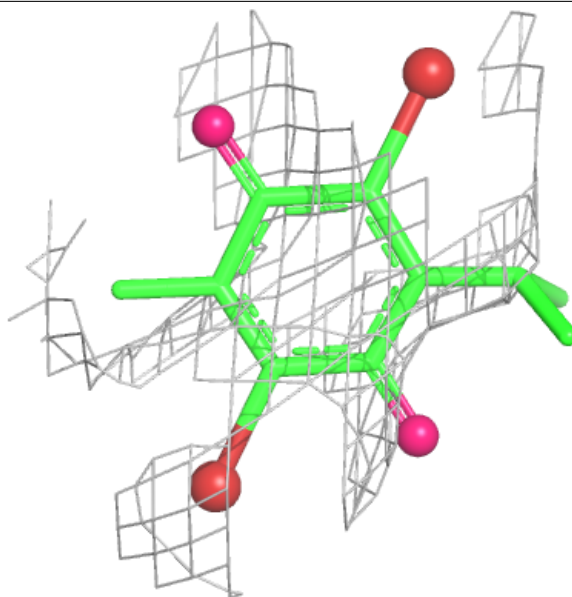
Electron density around HEC A 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



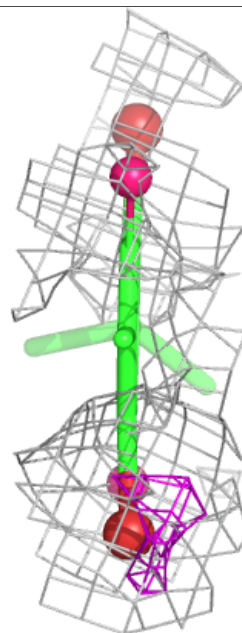
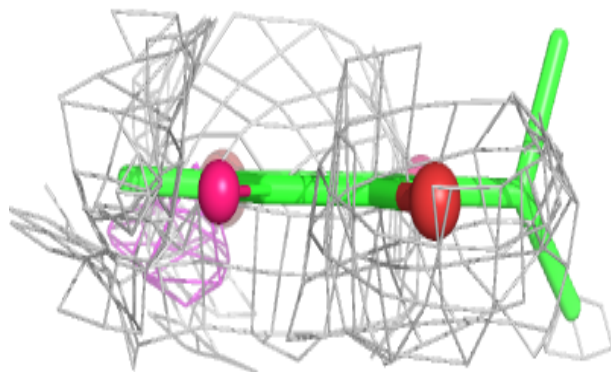
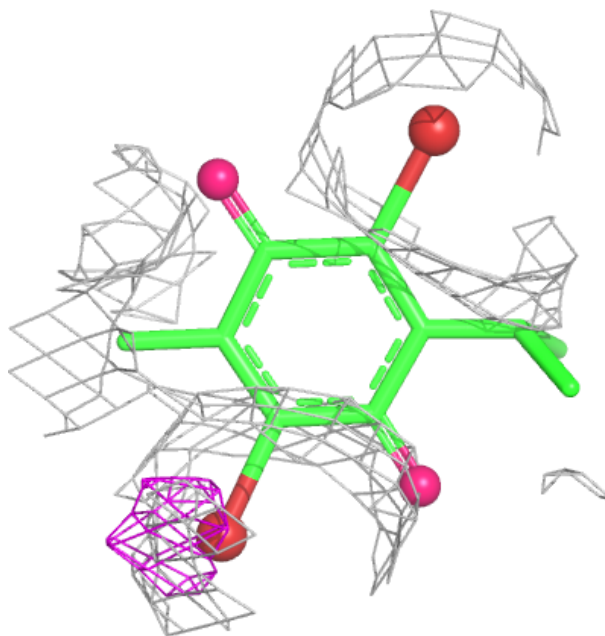
Electron density around BNT B 309:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



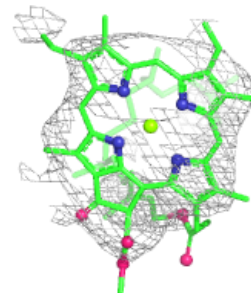
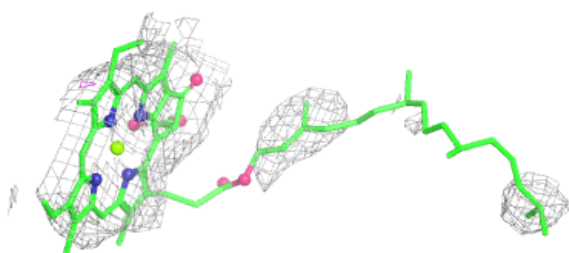
Electron density around BNT O 1309:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

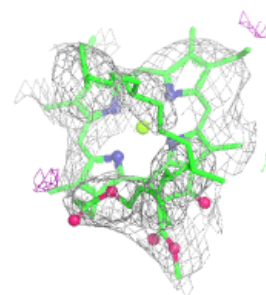
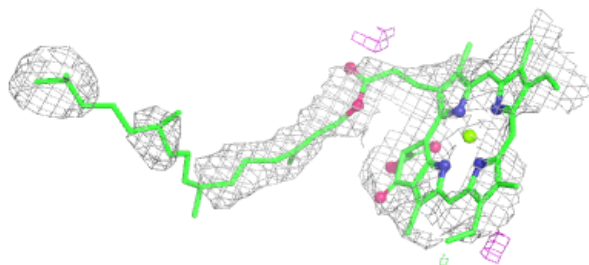
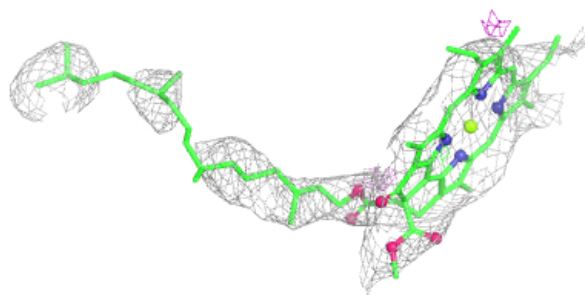


Electron density around CLA B 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

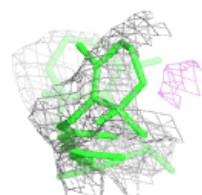
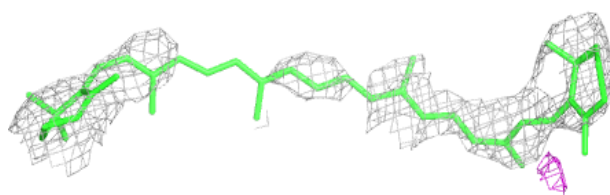
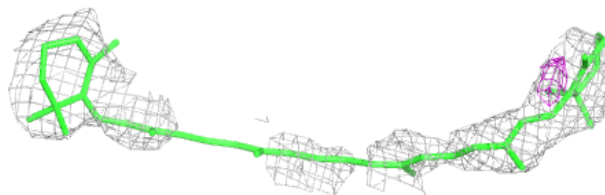
**Electron density around CLA O 1201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

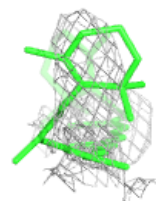
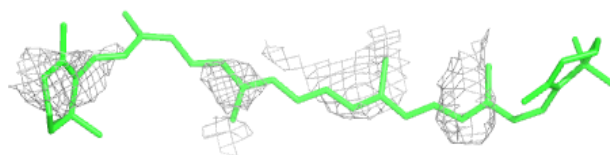
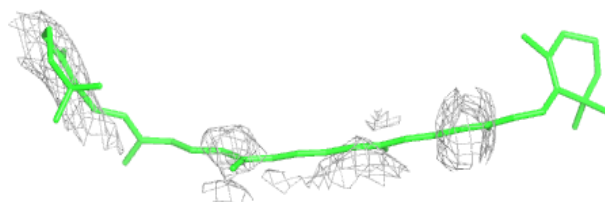


Electron density around BCR E 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

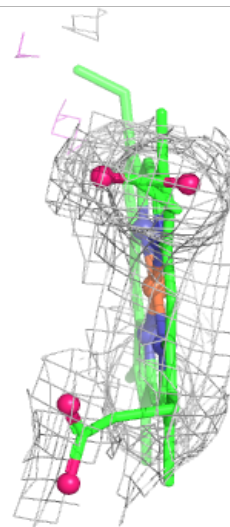
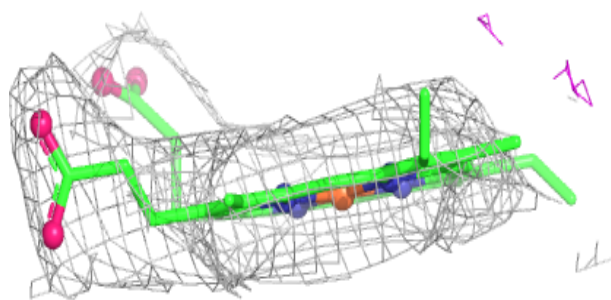
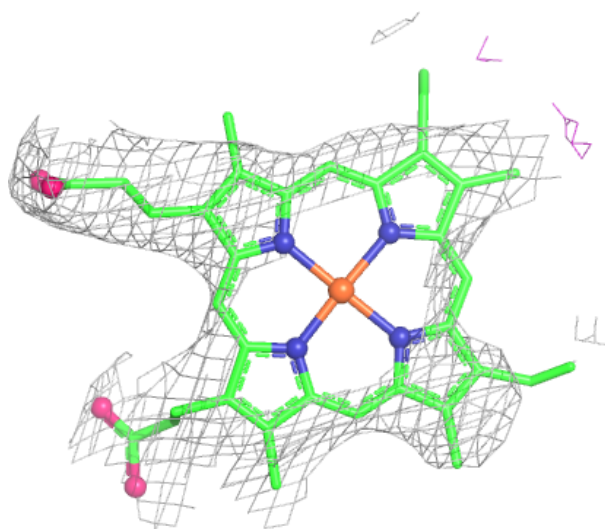
**Electron density around BCR R 1101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



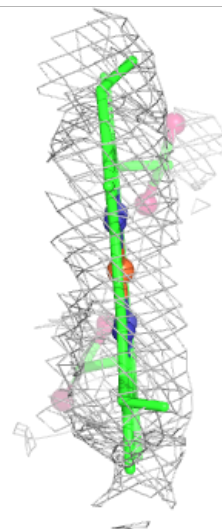
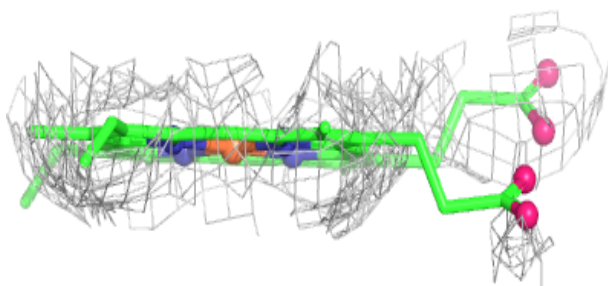
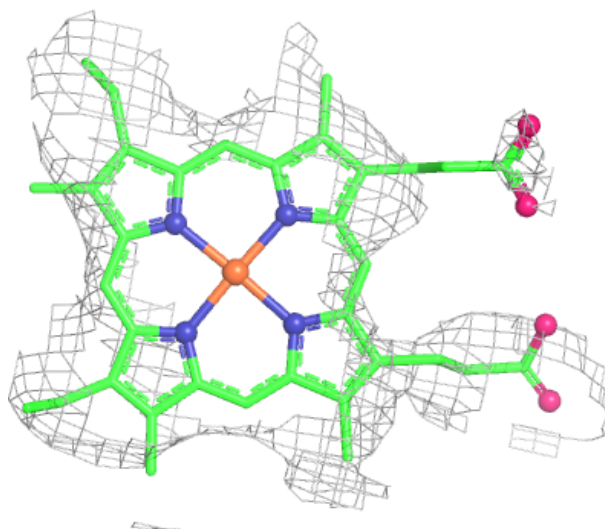
Electron density around HEC A 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



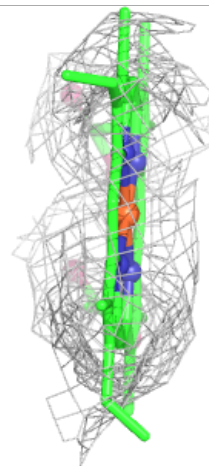
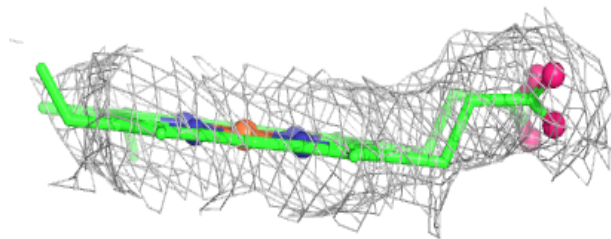
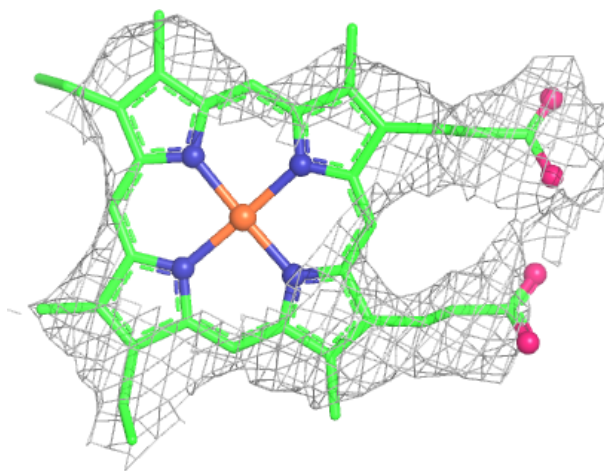
Electron density around HEC P 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



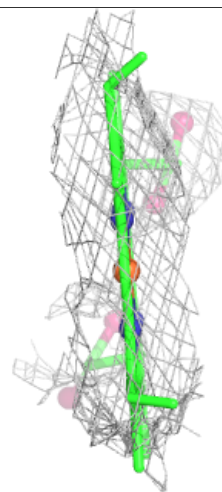
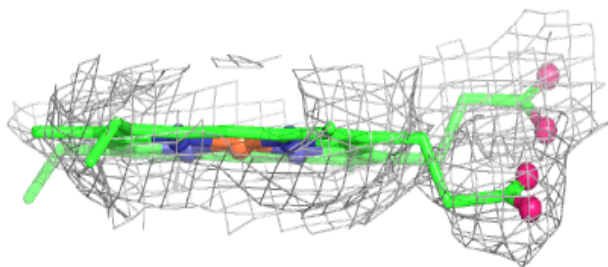
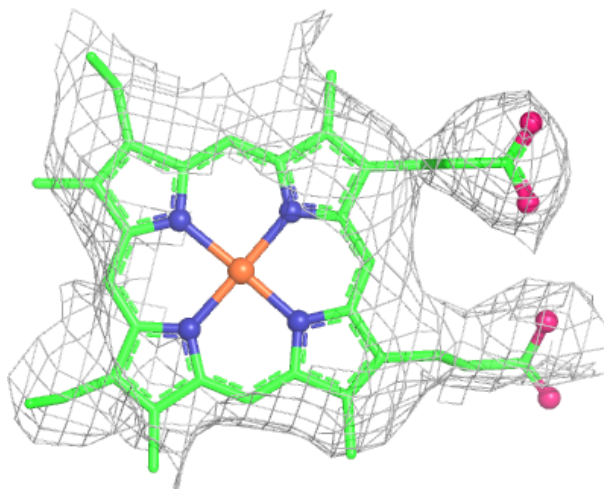
Electron density around HEC A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



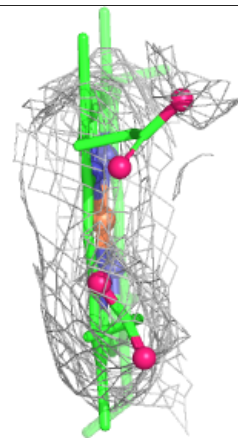
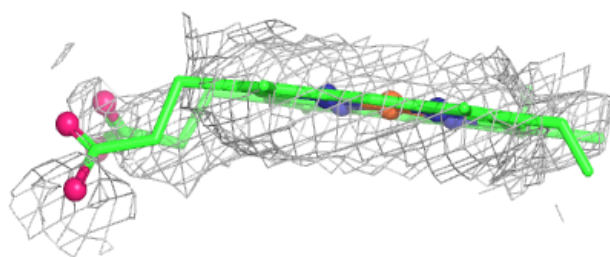
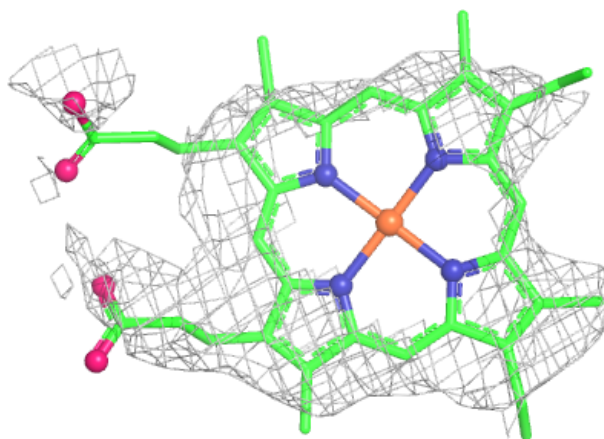
Electron density around HEC C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



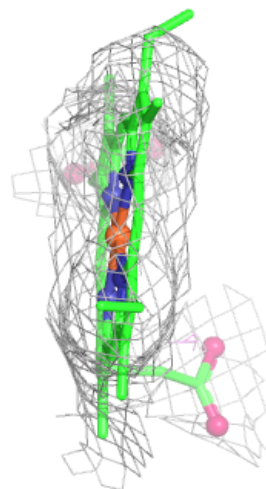
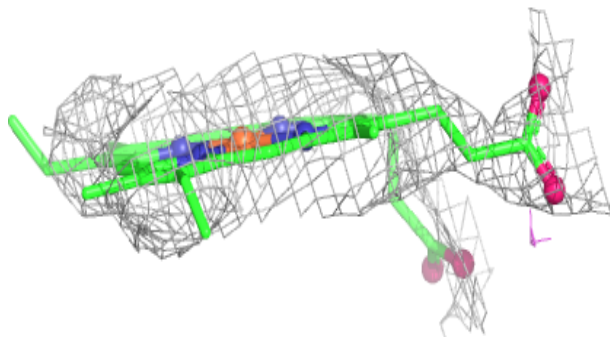
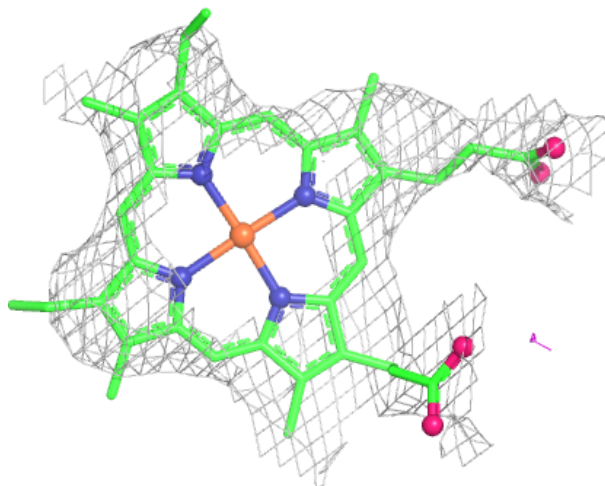
Electron density around HEC N 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC N 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.