Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 06:33 AM EDT

PDB ID	:	1BE3 / pdb_00001be3
Title	:	CYTOCHROME BC1 COMPLEX FROM BOVINE
Authors	:	Iwata, S.; Lee, J.W.; Okada, K.; Lee, J.K.; Iwata, M.; Ramaswamy, S.; Jap, B.K.
Deposited on	:	1998-05-19
Resolution	:	3.00 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 (i) 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 (1)) were used in the production of this report:

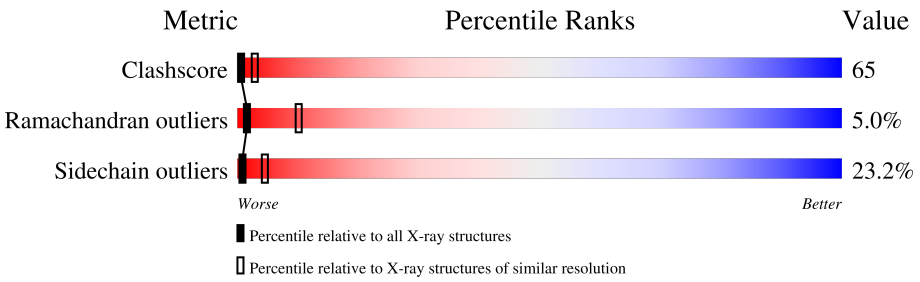
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	17% 50% 26% 7%
2	B	439	21% 46% 25% • 5%
3	C	379	22% 49% 26% •
4	D	241	23% 50% 22% 6%
5	E	196	20% 46% 28% 6%
6	F	110	25% 45% 23% • •
7	G	81	12% 56% 22% 10%
8	H	78	19% 40% 19% • 18%

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Mol	Chain	Length	Quality of chain
9	I	78	6% 21% 12% • 58%
10	J	62	31% 45% 21% •
11	K	56	12% 14% 12% 61%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 16222 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 BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3458	2161	609	668	20	0	0	0

- Molecule 2 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	419	3141	1972	556	606	7	0	0	0

- Molecule 3 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	379	3011	2018	472	502	19	0	0	0

- Molecule 4 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1919	1225	330	349	15	0	0	0

- Molecule 5 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1519	957	263	291	8	0	0	0

- Molecule 6 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	106	916	579	166	169	2	0	0	0

- Molecule 7 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	81	682	441	128	112	1	0	0	0

- Molecule 8 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	64	524	316	96	107	5	0	0	0

- Molecule 9 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	33	248	152	51	44	1	0	0	0

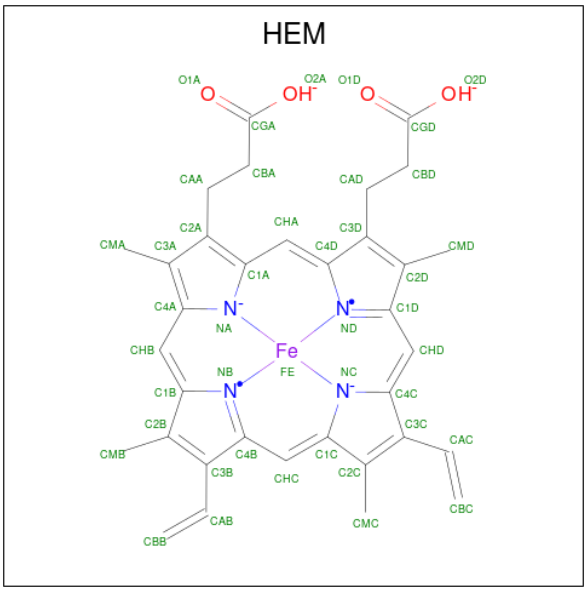
- Molecule 10 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	62	512	335	89	88	0	0	0

- Molecule 11 is a protein called CYTOCHROME BC1 COMPLEX.

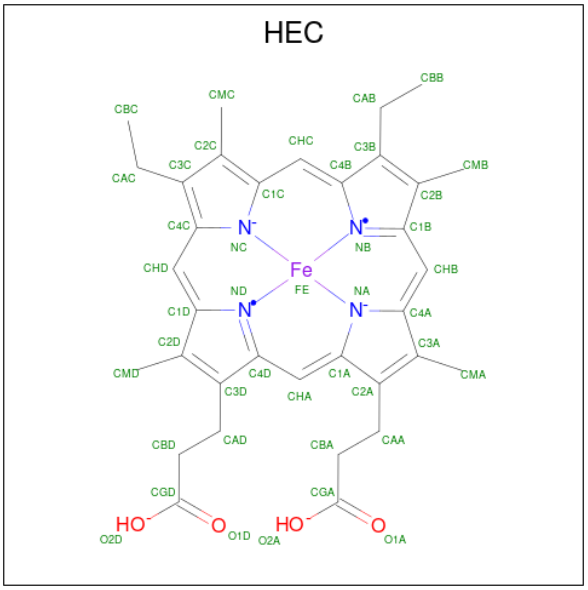
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	K	22	159	103	29	27	0	0	0

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



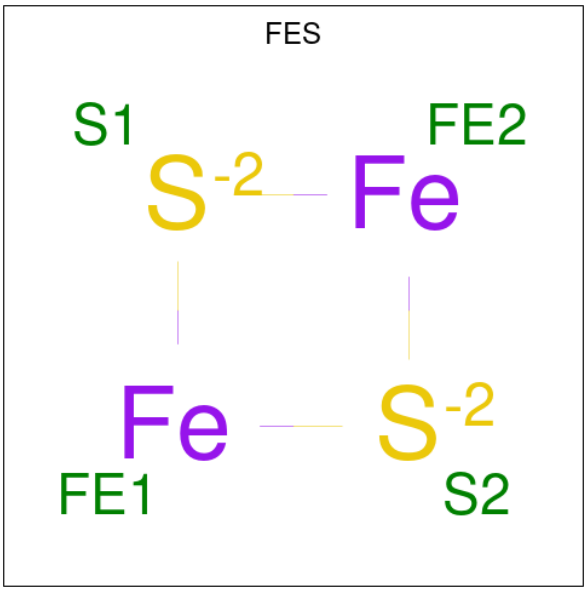
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0

- Molecule 13 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
13	D	1	43	34	1	4	4	0	0

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
14	E	1	4	2	2	0	0

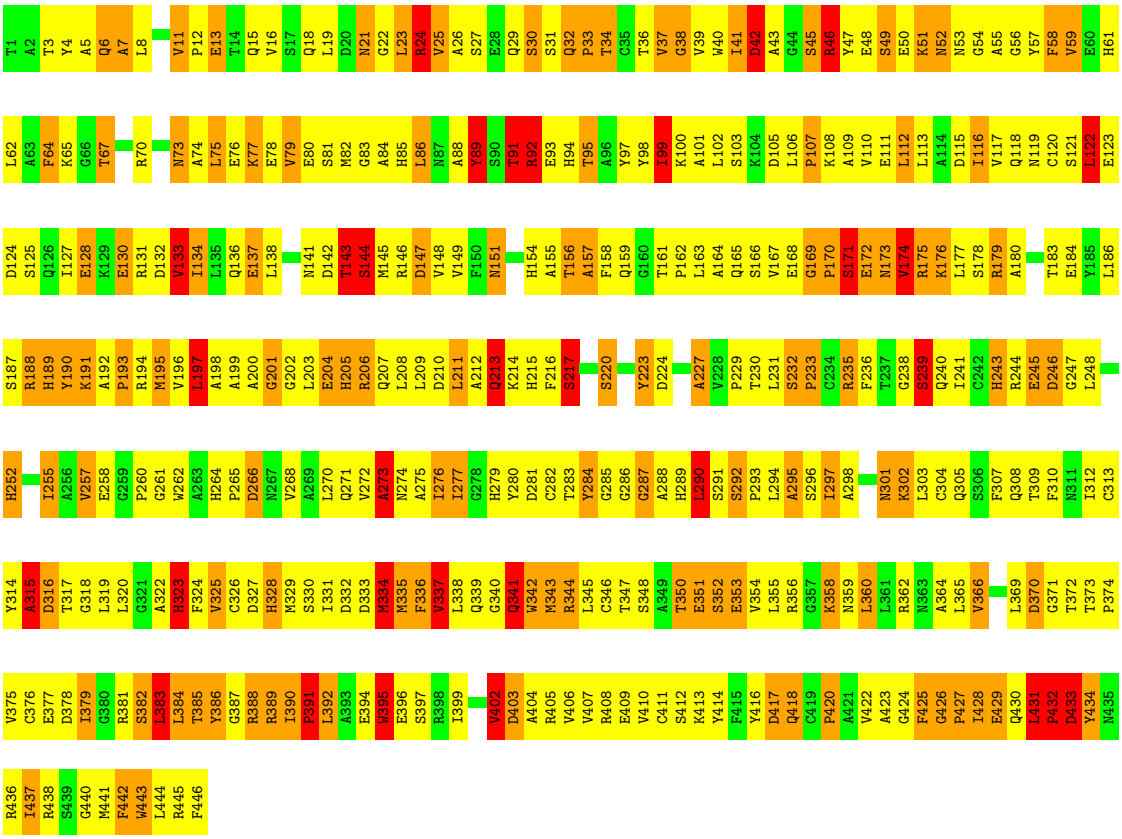
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

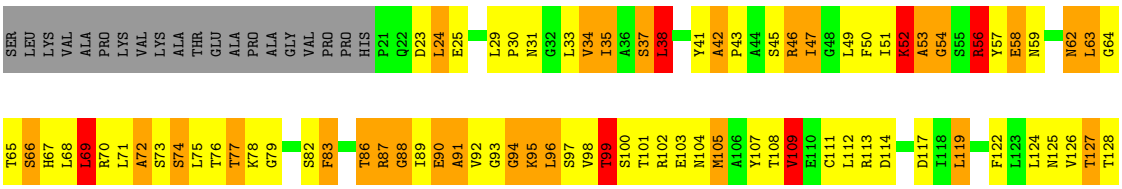
• Molecule 1: CYTOCHROME BC1 COMPLEX

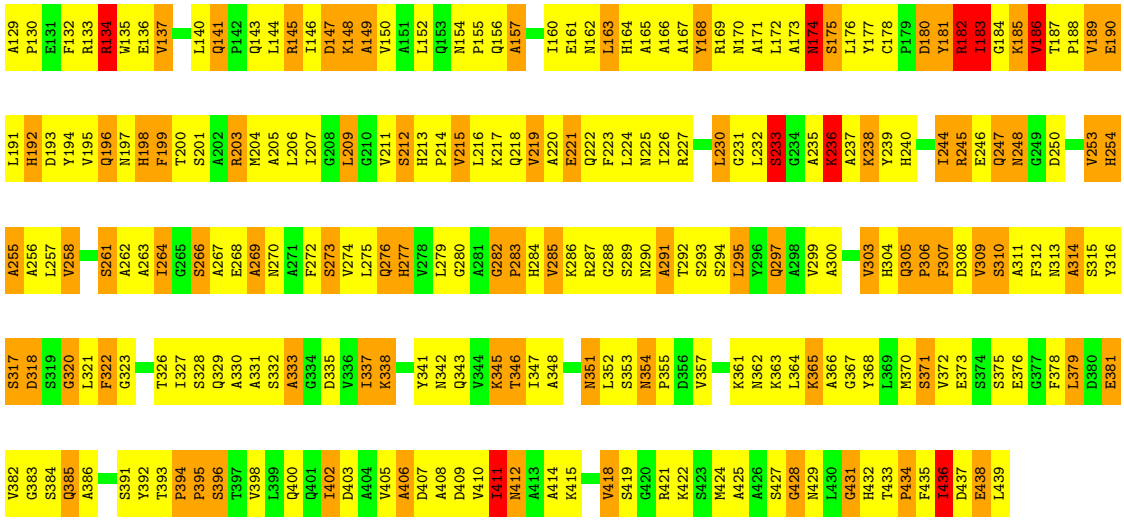
Chain A: 17% 50% 26% 7%



• Molecule 2: CYTOCHROME BC1 COMPLEX

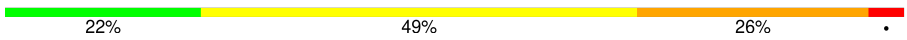
Chain B: 21% 46% 25% • 5%

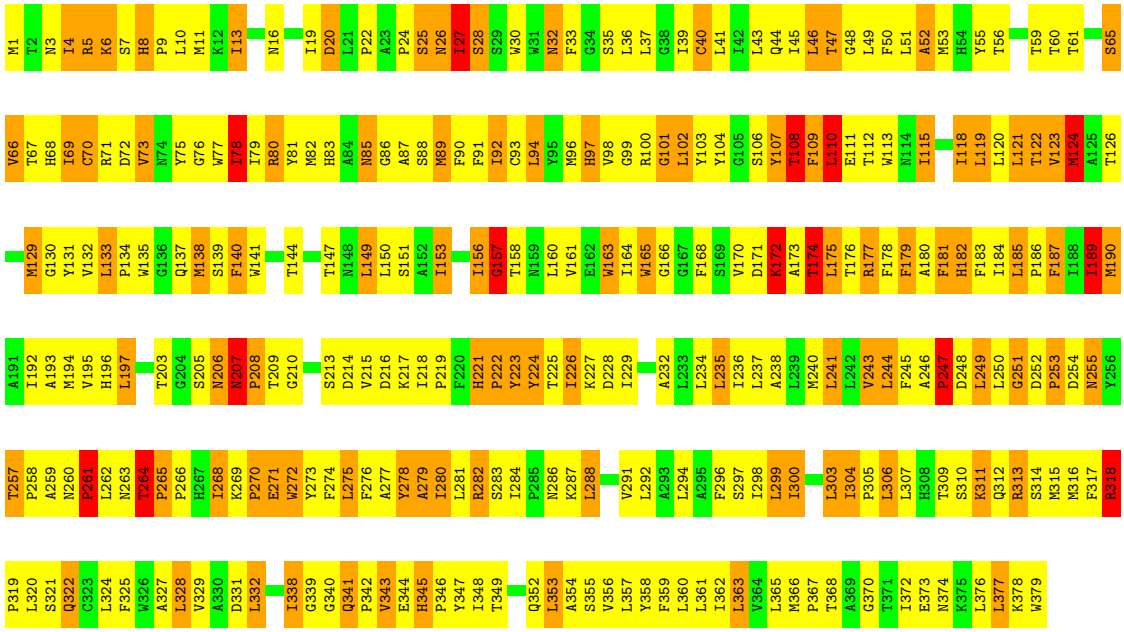




- Molecule 3: CYTOCHROME BC1 COMPLEX

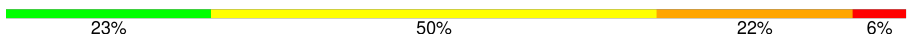
Chain C:

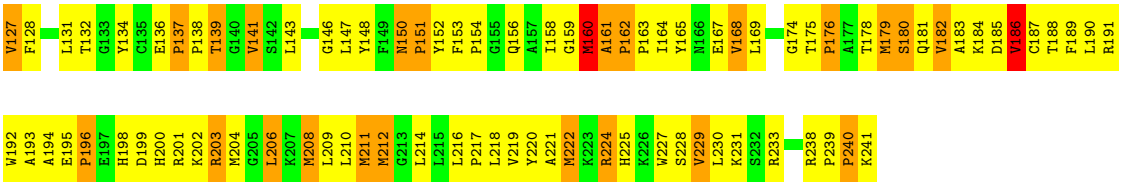




- Molecule 4: CYTOCHROME BC1 COMPLEX

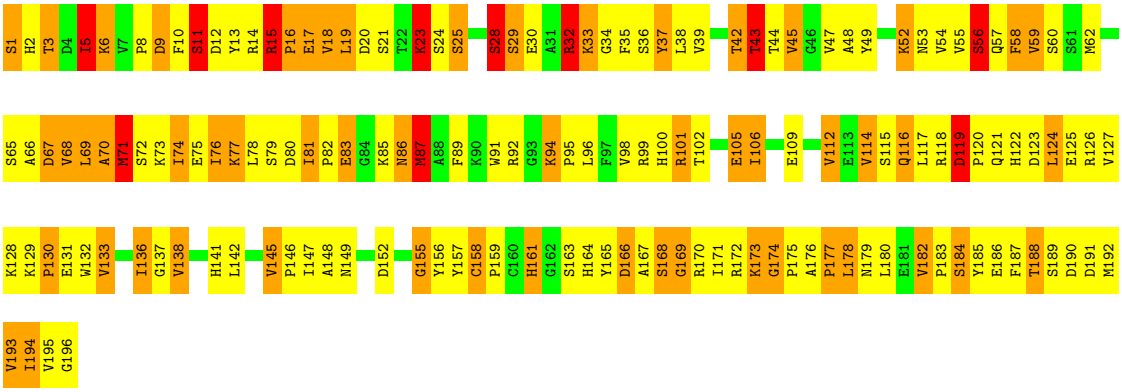
Chain D:





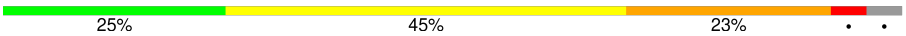
- Molecule 5: CYTOCHROME BC1 COMPLEX

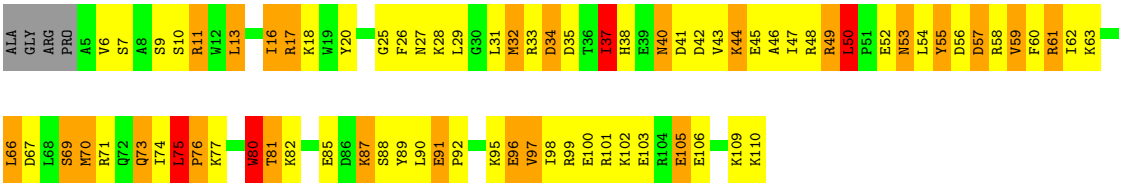
Chain E:



- Molecule 6: CYTOCHROME BC1 COMPLEX

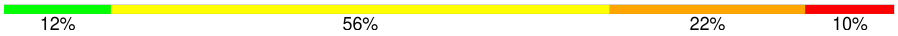
Chain F:

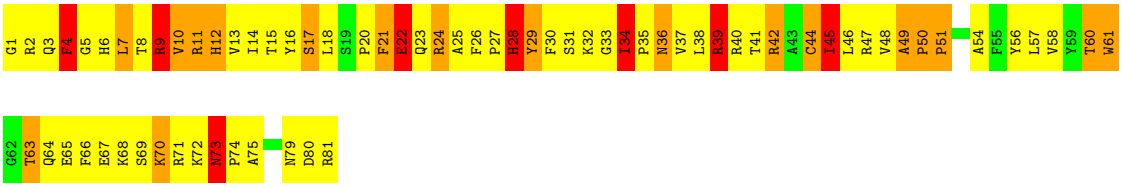




- Molecule 7: CYTOCHROME BC1 COMPLEX

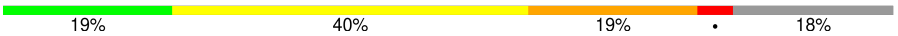
Chain G:

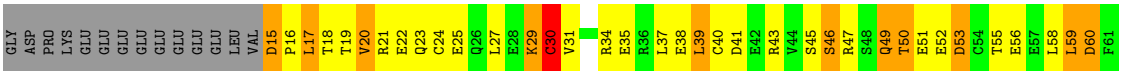


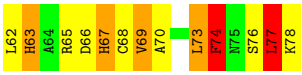


- Molecule 8: CYTOCHROME BC1 COMPLEX

Chain H:

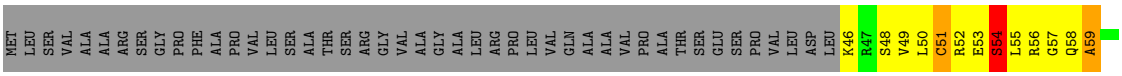






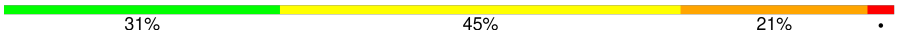
• Molecule 9: CYTOCHROME BC1 COMPLEX

Chain I:



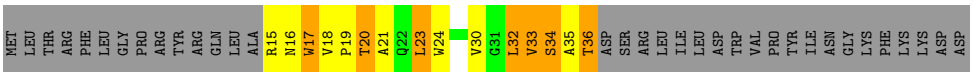
• Molecule 10: CYTOCHROME BC1 COMPLEX

Chain J:



• Molecule 11: CYTOCHROME BC1 COMPLEX

Chain K:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	211.20Å 211.20Å 339.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00	Depositor
% Data completeness (in resolution range)	81.7 (40.00-3.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.260 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16222	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, HEM, FES

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	0.82	6/3531 (0.2%)	2.10	151/4792 (3.2%)
2	B	0.78	4/3198 (0.1%)	2.03	100/4336 (2.3%)
3	C	0.88	8/3108 (0.3%)	2.00	96/4252 (2.3%)
4	D	0.73	4/1978 (0.2%)	1.84	54/2684 (2.0%)
5	E	0.72	2/1553 (0.1%)	1.92	52/2100 (2.5%)
6	F	0.70	0/935	2.00	29/1253 (2.3%)
7	G	0.78	1/704 (0.1%)	1.95	30/951 (3.2%)
8	H	0.74	4/529 (0.8%)	1.58	9/708 (1.3%)
9	I	0.78	0/250	2.07	11/335 (3.3%)
10	J	0.71	1/525 (0.2%)	1.68	12/707 (1.7%)
11	K	0.67	0/163	1.66	1/225 (0.4%)
All	All	0.79	30/16474 (0.2%)	1.98	545/22343 (2.4%)

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	14
2	B	0	17
3	C	0	8
4	D	0	5
5	E	0	5
6	F	0	5
7	G	0	2
8	H	0	1
All	All	0	57

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	LEU	C-O	8.77	1.34	1.23
3	C	174	THR	N-CA	-8.29	1.36	1.46
7	G	79	ASN	C-O	-8.13	1.15	1.23
3	C	280	ILE	CA-CB	-8.01	1.43	1.54
3	C	98	VAL	N-CA	-7.94	1.36	1.46
5	E	56	SER	C-O	7.46	1.33	1.24
2	B	436	ILE	CA-CB	7.36	1.62	1.54
4	D	101	ALA	CA-C	-7.32	1.43	1.52
4	D	26	ILE	N-CA	-7.27	1.38	1.46
8	H	77	LEU	C-O	-6.86	1.14	1.24
1	A	295	ALA	C-O	-6.78	1.16	1.24
2	B	436	ILE	CA-C	-6.69	1.44	1.52
8	H	77	LEU	C-N	6.46	1.42	1.33
1	A	252	HIS	CG-CD2	6.43	1.43	1.35
10	J	42	ILE	C-N	6.26	1.41	1.33
3	C	122	THR	N-CA	6.23	1.54	1.46
8	H	30	CYS	CA-C	6.20	1.60	1.52
1	A	252	HIS	CG-ND1	-6.16	1.31	1.38
1	A	343	MET	CA-C	6.16	1.60	1.52
2	B	261	SER	C-O	-6.09	1.15	1.23
8	H	30	CYS	C-O	-6.07	1.16	1.24
3	C	261	PRO	N-CD	-6.04	1.39	1.47
3	C	121	LEU	C-N	-6.03	1.25	1.34
3	C	102	LEU	C-O	-6.01	1.17	1.24
1	A	238	GLY	C-O	-6.00	1.15	1.23
4	D	26	ILE	CA-C	5.89	1.60	1.52
4	D	23	HIS	CA-CB	5.86	1.62	1.53
2	B	50	PHE	CA-C	-5.63	1.45	1.52
3	C	97	HIS	C-N	5.45	1.40	1.33
5	E	60	SER	CA-C	-5.22	1.46	1.52

All (545) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	196	HIS	CA-CB-CG	13.98	127.78	113.80
3	C	265	PRO	CB-CA-C	13.07	126.87	110.92
3	C	206	ASN	OD1-CG-ND2	12.37	134.97	122.60
1	A	268	VAL	N-CA-C	-12.07	100.89	112.96
5	E	182	VAL	N-CA-C	11.03	118.47	107.55
5	E	14	ARG	CD-NE-CZ	-10.43	109.80	124.40
5	E	119	ASP	CA-CB-CG	10.42	123.02	112.60
8	H	74	PHE	CA-CB-CG	-10.30	103.50	113.80
4	D	7	PRO	N-CA-C	10.12	123.05	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	431	LEU	CA-C-O	9.93	128.23	119.59
5	E	15	ARG	NE-CZ-NH2	9.90	128.11	119.20
6	F	49	ARG	CD-NE-CZ	9.85	138.19	124.40
9	I	75	SER	N-CA-C	9.80	120.87	107.73
2	B	436	ILE	N-CA-CB	-9.65	99.80	110.51
2	B	50	PHE	CA-CB-CG	9.51	123.31	113.80
7	G	28	HIS	N-CA-CB	9.44	120.93	110.35
3	C	245	PHE	CA-CB-CG	9.42	123.22	113.80
2	B	56	ARG	CD-NE-CZ	9.38	137.53	124.40
6	F	27	ASN	CA-CB-CG	-9.20	103.40	112.60
3	C	207	ASN	CA-CB-CG	9.19	121.79	112.60
1	A	235	ARG	NE-CZ-NH2	9.17	127.45	119.20
2	B	254	HIS	CA-CB-CG	9.15	122.95	113.80
1	A	45	SER	CA-C-O	9.07	129.11	119.14
2	B	54	GLY	N-CA-C	-9.06	101.92	112.79
3	C	153	ILE	CA-C-N	9.03	128.37	118.97
3	C	153	ILE	C-N-CA	9.03	128.37	118.97
2	B	109	VAL	O-C-N	-8.85	115.01	122.97
3	C	181	PHE	CA-C-N	8.75	131.82	120.44
3	C	181	PHE	C-N-CA	8.75	131.82	120.44
3	C	235	LEU	CA-C-O	-8.75	111.82	121.00
3	C	180	ALA	CA-C-O	8.73	129.67	120.42
7	G	4	PHE	CA-CB-CG	-8.71	105.09	113.80
1	A	413	LYS	O-C-N	8.53	131.87	122.15
10	J	42	ILE	CA-C-O	8.48	131.38	120.78
4	D	97	ASN	CA-C-N	8.38	130.32	119.84
4	D	97	ASN	C-N-CA	8.38	130.32	119.84
2	B	157	ALA	CA-C-O	-8.31	112.09	120.82
3	C	26	ASN	CA-C-O	-8.31	112.05	121.19
1	A	432	PRO	N-CA-CB	8.29	111.95	103.25
2	B	148	LYS	CA-C-N	8.26	131.34	120.28
2	B	148	LYS	C-N-CA	8.26	131.34	120.28
1	A	235	ARG	NE-CZ-NH1	-8.19	113.31	121.50
2	B	245	ARG	CD-NE-CZ	-8.18	112.95	124.40
7	G	26	PHE	CA-CB-CG	8.10	121.89	113.80
2	B	232	LEU	CA-C-N	8.04	131.38	120.44
2	B	232	LEU	C-N-CA	8.04	131.38	120.44
1	A	442	PHE	CA-C-O	-8.03	112.49	121.40
2	B	317	SER	N-CA-C	8.01	119.64	111.07
1	A	337	VAL	CA-C-O	-7.97	112.66	120.95
3	C	80	ARG	NE-CZ-NH1	-7.97	113.53	121.50
1	A	315	ALA	CA-C-O	7.76	131.61	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	14	PHE	CA-CB-CG	7.76	121.56	113.80
2	B	134	ARG	NE-CZ-NH2	7.70	126.13	119.20
1	A	433	ASP	CA-C-O	-7.67	112.66	121.72
1	A	390	ILE	CA-C-O	7.63	130.17	119.95
2	B	134	ARG	NE-CZ-NH1	-7.62	113.89	121.50
1	A	46	ARG	NE-CZ-NH2	7.60	126.04	119.20
2	B	83	PHE	CA-CB-CG	-7.59	106.21	113.80
1	A	223	TYR	CA-C-N	7.58	132.73	120.60
1	A	223	TYR	C-N-CA	7.58	132.73	120.60
1	A	343	MET	N-CA-CB	7.55	121.20	109.94
3	C	280	ILE	CA-C-N	7.51	130.20	120.44
3	C	280	ILE	C-N-CA	7.51	130.20	120.44
4	D	49	ARG	NE-CZ-NH1	-7.50	114.00	121.50
2	B	189	VAL	N-CA-CB	7.50	118.49	110.62
1	A	417	ASP	CA-CB-CG	-7.48	105.12	112.60
1	A	431	LEU	O-C-N	-7.48	115.64	121.47
2	B	62	ASN	CA-CB-CG	-7.45	105.15	112.60
6	F	27	ASN	OD1-CG-ND2	7.42	130.02	122.60
4	D	83	ARG	CA-C-N	7.36	129.03	119.84
4	D	83	ARG	C-N-CA	7.36	129.03	119.84
2	B	255	ALA	O-C-N	-7.31	114.79	123.27
7	G	6	HIS	CA-C-N	-7.25	110.77	120.63
7	G	6	HIS	C-N-CA	-7.25	110.77	120.63
1	A	230	THR	N-CA-C	-7.24	103.92	112.89
1	A	418	GLN	CA-C-N	-7.18	111.15	121.20
1	A	418	GLN	C-N-CA	-7.18	111.15	121.20
3	C	177	ARG	NE-CZ-NH2	-7.18	112.74	119.20
1	A	169	GLY	CA-C-N	7.17	128.81	119.84
1	A	169	GLY	C-N-CA	7.17	128.81	119.84
1	A	268	VAL	CA-C-O	7.12	125.27	119.29
4	D	86	LYS	N-CA-C	7.11	120.01	110.35
4	D	30	PHE	O-C-N	7.09	129.75	122.09
5	E	58	PHE	CA-CB-CG	7.08	120.88	113.80
2	B	394	PRO	CA-C-N	7.06	126.31	118.97
2	B	394	PRO	C-N-CA	7.06	126.31	118.97
5	E	52	LYS	CA-C-N	-7.02	111.31	120.44
5	E	52	LYS	C-N-CA	-7.02	111.31	120.44
6	F	60	PHE	CA-CB-CG	-7.01	106.79	113.80
5	E	194	ILE	N-CA-C	7.01	116.80	106.85
1	A	151	ASN	CA-CB-CG	7.01	119.61	112.60
7	G	50	PRO	N-CA-C	6.99	119.23	110.70
7	G	12	HIS	CA-C-N	-6.98	113.47	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	12	HIS	C-N-CA	-6.98	113.47	123.11
5	E	15	ARG	NH1-CZ-NH2	-6.96	110.25	119.30
2	B	119	LEU	N-CA-C	6.93	118.83	111.28
2	B	431	GLY	N-CA-C	-6.92	106.08	114.66
2	B	277	HIS	N-CA-C	6.91	120.59	111.75
6	F	53	ASN	CA-C-O	6.90	128.66	121.07
3	C	268	ILE	CB-CA-C	-6.89	102.19	111.15
4	D	160	MET	N-CA-C	6.89	120.18	107.99
3	C	235	LEU	O-C-N	6.88	129.19	122.03
2	B	250	ASP	CA-C-N	6.88	129.50	120.28
2	B	250	ASP	C-N-CA	6.88	129.50	120.28
3	C	78	ILE	N-CA-CB	6.83	119.31	110.57
6	F	61	ARG	CA-CB-CG	6.82	127.73	114.10
1	A	21	ASN	OD1-CG-ND2	6.71	129.31	122.60
3	C	303	LEU	N-CA-CB	6.70	120.38	110.53
2	B	45	SER	O-C-N	-6.69	115.39	123.29
8	H	67	HIS	CA-CB-CG	6.67	120.47	113.80
1	A	273	ALA	CA-C-O	-6.63	113.45	120.55
1	A	403	ASP	CA-CB-CG	6.62	119.22	112.60
6	F	57	ASP	CA-CB-CG	-6.61	105.99	112.60
4	D	10	TYR	CA-CB-CG	-6.60	102.03	113.90
1	A	335	MET	CA-C-O	6.59	127.46	119.49
1	A	230	THR	CA-C-N	6.58	131.95	122.08
1	A	230	THR	C-N-CA	6.58	131.95	122.08
1	A	133	VAL	CA-C-O	6.57	127.74	120.71
2	B	167	ALA	O-C-N	-6.56	113.64	122.43
2	B	167	ALA	CA-C-O	6.55	127.43	119.38
5	E	145	VAL	CB-CA-C	-6.55	103.25	110.52
1	A	214	LYS	CA-C-O	-6.54	114.45	122.36
1	A	295	ALA	CA-C-O	6.53	127.89	120.90
3	C	168	PHE	CA-C-O	6.50	126.56	119.15
3	C	140	PHE	N-CA-C	6.50	118.44	111.36
3	C	66	VAL	N-CA-CB	6.46	117.68	110.51
2	B	381	GLU	O-C-N	6.45	128.96	122.12
6	F	27	ASN	CA-C-N	6.44	129.56	120.28
6	F	27	ASN	C-N-CA	6.44	129.56	120.28
3	C	78	ILE	CB-CA-C	-6.44	103.59	112.02
2	B	42	ALA	CA-C-N	6.43	127.26	120.12
2	B	42	ALA	C-N-CA	6.43	127.26	120.12
1	A	390	ILE	CA-C-N	6.43	127.87	119.84
1	A	390	ILE	C-N-CA	6.43	127.87	119.84
1	A	42	ASP	N-CA-C	6.42	120.73	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	50	LEU	CA-C-O	-6.41	113.69	120.23
3	C	216	ASP	N-CA-C	6.41	118.31	109.54
1	A	276	ILE	N-CA-C	6.40	116.55	110.53
2	B	53	ALA	CA-C-O	6.40	127.60	120.43
4	D	109	LEU	CA-C-N	6.40	126.97	120.38
4	D	109	LEU	C-N-CA	6.40	126.97	120.38
2	B	163	LEU	O-C-N	-6.37	115.41	122.03
3	C	241	LEU	CA-C-O	6.37	127.51	120.63
4	D	168	VAL	N-CA-CB	6.36	121.18	110.56
2	B	69	LEU	CA-C-N	6.36	128.80	120.28
2	B	69	LEU	C-N-CA	6.36	128.80	120.28
2	B	174	ASN	OD1-CG-ND2	6.35	128.95	122.60
3	C	232	ALA	CA-C-O	6.34	127.14	120.42
1	A	392	LEU	CA-C-O	6.34	127.47	120.63
1	A	390	ILE	N-CA-CB	6.32	120.06	111.21
5	E	29	SER	N-CA-C	6.31	119.83	111.75
1	A	189	HIS	CA-CB-CG	6.31	120.11	113.80
6	F	34	ASP	CA-CB-CG	-6.30	106.30	112.60
7	G	50	PRO	N-CA-CB	6.29	109.19	103.08
3	C	108	THR	N-CA-C	-6.28	104.54	111.82
1	A	11	VAL	CA-C-N	6.28	127.68	119.84
1	A	11	VAL	C-N-CA	6.28	127.68	119.84
5	E	182	VAL	CB-CA-C	-6.27	103.64	111.04
1	A	276	ILE	CA-C-N	6.26	128.97	120.77
1	A	276	ILE	C-N-CA	6.26	128.97	120.77
1	A	276	ILE	CA-C-O	-6.25	114.11	121.05
1	A	95	THR	CA-C-O	-6.25	114.35	121.72
1	A	13	GLU	N-CA-CB	6.25	119.19	110.26
1	A	147	ASP	CA-CB-CG	-6.25	106.35	112.60
1	A	92	ARG	CD-NE-CZ	6.23	133.12	124.40
2	B	327	ILE	CB-CA-C	-6.23	101.08	111.29
3	C	107	TYR	N-CA-C	-6.21	105.57	113.02
3	C	123	VAL	CA-C-N	6.20	128.92	120.54
3	C	123	VAL	C-N-CA	6.20	128.92	120.54
1	A	38	GLY	CA-C-O	6.20	126.83	121.19
7	G	36	ASN	CA-CB-CG	6.20	118.80	112.60
6	F	50	LEU	O-C-N	6.19	130.06	121.64
10	J	55	ILE	O-C-N	-6.18	116.15	122.14
1	A	24	ARG	CB-CA-C	6.17	119.94	109.75
1	A	316	ASP	N-CA-C	6.17	120.54	112.89
2	B	198	HIS	CA-CB-CG	-6.17	107.63	113.80
5	E	14	ARG	NH1-CZ-NH2	6.16	127.30	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	LEU	CA-C-N	-6.11	114.29	122.72
1	A	23	LEU	C-N-CA	-6.11	114.29	122.72
1	A	434	TYR	N-CA-C	-6.10	104.71	111.36
1	A	328	HIS	CA-C-N	6.10	132.41	122.65
1	A	328	HIS	C-N-CA	6.10	132.41	122.65
1	A	391	PRO	CA-C-N	6.10	128.74	120.38
1	A	391	PRO	C-N-CA	6.10	128.74	120.38
5	E	56	SER	O-C-N	-6.10	114.26	122.43
3	C	354	ALA	CA-C-N	-6.10	112.60	120.65
3	C	354	ALA	C-N-CA	-6.10	112.60	120.65
7	G	11	ARG	NE-CZ-NH2	-6.09	113.72	119.20
2	B	403	ASP	CA-CB-CG	-6.09	106.51	112.60
5	E	14	ARG	CA-C-N	-6.09	115.20	123.96
5	E	14	ARG	C-N-CA	-6.09	115.20	123.96
6	F	31	LEU	CA-C-O	-6.08	114.94	121.94
2	B	303	VAL	N-CA-C	6.08	118.54	109.17
3	C	282	ARG	CD-NE-CZ	-6.08	115.88	124.40
3	C	13	ILE	CB-CA-C	-6.08	103.93	112.14
5	E	59	VAL	CB-CA-C	-6.08	103.07	111.65
1	A	64	PHE	CA-C-O	-6.08	112.55	119.78
1	A	277	ILE	CB-CA-C	-6.07	103.93	111.70
1	A	366	VAL	N-CA-CB	6.07	120.02	110.31
1	A	213	GLN	CB-CG-CD	6.06	122.90	112.60
1	A	395	TRP	CD2-CE2-CZ2	-6.05	116.35	122.40
1	A	67	THR	CA-C-O	-6.04	113.11	120.54
4	D	26	ILE	N-CA-CB	6.04	117.61	110.55
2	B	62	ASN	CA-C-O	6.03	125.42	118.97
7	G	49	ALA	CA-C-N	6.02	126.58	120.38
7	G	49	ALA	C-N-CA	6.02	126.58	120.38
4	D	120	ARG	CD-NE-CZ	6.01	132.82	124.40
5	E	11	SER	CA-C-O	-5.99	114.01	121.02
1	A	290	LEU	CA-C-O	5.99	129.07	120.51
1	A	220	SER	N-CA-C	5.98	118.31	109.69
4	D	38	SER	CA-C-N	5.96	128.59	120.54
4	D	38	SER	C-N-CA	5.96	128.59	120.54
5	E	32	ARG	NE-CZ-NH1	-5.95	115.55	121.50
1	A	323	HIS	CA-C-N	-5.94	113.35	122.62
1	A	323	HIS	C-N-CA	-5.94	113.35	122.62
2	B	199	PHE	CA-CB-CG	5.94	119.74	113.80
1	A	403	ASP	N-CA-C	-5.93	101.70	110.48
3	C	322	GLN	CA-C-N	5.93	128.16	120.44
3	C	322	GLN	C-N-CA	5.93	128.16	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	VAL	CB-CA-C	-5.92	101.42	110.95
4	D	150	ASN	CA-C-N	5.92	125.62	119.82
4	D	150	ASN	C-N-CA	5.92	125.62	119.82
2	B	254	HIS	CA-C-O	-5.91	114.45	120.71
4	D	238	ARG	CA-C-N	5.90	126.46	120.38
4	D	238	ARG	C-N-CA	5.90	126.46	120.38
1	A	425	PHE	CA-C-O	-5.89	113.01	120.20
7	G	21	PHE	O-C-N	-5.89	115.33	122.22
5	E	169	GLY	CA-C-N	5.89	129.12	120.82
5	E	169	GLY	C-N-CA	5.89	129.12	120.82
4	D	26	ILE	CB-CA-C	-5.89	104.44	111.97
3	C	180	ALA	O-C-N	-5.88	115.45	122.15
3	C	318	ARG	CA-CB-CG	5.88	125.86	114.10
1	A	336	PHE	CA-C-N	5.86	128.49	120.46
1	A	336	PHE	C-N-CA	5.86	128.49	120.46
1	A	213	GLN	OE1-CD-NE2	-5.84	116.75	122.60
9	I	72	VAL	CA-C-N	5.84	127.14	119.84
9	I	72	VAL	C-N-CA	5.84	127.14	119.84
1	A	188	ARG	CA-C-O	-5.83	113.52	120.10
2	B	53	ALA	CA-C-N	-5.82	115.81	122.85
2	B	53	ALA	C-N-CA	-5.82	115.81	122.85
1	A	402	VAL	N-CA-C	5.82	121.44	109.34
3	C	101	GLY	O-C-N	5.82	127.77	122.19
2	B	309	VAL	CA-C-O	5.81	125.84	120.96
2	B	310	SER	CA-C-O	5.81	127.69	120.54
4	D	74	PRO	CA-C-N	5.81	129.15	120.31
4	D	74	PRO	C-N-CA	5.81	129.15	120.31
3	C	16	ASN	CA-C-N	5.81	129.89	120.60
3	C	16	ASN	C-N-CA	5.81	129.89	120.60
2	B	253	VAL	CA-C-N	-5.80	114.51	122.93
2	B	253	VAL	C-N-CA	-5.80	114.51	122.93
1	A	161	THR	CA-C-N	5.80	126.20	119.47
1	A	161	THR	C-N-CA	5.80	126.20	119.47
1	A	91	THR	O-C-N	-5.80	116.46	122.84
10	J	42	ILE	O-C-N	-5.79	115.33	122.57
1	A	32	GLN	CA-C-N	5.79	124.99	118.97
1	A	32	GLN	C-N-CA	5.79	124.99	118.97
7	G	11	ARG	NH1-CZ-NH2	5.78	126.82	119.30
2	B	91	ALA	CA-C-N	5.78	129.44	122.16
2	B	91	ALA	C-N-CA	5.78	129.44	122.16
1	A	89	TYR	CA-CB-CG	5.78	124.30	113.90
5	E	133	VAL	CA-C-O	5.77	126.39	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	48	ALA	O-C-N	5.76	128.22	122.12
9	I	68	VAL	CB-CA-C	-5.75	102.06	110.81
2	B	86	THR	N-CA-CB	5.75	118.31	109.91
1	A	364	ALA	CA-C-O	5.74	126.50	120.42
4	D	53	GLY	N-CA-C	-5.74	107.55	114.66
4	D	23	HIS	N-CA-C	5.73	117.53	111.28
5	E	5	ILE	CB-CA-C	-5.73	103.20	111.34
3	C	182	HIS	N-CA-C	-5.73	104.94	111.07
9	I	67	SER	O-C-N	-5.72	116.80	123.27
1	A	417	ASP	O-C-N	5.72	129.72	122.57
1	A	443	TRP	N-CA-C	5.72	119.62	107.67
4	D	196	PRO	N-CA-CB	5.71	109.25	103.25
3	C	16	ASN	CA-CB-CG	-5.71	106.89	112.60
1	A	383	LEU	N-CA-CB	5.71	119.34	110.44
1	A	172	GLU	N-CA-C	5.70	117.50	111.28
2	B	309	VAL	N-CA-C	5.70	115.75	107.88
1	A	389	ARG	CB-CA-C	5.70	119.82	109.62
2	B	314	ALA	N-CA-CB	-5.70	101.82	110.77
3	C	221	HIS	CA-CB-CG	-5.69	108.11	113.80
8	H	30	CYS	O-C-N	5.69	129.05	122.17
3	C	207	ASN	OD1-CG-ND2	-5.68	116.92	122.60
3	C	264	THR	CA-C-N	-5.68	114.53	120.38
3	C	264	THR	C-N-CA	-5.68	114.53	120.38
1	A	345	LEU	CA-C-O	-5.68	114.85	120.70
1	A	285	GLY	CA-C-O	5.68	126.53	120.40
6	F	58	ARG	CD-NE-CZ	-5.67	116.46	124.40
1	A	33	PRO	N-CA-CB	5.67	109.29	103.23
4	D	186	VAL	CB-CA-C	-5.67	104.60	112.02
10	J	57	HIS	N-CA-C	5.67	117.91	111.11
3	C	68	HIS	CA-CB-CG	-5.66	108.14	113.80
5	E	189	SER	CA-C-N	5.66	128.14	120.38
5	E	189	SER	C-N-CA	5.66	128.14	120.38
2	B	168	TYR	CA-C-O	5.66	128.08	121.46
2	B	285	VAL	N-CA-C	5.66	116.04	108.11
2	B	395	PRO	CA-C-N	5.66	128.18	120.54
2	B	395	PRO	C-N-CA	5.66	128.18	120.54
4	D	48	TYR	CA-C-N	5.65	132.33	121.54
4	D	48	TYR	C-N-CA	5.65	132.33	121.54
3	C	226	ILE	N-CA-CB	5.64	117.80	110.57
1	A	119	ASN	CA-CB-CG	-5.63	106.97	112.60
3	C	99	GLY	O-C-N	5.63	127.64	122.17
1	A	362	ARG	O-C-N	5.63	128.11	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	124	MET	CA-CB-CG	5.63	125.36	114.10
3	C	332	LEU	CA-C-O	5.63	126.50	120.20
4	D	73	GLY	O-C-N	-5.63	116.14	121.77
5	E	168	SER	N-CA-C	5.62	117.41	111.28
3	C	189	ILE	CB-CA-C	-5.62	104.78	111.97
4	D	55	CYS	CA-CB-SG	-5.62	101.48	114.40
4	D	10	TYR	N-CA-C	5.60	117.66	109.71
1	A	301	ASN	CB-CG-ND2	-5.59	108.01	116.40
6	F	32	MET	CA-CB-CG	5.59	125.29	114.10
3	C	122	THR	CA-CB-CG2	-5.59	100.99	110.50
6	F	40	ASN	CA-C-N	5.59	128.09	120.54
6	F	40	ASN	C-N-CA	5.59	128.09	120.54
6	F	80	TRP	N-CA-C	5.59	118.84	109.95
1	A	122	LEU	N-CA-C	5.58	118.62	107.62
2	B	245	ARG	CA-C-N	-5.58	115.24	123.05
2	B	245	ARG	C-N-CA	-5.58	115.24	123.05
3	C	205	SER	N-CA-C	-5.57	102.22	110.46
1	A	326	CYS	N-CA-C	5.56	115.89	108.38
7	G	22	GLU	CB-CA-C	-5.56	99.55	110.11
3	C	247	PRO	N-CA-CB	5.55	109.08	103.25
9	I	64	LEU	N-CA-C	5.55	117.48	108.26
1	A	266	ASP	CA-CB-CG	-5.55	107.05	112.60
2	B	183	ILE	CB-CG1-CD1	5.54	125.44	113.80
1	A	325	VAL	O-C-N	-5.54	117.36	123.18
3	C	253	PRO	N-CA-CB	5.54	108.10	103.17
1	A	144	SER	CA-C-O	5.54	126.30	120.54
3	C	264	THR	N-CA-C	5.53	120.61	108.66
4	D	6	HIS	CA-C-N	5.53	126.08	120.38
4	D	6	HIS	C-N-CA	5.53	126.08	120.38
4	D	64	LEU	CA-C-O	5.53	126.28	120.42
3	C	207	ASN	CB-CG-ND2	5.53	124.69	116.40
5	E	174	GLY	CA-C-N	5.53	125.62	119.32
5	E	174	GLY	C-N-CA	5.53	125.62	119.32
2	B	87	ARG	O-C-N	5.52	127.97	122.12
3	C	118	ILE	N-CA-CB	5.52	116.64	110.51
3	C	318	ARG	NE-CZ-NH1	-5.52	115.98	121.50
5	E	15	ARG	CA-C-N	5.51	126.73	119.84
5	E	15	ARG	C-N-CA	5.51	126.73	119.84
1	A	440	GLY	N-CA-C	-5.51	108.10	115.32
2	B	157	ALA	N-CA-C	5.51	116.97	111.07
6	F	55	TYR	O-C-N	-5.51	115.87	122.15
2	B	233	SER	N-CA-C	5.50	117.08	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	63	HIS	CA-CB-CG	-5.50	108.30	113.80
5	E	161	HIS	CA-CB-CG	-5.49	108.31	113.80
1	A	173	ASN	OD1-CG-ND2	-5.49	117.11	122.60
4	D	202	LYS	CA-C-N	-5.49	113.31	120.44
4	D	202	LYS	C-N-CA	-5.49	113.31	120.44
7	G	73	ASN	CA-C-N	5.48	126.34	120.47
7	G	73	ASN	C-N-CA	5.48	126.34	120.47
2	B	94	GLY	CA-C-O	-5.48	115.31	121.23
3	C	325	PHE	CA-CB-CG	-5.47	108.33	113.80
5	E	128	LYS	N-CA-C	-5.47	106.44	113.23
5	E	13	TYR	CA-C-O	5.46	126.24	119.79
2	B	385	GLN	OE1-CD-NE2	5.46	128.06	122.60
3	C	85	ASN	CB-CG-ND2	-5.46	108.22	116.40
6	F	52	GLU	O-C-N	-5.45	116.42	122.09
6	F	66	LEU	N-CA-C	-5.44	105.43	111.36
6	F	56	ASP	CA-CB-CG	-5.44	107.16	112.60
3	C	187	PHE	N-CA-C	-5.42	105.45	111.36
10	J	47	ASN	CA-CB-CG	5.41	118.01	112.60
1	A	195	MET	N-CA-CB	-5.41	102.09	110.04
2	B	38	LEU	CA-C-O	-5.41	114.72	120.40
6	F	96	GLU	N-CA-CB	5.41	118.91	109.72
1	A	420	PRO	CA-C-N	5.41	130.62	123.05
1	A	420	PRO	C-N-CA	5.41	130.62	123.05
2	B	137	VAL	CB-CA-C	-5.40	103.36	112.16
3	C	49	LEU	CB-CA-C	-5.40	101.77	110.74
4	D	47	ALA	N-CA-C	-5.40	101.49	109.86
4	D	110	PRO	CA-C-N	5.40	125.66	119.83
4	D	110	PRO	C-N-CA	5.40	125.66	119.83
3	C	255	ASN	CA-CB-CG	-5.38	107.22	112.60
3	C	185	LEU	CA-C-N	5.38	125.71	119.47
3	C	185	LEU	C-N-CA	5.38	125.71	119.47
1	A	195	MET	CA-C-N	5.38	130.47	122.99
1	A	195	MET	C-N-CA	5.38	130.47	122.99
4	D	229	VAL	CA-C-O	-5.38	115.68	121.27
3	C	203	THR	N-CA-CB	5.37	118.14	111.00
3	C	110	LEU	CA-C-N	5.37	127.42	120.44
3	C	110	LEU	C-N-CA	5.37	127.42	120.44
3	C	98	VAL	N-CA-C	5.36	116.14	110.72
7	G	39	ARG	N-CA-C	5.36	117.88	111.71
1	A	209	LEU	O-C-N	5.35	127.66	122.09
7	G	9	ARG	NE-CZ-NH2	5.35	124.02	119.20
3	C	177	ARG	NH1-CZ-NH2	5.34	126.24	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	425	PHE	CA-CB-CG	5.33	119.14	113.80
2	B	96	LEU	CB-CA-C	-5.33	104.21	111.95
2	B	309	VAL	O-C-N	-5.33	118.33	122.97
1	A	204	GLU	CA-C-O	5.33	126.06	120.36
2	B	134	ARG	CA-CB-CG	5.32	124.74	114.10
5	E	94	LYS	CA-C-N	5.32	126.77	120.23
5	E	94	LYS	C-N-CA	5.32	126.77	120.23
2	B	247	GLN	O-C-N	-5.31	117.00	123.16
1	A	389	ARG	CA-C-N	5.30	131.94	122.13
1	A	389	ARG	C-N-CA	5.30	131.94	122.13
1	A	118	GLN	CA-C-N	-5.30	115.72	122.77
1	A	118	GLN	C-N-CA	-5.30	115.72	122.77
1	A	348	SER	CA-C-O	-5.30	114.91	120.32
1	A	33	PRO	N-CA-C	5.30	121.05	113.47
3	C	101	GLY	N-CA-C	-5.30	106.37	112.73
5	E	133	VAL	N-CA-C	5.30	115.48	107.75
4	D	203	ARG	N-CA-C	-5.30	105.40	111.07
2	B	38	LEU	CA-C-N	-5.29	113.59	122.17
2	B	38	LEU	C-N-CA	-5.29	113.59	122.17
7	G	51	PRO	N-CA-CB	5.29	109.10	103.39
8	H	15	ASP	CA-C-N	5.28	126.44	119.84
8	H	15	ASP	C-N-CA	5.28	126.44	119.84
4	D	14	HIS	CA-CB-CG	-5.28	108.52	113.80
1	A	362	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	A	423	ALA	CA-C-O	-5.26	114.06	120.54
10	J	33	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	A	403	ASP	CA-C-O	-5.26	115.42	121.47
2	B	411	ILE	CB-CA-C	-5.26	105.14	111.88
3	C	78	ILE	CA-CB-CG1	5.26	119.35	110.40
1	A	392	LEU	N-CA-C	5.26	117.69	111.33
11	K	17	TRP	CA-CB-CG	-5.26	103.61	113.60
1	A	417	ASP	N-CA-C	5.25	118.44	111.30
5	E	130	PRO	CA-C-N	5.25	128.04	120.38
5	E	130	PRO	C-N-CA	5.25	128.04	120.38
3	C	133	LEU	CA-C-N	5.24	125.05	119.28
3	C	133	LEU	C-N-CA	5.24	125.05	119.28
4	D	44	ASP	N-CA-C	5.24	116.99	111.28
1	A	58	PHE	CA-C-O	5.24	126.10	120.70
5	E	28	SER	CA-C-N	5.24	128.03	120.38
5	E	28	SER	C-N-CA	5.24	128.03	120.38
2	B	194	TYR	CG-CD2-CE2	-5.24	113.34	121.20
6	F	81	THR	CA-CB-OG1	-5.24	101.75	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	23	HIS	CB-CA-C	-5.23	102.10	110.79
2	B	64	GLY	CA-C-O	5.23	124.82	119.01
2	B	87	ARG	CA-C-O	-5.23	115.00	120.55
2	B	230	LEU	CA-C-N	5.23	131.16	120.80
2	B	230	LEU	C-N-CA	5.23	131.16	120.80
2	B	436	ILE	CA-CB-CG2	-5.23	101.61	110.50
5	E	81	ILE	CA-C-N	5.23	124.99	119.76
5	E	81	ILE	C-N-CA	5.23	124.99	119.76
7	G	34	ILE	CA-C-N	5.22	124.73	119.19
7	G	34	ILE	C-N-CA	5.22	124.73	119.19
9	I	76	VAL	N-CA-C	5.22	116.20	107.18
2	B	34	VAL	CB-CA-C	-5.21	104.07	111.21
4	D	7	PRO	CA-C-N	5.21	126.35	119.84
4	D	7	PRO	C-N-CA	5.21	126.35	119.84
6	F	62	ILE	CA-C-N	5.21	127.69	120.29
6	F	62	ILE	C-N-CA	5.21	127.69	120.29
1	A	201	GLY	N-CA-C	5.21	125.52	113.18
4	D	30	PHE	CA-CB-CG	-5.20	108.60	113.80
1	A	41	ILE	CA-C-N	-5.20	114.91	122.86
1	A	41	ILE	C-N-CA	-5.20	114.91	122.86
2	B	337	ILE	CA-C-O	-5.19	115.87	121.27
3	C	322	GLN	OE1-CD-NE2	5.19	127.79	122.60
1	A	174	VAL	CB-CA-C	-5.19	102.78	111.29
2	B	428	GLY	N-CA-C	5.19	118.18	110.60
1	A	239	SER	CA-C-O	-5.18	115.33	121.60
2	B	182	ARG	CA-CB-CG	5.18	124.46	114.10
6	F	57	ASP	N-CA-C	5.18	117.32	111.11
1	A	323	HIS	CA-CB-CG	5.18	118.98	113.80
2	B	63	LEU	O-C-N	-5.18	117.31	123.11
1	A	428	ILE	CB-CG1-CD1	-5.17	102.94	113.80
3	C	297	SER	CA-C-N	5.17	128.14	120.74
3	C	297	SER	C-N-CA	5.17	128.14	120.74
2	B	75	LEU	N-CA-CB	5.17	118.28	110.42
5	E	39	VAL	CB-CA-C	-5.17	105.16	112.14
9	I	74	ALA	N-CA-C	5.17	116.26	108.46
2	B	238	LYS	CA-C-O	-5.17	115.21	120.89
2	B	306	PRO	N-CA-CB	5.16	107.43	103.30
9	I	54	SER	CA-C-N	5.15	128.00	119.35
9	I	54	SER	C-N-CA	5.15	128.00	119.35
1	A	427	PRO	N-CA-CB	5.15	108.26	102.60
3	C	157	GLY	CA-C-N	5.15	129.37	121.19
3	C	157	GLY	C-N-CA	5.15	129.37	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	168	VAL	CB-CA-C	-5.14	105.35	112.24
2	B	394	PRO	N-CA-CB	5.14	108.07	103.08
2	B	181	TYR	N-CA-C	5.14	119.26	113.15
8	H	18	THR	N-CA-C	5.13	118.32	111.75
4	D	240	PRO	N-CA-C	-5.13	106.85	113.57
5	E	37	TYR	CA-C-O	5.13	125.67	119.31
1	A	217	SER	N-CA-CB	-5.13	103.32	111.62
5	E	29	SER	O-C-N	-5.12	116.36	122.20
7	G	7	LEU	CA-C-O	-5.12	115.62	120.90
1	A	342	TRP	O-C-N	-5.12	116.01	122.20
1	A	411	CYS	N-CA-C	5.11	116.85	111.28
10	J	8	ARG	CA-C-N	5.11	127.44	120.54
10	J	8	ARG	C-N-CA	5.11	127.44	120.54
1	A	205	HIS	CA-CB-CG	-5.11	108.69	113.80
3	C	275	LEU	CA-C-O	-5.11	115.45	121.07
10	J	55	ILE	N-CA-C	5.10	117.88	112.83
1	A	341	GLN	O-C-N	-5.10	115.59	122.23
9	I	51	CYS	N-CA-C	5.10	117.86	110.17
2	B	395	PRO	N-CA-CB	5.09	108.68	103.23
2	B	72	ALA	N-CA-C	5.09	118.63	112.93
1	A	157	ALA	N-CA-C	-5.09	105.73	111.28
5	E	9	ASP	CA-CB-CG	-5.09	107.51	112.60
8	H	17	LEU	CA-C-N	5.09	127.81	120.38
8	H	17	LEU	C-N-CA	5.09	127.81	120.38
3	C	69	ILE	CA-C-N	-5.08	114.37	122.66
3	C	69	ILE	C-N-CA	-5.08	114.37	122.66
1	A	13	GLU	CA-C-O	5.08	127.46	121.87
1	A	170	PRO	N-CA-CB	5.08	108.58	103.25
2	B	174	ASN	CB-CA-C	5.08	117.82	109.90
2	B	412	ASN	CA-CB-CG	5.08	117.68	112.60
4	D	73	GLY	N-CA-C	5.08	122.70	112.34
3	C	55	TYR	CA-C-O	-5.08	115.38	121.11
7	G	61	TRP	CA-C-N	5.07	125.71	120.03
7	G	61	TRP	C-N-CA	5.07	125.71	120.03
6	F	45	GLU	O-C-N	5.07	127.29	122.07
10	J	25	VAL	CA-C-N	5.07	126.94	120.56
10	J	25	VAL	C-N-CA	5.07	126.94	120.56
3	C	20	ASP	CA-C-N	5.06	130.56	120.94
3	C	20	ASP	C-N-CA	5.06	130.56	120.94
3	C	182	HIS	O-C-N	5.06	127.28	122.07
1	A	144	SER	N-CA-C	5.06	116.85	108.20
4	D	229	VAL	O-C-N	5.06	127.00	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	136	ILE	O-C-N	5.06	128.49	123.18
3	C	284	ILE	CA-C-N	5.05	126.16	119.84
3	C	284	ILE	C-N-CA	5.05	126.16	119.84
2	B	291	ALA	N-CA-C	-5.05	106.28	112.90
3	C	179	PHE	O-C-N	-5.05	116.84	122.09
7	G	13	VAL	CA-C-N	-5.05	115.69	122.91
7	G	13	VAL	C-N-CA	-5.05	115.69	122.91
1	A	364	ALA	N-CA-C	-5.05	105.86	111.36
3	C	129	MET	CA-CB-CG	-5.05	104.00	114.10
2	B	247	GLN	CA-C-O	5.04	126.72	120.92
4	D	151	PRO	N-CA-CB	5.04	108.31	103.52
1	A	173	ASN	CB-CG-ND2	5.04	123.96	116.40
7	G	4	PHE	N-CA-CB	5.04	117.77	110.26
2	B	77	THR	CA-CB-OG1	-5.03	102.05	109.60
5	E	158	CYS	CA-C-O	5.03	122.56	119.29
7	G	5	GLY	CA-C-O	-5.03	111.82	120.57
3	C	206	ASN	CB-CG-OD1	-5.03	110.75	120.80
1	A	193	PRO	N-CA-CB	5.02	108.12	102.60
1	A	205	HIS	CA-C-N	5.01	131.12	121.54
1	A	205	HIS	C-N-CA	5.01	131.12	121.54
1	A	340	GLY	O-C-N	5.01	127.75	122.28
6	F	91	GLU	CA-C-O	5.01	123.24	118.63
3	C	184	ILE	CA-CB-CG1	5.01	118.92	110.40
2	B	180	ASP	N-CA-CB	5.01	117.57	110.06
5	E	23	LYS	N-CA-C	5.01	116.81	109.24
5	E	25	SER	CA-C-N	5.01	127.92	120.31
5	E	25	SER	C-N-CA	5.01	127.92	120.31
1	A	243	HIS	CA-C-N	5.01	127.96	120.95
1	A	243	HIS	C-N-CA	5.01	127.96	120.95
1	A	290	LEU	O-C-N	-5.01	115.93	122.59
1	A	337	VAL	O-C-N	5.00	126.72	121.87
1	A	99	ILE	CB-CA-C	-5.00	103.23	110.63

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	THR	Mainchain
1	A	190	TYR	Mainchain
1	A	197	LEU	Mainchain
1	A	210	ASP	Mainchain
1	A	273	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	A	284	TYR	Mainchain
1	A	297	ILE	Mainchain
1	A	304	CYS	Mainchain
1	A	323	HIS	Mainchain
1	A	334	MET	Mainchain
1	A	341	GLN	Mainchain
1	A	433	ASP	Mainchain
1	A	437	ILE	Mainchain
1	A	47	TYR	Mainchain
2	B	105	MET	Mainchain
2	B	147	ASP	Mainchain
2	B	149	ALA	Mainchain
2	B	172	LEU	Mainchain
2	B	174	ASN	Mainchain
2	B	186	VAL	Mainchain
2	B	244	ILE	Mainchain
2	B	246	GLU	Mainchain
2	B	248	ASN	Mainchain
2	B	282	GLY	Mainchain
2	B	320	GLY	Mainchain
2	B	379	LEU	Mainchain
2	B	391	SER	Mainchain
2	B	406	ALA	Mainchain
2	B	69	LEU	Mainchain
2	B	90	GLU	Mainchain
2	B	99	THR	Mainchain
3	C	108	THR	Mainchain
3	C	149	LEU	Mainchain
3	C	163	TRP	Mainchain
3	C	165	TRP	Mainchain
3	C	213	SER	Mainchain
3	C	264	THR	Mainchain
3	C	40	CYS	Mainchain
3	C	75	TYR	Mainchain
4	D	24	THR	Mainchain
4	D	31	GLN	Mainchain
4	D	41	HIS	Mainchain
4	D	5	LEU	Mainchain
4	D	6	HIS	Mainchain
5	E	155	GLY	Mainchain
5	E	184	SER	Mainchain
5	E	43	THR	Mainchain

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Mol	Chain	Res	Type	Group
5	E	56	SER	Mainchain
5	E	71	MET	Mainchain
6	F	17	ARG	Mainchain
6	F	37	ILE	Mainchain
6	F	73	GLN	Mainchain
6	F	75	LEU	Mainchain
6	F	80	TRP	Mainchain
7	G	22	GLU	Mainchain
7	G	73	ASN	Mainchain
8	H	59	LEU	Mainchain

5.2 Too-close contacts (i)

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	3458	0	3356	511	0
2	B	3141	0	3123	421	1
3	C	3011	0	3077	409	2
4	D	1919	0	1868	313	0
5	E	1519	0	1503	193	2
6	F	916	0	909	90	0
7	G	682	0	679	107	0
8	H	524	0	504	60	0
9	I	248	0	265	75	0
10	J	512	0	518	71	0
11	K	159	0	159	23	0
12	C	86	0	60	19	0
13	D	43	0	30	3	0
14	E	4	0	0	1	0
All	All	16222	0	16051	2085	3

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 65.

All (2085) 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:158:PHE:CE1	1:A:317:THR:HG21	1.71	1.26
1:A:21:ASN:CB	1:A:217:SER:HB2	1.70	1.20
1:A:392:LEU:HA	1:A:395:TRP:CD1	1.79	1.17
2:B:29:LEU:HD12	2:B:33:LEU:HD21	1.19	1.15
1:A:158:PHE:HE1	1:A:317:THR:HG21	0.97	1.12
4:D:233:ARG:HG2	7:G:17:SER:HB2	1.29	1.12
3:C:26:ASN:HD21	3:C:207:ASN:HB2	1.11	1.11
3:C:174:THR:HG23	3:C:178:PHE:HE1	1.13	1.10
1:A:34:THR:HG21	2:B:370:MET:HG2	1.31	1.09
2:B:304:HIS:CD2	2:B:306:PRO:HD2	1.85	1.09
4:D:83:ARG:HB3	4:D:84:PRO:CD	1.82	1.09
2:B:24:LEU:H	2:B:24:LEU:HD12	1.18	1.08
4:D:83:ARG:CB	4:D:84:PRO:HD2	1.85	1.07
1:A:42:ASP:HB3	1:A:384:LEU:HD22	1.13	1.06
1:A:18:GLN:HE21	1:A:22:GLY:HA2	1.10	1.06
7:G:72:LYS:HB3	7:G:75:ALA:HB2	1.32	1.06
7:G:8:THR:HG22	7:G:9:ARG:H	1.15	1.05
1:A:64:PHE:HE1	1:A:86:LEU:HG	1.19	1.04
9:I:78:TYR:OXT	9:I:78:TYR:HD1	1.38	1.04
3:C:206:ASN:HB2	3:C:313:ARG:NH2	1.72	1.04
3:C:129:MET:HG2	3:C:178:PHE:HD2	1.20	1.03
3:C:108:THR:HB	3:C:313:ARG:HH11	1.21	1.03
1:A:21:ASN:HB3	1:A:217:SER:CB	1.89	1.02
1:A:213:GLN:HB3	1:A:215:HIS:NE2	1.73	1.01
3:C:265:PRO:HB2	3:C:268:ILE:HG12	1.02	1.01
3:C:310:SER:HA	3:C:374:ASN:HD21	1.25	1.01
4:D:70:VAL:HG23	4:D:84:PRO:HD3	1.41	1.01
4:D:57:THR:HG22	4:D:59:ASP:H	1.26	1.01
2:B:305:GLN:HB2	2:B:306:PRO:HD3	1.39	1.00
3:C:26:ASN:HD21	3:C:207:ASN:CB	1.75	1.00
1:A:64:PHE:CE1	1:A:86:LEU:HG	1.96	1.00
1:A:67:THR:HG22	1:A:70:ARG:HB2	1.43	1.00
3:C:265:PRO:HB2	3:C:268:ILE:CG1	1.93	0.99
1:A:383:LEU:HA	1:A:387:GLY:O	1.63	0.98
1:A:378:ASP:O	1:A:382:SER:HB2	1.63	0.97
3:C:174:THR:HG23	3:C:178:PHE:CE1	1.98	0.97
2:B:279:LEU:HD22	2:B:295:LEU:HD13	1.43	0.97
12:C:381:HEM:HBC2	12:C:381:HEM:HMC2	1.46	0.97
1:A:248:LEU:HD11	1:A:425:PHE:HE2	1.27	0.97
9:I:78:TYR:OXT	9:I:78:TYR:CD1	2.19	0.95
2:B:385:GLN:HG2	9:I:62:ARG:HH12	1.31	0.95
4:D:74:PRO:HG2	4:D:82:MET:SD	2.06	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:HG21	2:B:199:PHE:HA	1.46	0.95
1:A:248:LEU:HD11	1:A:425:PHE:CE2	2.02	0.94
3:C:3:ASN:N	3:C:8:HIS:NE2	2.14	0.94
2:B:248:ASN:HB2	2:B:428:GLY:HA2	1.47	0.94
3:C:348:ILE:O	3:C:352:GLN:HG3	1.67	0.94
3:C:106:SER:HB3	12:C:381:HEM:HBD2	1.49	0.94
1:A:36:THR:OG1	1:A:372:THR:HG22	1.69	0.93
1:A:21:ASN:HB3	1:A:217:SER:HB2	0.93	0.92
4:D:233:ARG:CG	7:G:17:SER:HB2	1.98	0.92
3:C:270:PRO:HB2	3:C:274:PHE:HB2	1.51	0.92
1:A:27:SER:HA	1:A:199:ALA:O	1.69	0.92
2:B:283:PRO:HG3	9:I:55:LEU:HD22	1.49	0.92
4:D:219:VAL:HA	4:D:222:MET:HG3	1.50	0.92
3:C:10:LEU:HD12	3:C:13:ILE:HD12	1.51	0.92
1:A:408:ARG:HH12	11:K:15:ARG:HG2	1.34	0.92
2:B:169:ARG:HH11	2:B:238:LYS:NZ	1.68	0.92
3:C:26:ASN:ND2	3:C:207:ASN:HB2	1.84	0.92
1:A:45:SER:HB3	1:A:92:ARG:HA	1.50	0.92
2:B:297:GLN:OE1	2:B:297:GLN:HA	1.67	0.92
2:B:341:TYR:CE2	2:B:345:LYS:HE3	2.05	0.91
4:D:224:ARG:HB2	7:G:25:ALA:HB1	1.53	0.91
12:C:380:HEM:HBB2	12:C:380:HEM:HHC	1.50	0.91
2:B:341:TYR:HE2	2:B:345:LYS:HE3	1.32	0.91
9:I:62:ARG:HB3	9:I:63:PRO:HD3	1.51	0.91
1:A:91:THR:HG22	1:A:93:GLU:H	1.36	0.91
2:B:304:HIS:HD2	2:B:306:PRO:HD2	1.25	0.91
7:G:36:ASN:HA	7:G:39:ARG:HD3	1.52	0.91
4:D:83:ARG:HB3	4:D:84:PRO:HD2	0.94	0.90
2:B:182:ARG:NH1	2:B:185:LYS:HE2	1.86	0.90
3:C:1:MET:SD	3:C:7:SER:HB2	2.12	0.90
10:J:29:LEU:HD13	11:K:34:SER:HB2	1.54	0.90
7:G:29:TYR:HD2	7:G:30:PHE:CD2	1.90	0.90
3:C:210:GLY:HA3	3:C:314:SER:HB2	1.54	0.90
5:E:19:LEU:HD12	5:E:19:LEU:O	1.71	0.90
2:B:237:ALA:HB2	2:B:318:ASP:OD2	1.70	0.89
1:A:236:PHE:CE2	1:A:317:THR:HG23	2.07	0.89
4:D:178:THR:HB	4:D:181:GLN:HG3	1.53	0.89
8:H:70:ALA:HA	8:H:73:LEU:HD22	1.53	0.89
2:B:305:GLN:HB2	2:B:306:PRO:CD	2.03	0.88
4:D:211:MET:HA	4:D:211:MET:HE3	1.53	0.88
3:C:345:HIS:HB3	3:C:346:PRO:CD	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PHE:CE2	1:A:258:GLU:HB3	2.08	0.88
2:B:47:ILE:HD11	2:B:211:VAL:HG21	1.55	0.88
3:C:170:VAL:HG13	3:C:174:THR:HG21	1.56	0.88
3:C:108:THR:HB	3:C:313:ARG:NH1	1.88	0.88
4:D:165:TYR:O	4:D:168:VAL:HG23	1.74	0.88
7:G:73:ASN:N	7:G:74:PRO:HD2	1.89	0.88
4:D:27:ARG:HH12	10:J:58:LYS:HG3	1.40	0.87
9:I:72:VAL:HB	9:I:73:PRO:HD3	1.55	0.87
2:B:132:PHE:CD2	2:B:191:LEU:HD13	2.10	0.87
6:F:42:ASP:OD2	6:F:101:ARG:NH1	2.07	0.87
1:A:75:LEU:HD21	1:A:116:ILE:HD11	1.55	0.87
4:D:181:GLN:HA	8:H:77:LEU:HD13	1.56	0.87
6:F:37:ILE:HD11	6:F:90:LEU:CD2	2.05	0.87
1:A:18:GLN:NE2	1:A:22:GLY:HA2	1.90	0.87
1:A:151:ASN:ND2	5:E:2:HIS:NE2	2.23	0.86
1:A:155:ALA:HA	1:A:164:ALA:HB1	1.54	0.86
3:C:185:LEU:HB3	3:C:186:PRO:HD3	1.56	0.86
2:B:331:ALA:HA	2:B:432:HIS:ND1	1.89	0.86
1:A:53:ASN:OD1	1:A:165:GLN:HB2	1.75	0.86
1:A:224:ASP:OD1	1:A:227:ALA:HB3	1.76	0.86
3:C:1:MET:SD	3:C:4:ILE:HB	2.14	0.86
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.58	0.86
3:C:310:SER:HB3	3:C:318:ARG:NH1	1.91	0.85
1:A:61:HIS:CD2	1:A:134:ILE:HD11	2.11	0.85
4:D:26:ILE:HG22	4:D:54:VAL:HG13	1.57	0.85
4:D:74:PRO:HB2	4:D:79:GLU:HB2	1.58	0.85
7:G:8:THR:HG22	7:G:9:ARG:N	1.91	0.85
1:A:30:SER:N	1:A:201:GLY:O	2.09	0.85
9:I:72:VAL:HB	9:I:73:PRO:CD	2.05	0.85
1:A:317:THR:HG22	1:A:318:GLY:N	1.87	0.85
3:C:129:MET:HG2	3:C:178:PHE:CD2	2.10	0.85
1:A:39:VAL:HG23	1:A:113:LEU:HD23	1.59	0.85
2:B:29:LEU:HD12	2:B:33:LEU:CD2	2.06	0.85
4:D:27:ARG:HH11	10:J:58:LYS:HZ1	1.23	0.85
1:A:408:ARG:NH1	11:K:15:ARG:HG2	1.91	0.85
4:D:10:TYR:CD1	4:D:11:PRO:HD2	2.11	0.84
4:D:51:LEU:HA	4:D:56:TYR:O	1.77	0.84
4:D:10:TYR:HB2	4:D:125:ASP:OD1	1.75	0.84
1:A:106:LEU:HD22	1:A:203:LEU:HD22	1.59	0.84
4:D:50:HIS:HB3	4:D:54:VAL:HB	1.60	0.84
6:F:50:LEU:HB2	6:F:55:TYR:HB2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:GLU:HA	8:H:30:CYS:SG	2.17	0.84
2:B:217:LYS:O	2:B:221:GLU:HG3	1.77	0.84
7:G:9:ARG:NH2	7:G:11:ARG:HD2	1.93	0.83
9:I:70:LEU:HD12	9:I:71:ASN:N	1.92	0.83
2:B:200:THR:HG22	2:B:203:ARG:HD2	1.58	0.83
4:D:27:ARG:HH11	10:J:58:LYS:NZ	1.74	0.83
3:C:265:PRO:CB	3:C:268:ILE:HG12	1.98	0.83
6:F:28:LYS:HD3	6:F:74:ILE:HD11	1.58	0.83
3:C:264:THR:O	3:C:266:PRO:HD3	1.78	0.83
3:C:341:GLN:HB3	3:C:347:TYR:CD2	2.14	0.83
1:A:42:ASP:HB3	1:A:384:LEU:CD2	2.05	0.83
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.61	0.83
3:C:278:TYR:O	3:C:279:ALA:C	2.22	0.82
3:C:59:THR:HG23	3:C:135:TRP:HE1	1.43	0.82
3:C:215:VAL:HG11	6:F:59:VAL:HG13	1.61	0.82
4:D:208:MET:HE3	4:D:208:MET:C	2.05	0.82
1:A:335:MET:HE2	1:A:339:GLN:HG3	1.59	0.82
3:C:345:HIS:HB3	3:C:346:PRO:HD3	1.60	0.82
1:A:134:ILE:HD13	1:A:134:ILE:N	1.93	0.82
2:B:24:LEU:HD12	2:B:24:LEU:N	1.94	0.82
3:C:138:MET:HE1	3:C:268:ILE:HA	1.61	0.82
1:A:236:PHE:HD2	1:A:258:GLU:HG2	1.42	0.82
1:A:360:LEU:HD13	2:B:93:GLY:HA2	1.61	0.82
2:B:263:ALA:O	2:B:269:ALA:HB2	1.80	0.81
5:E:2:HIS:O	5:E:5:ILE:HG12	1.80	0.81
1:A:334:MET:HA	1:A:334:MET:CE	2.11	0.81
2:B:165:ALA:HA	2:B:173:ALA:HB1	1.61	0.81
4:D:229:VAL:O	4:D:233:ARG:HG3	1.79	0.81
1:A:144:SER:O	1:A:148:VAL:HG23	1.80	0.81
1:A:428:ILE:HG23	1:A:431:LEU:CB	2.11	0.81
9:I:64:LEU:HD12	9:I:65:VAL:N	1.94	0.81
1:A:134:ILE:HA	1:A:137:GLU:HG3	1.63	0.81
2:B:257:LEU:HD13	2:B:424:MET:HE2	1.63	0.81
4:D:178:THR:OG1	4:D:181:GLN:NE2	2.11	0.81
1:A:293:PRO:O	1:A:297:ILE:HG13	1.81	0.80
1:A:143:THR:HG21	9:I:48:SER:H	1.43	0.80
2:B:169:ARG:HH11	2:B:238:LYS:HZ2	1.26	0.80
3:C:309:THR:CG2	3:C:370:GLY:HA3	2.11	0.80
3:C:309:THR:HG23	3:C:370:GLY:HA3	1.62	0.80
2:B:209:LEU:HD22	2:B:375:SER:HB2	1.64	0.80
4:D:30:PHE:HD1	4:D:189:PHE:CE2	2.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:359:PHE:O	3:C:363:LEU:HB2	1.82	0.79
1:A:420:PRO:HG3	1:A:441:MET:HE2	1.64	0.79
2:B:99:THR:OG1	9:I:68:VAL:HG22	1.81	0.79
4:D:11:PRO:HG3	8:H:70:ALA:O	1.82	0.79
4:D:57:THR:HG22	4:D:59:ASP:N	1.98	0.79
5:E:177:PRO:HB2	5:E:178:LEU:HD23	1.62	0.79
3:C:108:THR:CB	3:C:313:ARG:HH11	1.96	0.79
7:G:9:ARG:HH21	7:G:11:ARG:HD2	1.47	0.79
2:B:111:CYS:HB3	2:B:119:LEU:HD22	1.65	0.79
1:A:236:PHE:CD2	1:A:258:GLU:HG2	2.18	0.79
3:C:137:GLN:OE1	3:C:259:ALA:HA	1.83	0.79
2:B:338:LYS:HG2	2:B:439:LEU:HD21	1.65	0.79
3:C:206:ASN:HB2	3:C:313:ARG:HH21	1.48	0.79
8:H:49:GLN:HB2	8:H:52:GLU:HG2	1.63	0.79
4:D:27:ARG:NH1	10:J:58:LYS:NZ	2.31	0.79
4:D:228:SER:HB2	7:G:23:GLN:NE2	1.98	0.79
2:B:31:ASN:HB3	2:B:201:SER:HB3	1.65	0.79
2:B:308:ASP:OD1	2:B:309:VAL:N	2.16	0.79
10:J:18:SER:OG	11:K:23:LEU:HB2	1.83	0.79
1:A:260:PRO:HG3	1:A:414:TYR:CE1	2.18	0.78
6:F:37:ILE:HD11	6:F:90:LEU:HD21	1.64	0.78
10:J:51:LEU:HB3	10:J:52:TRP:CZ3	2.18	0.78
1:A:106:LEU:HD22	1:A:203:LEU:CD2	2.13	0.78
1:A:392:LEU:HA	1:A:395:TRP:NE1	1.98	0.78
2:B:385:GLN:CG	9:I:62:ARG:HH12	1.96	0.78
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.19	0.78
1:A:52:ASN:HB2	1:A:55:ALA:HB2	1.64	0.78
2:B:156:GLN:HE22	9:I:56:ARG:HD3	1.47	0.78
5:E:76:ILE:HG23	5:E:194:ILE:HD13	1.65	0.78
1:A:245:GLU:H	1:A:426:GLY:HA3	1.47	0.78
6:F:75:LEU:O	6:F:80:TRP:NE1	2.17	0.78
1:A:102:LEU:HB2	1:A:105:ASP:OD2	1.84	0.77
5:E:169:GLY:HA2	5:E:180:LEU:HD12	1.66	0.77
5:E:164:HIS:CD2	5:E:173:LYS:HG2	2.19	0.77
1:A:39:VAL:HG12	1:A:41:ILE:HD11	1.66	0.77
2:B:203:ARG:NE	2:B:230:LEU:HD23	1.98	0.77
2:B:274:VAL:HG21	2:B:405:VAL:HG21	1.65	0.77
1:A:244:ARG:HG2	7:G:10:VAL:HG12	1.65	0.77
1:A:436:ARG:HE	3:C:222:PRO:HD3	1.50	0.77
2:B:74:SER:O	2:B:82:SER:HB2	1.85	0.77
2:B:200:THR:O	2:B:204:MET:HG3	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:74:PRO:CB	4:D:79:GLU:HB2	2.15	0.77
3:C:103:TYR:O	3:C:315:MET:HB2	1.83	0.77
7:G:29:TYR:CD2	7:G:30:PHE:CD2	2.73	0.77
1:A:240:GLN:HG3	1:A:422:VAL:HB	1.67	0.76
3:C:7:SER:HA	3:C:13:ILE:HG12	1.65	0.76
2:B:306:PRO:HB2	2:B:329:GLN:NE2	2.00	0.76
1:A:445:ARG:O	1:A:446:PHE:HB2	1.83	0.76
2:B:54:GLY:H	2:B:57:TYR:HD2	1.31	0.76
2:B:67:HIS:HD2	2:B:144:LEU:HD22	1.49	0.76
4:D:97:ASN:OD1	4:D:98:PRO:HD2	1.86	0.76
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.68	0.76
2:B:304:HIS:HD2	2:B:306:PRO:CD	1.99	0.76
1:A:262:TRP:CD2	1:A:385:THR:HG23	2.21	0.76
2:B:200:THR:CG2	2:B:203:ARG:HD2	2.16	0.76
5:E:67:ASP:C	5:E:67:ASP:OD1	2.29	0.75
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.68	0.75
2:B:56:ARG:NH2	2:B:318:ASP:OD1	2.16	0.75
4:D:113:LEU:CD2	4:D:116:ILE:HD12	2.16	0.75
5:E:73:LYS:HG3	5:E:196:GLY:O	1.86	0.75
9:I:70:LEU:HD12	9:I:71:ASN:H	1.49	0.75
1:A:73:ASN:O	1:A:77:LYS:HG3	1.86	0.75
2:B:248:ASN:HB2	2:B:428:GLY:CA	2.17	0.75
2:B:262:ALA:HB2	2:B:272:PHE:HE2	1.52	0.74
2:B:162:ASN:HD22	2:B:244:ILE:CG2	2.00	0.74
3:C:8:HIS:HB3	3:C:9:PRO:HD3	1.69	0.74
3:C:100:ARG:HH21	12:C:381:HEM:HBD1	1.52	0.74
4:D:70:VAL:HG23	4:D:84:PRO:CD	2.16	0.74
1:A:286:GLY:O	1:A:287:GLY:C	2.31	0.74
1:A:332:ASP:CG	1:A:430:GLN:HE21	1.95	0.74
2:B:198:HIS:HE1	2:B:233:SER:HB3	1.53	0.74
1:A:158:PHE:HE1	1:A:317:THR:CG2	1.91	0.74
1:A:240:GLN:NE2	1:A:431:LEU:HD21	2.01	0.74
1:A:418:GLN:O	1:A:420:PRO:HD3	1.88	0.74
2:B:42:ALA:HB1	2:B:43:PRO:HD2	1.67	0.74
2:B:129:ALA:N	2:B:130:PRO:HD3	2.02	0.74
2:B:264:ILE:CG2	2:B:317:SER:HA	2.17	0.74
3:C:237:LEU:HD13	4:D:212:MET:HG2	1.69	0.74
4:D:54:VAL:O	4:D:54:VAL:HG12	1.87	0.74
1:A:106:LEU:CD2	1:A:203:LEU:HD13	2.16	0.74
2:B:267:ALA:O	2:B:268:GLU:C	2.30	0.74
1:A:236:PHE:CZ	1:A:317:THR:HG23	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HA	1:A:199:ALA:HB2	1.70	0.73
3:C:10:LEU:HD12	3:C:13:ILE:CD1	2.17	0.73
2:B:435:PHE:HB2	2:B:438:GLU:OE1	1.88	0.73
1:A:334:MET:HA	1:A:334:MET:HE2	1.70	0.73
1:A:428:ILE:HG23	1:A:431:LEU:HB2	1.68	0.73
2:B:169:ARG:HD3	2:B:238:LYS:HZ2	1.52	0.73
10:J:51:LEU:HB3	10:J:52:TRP:CE3	2.23	0.73
2:B:385:GLN:HG2	9:I:62:ARG:NH1	2.02	0.73
4:D:100:ALA:O	4:D:103:ALA:N	2.22	0.73
2:B:300:ALA:HA	2:B:307:PHE:CZ	2.24	0.73
2:B:308:ASP:OD2	9:I:55:LEU:HA	1.89	0.73
7:G:72:LYS:CB	7:G:75:ALA:HB2	2.13	0.73
1:A:198:ALA:HB1	1:A:379:ILE:HG22	1.68	0.73
1:A:73:ASN:ND2	1:A:73:ASN:H	1.85	0.73
3:C:135:TRP:HH2	3:C:170:VAL:HG12	1.54	0.73
1:A:184:GLU:O	1:A:188:ARG:HG3	1.88	0.73
2:B:76:THR:HG21	2:B:133:ARG:NH2	2.04	0.73
2:B:83:PHE:CE1	2:B:87:ARG:HG3	2.23	0.73
3:C:78:ILE:HD11	5:E:57:GLN:NE2	2.03	0.73
4:D:164:ILE:HG22	4:D:179:MET:HG2	1.69	0.73
8:H:21:ARG:HB3	8:H:65:ARG:HH21	1.53	0.73
1:A:213:GLN:HB3	1:A:215:HIS:CD2	2.24	0.72
1:A:386:TYR:HD1	1:A:386:TYR:H	1.36	0.72
3:C:138:MET:CE	3:C:269:LYS:H	2.02	0.72
5:E:117:LEU:HD12	5:E:120:PRO:HA	1.71	0.72
1:A:426:GLY:HA2	1:A:428:ILE:N	2.04	0.72
2:B:102:ARG:NH1	2:B:175:SER:HA	2.04	0.72
1:A:64:PHE:HE2	1:A:88:ALA:HB2	1.53	0.72
3:C:248:ASP:O	3:C:249:LEU:C	2.27	0.72
4:D:102:ARG:HE	4:D:109:LEU:HD22	1.54	0.72
2:B:77:THR:HG22	2:B:130:PRO:HA	1.72	0.72
2:B:309:VAL:HG22	2:B:326:THR:HA	1.71	0.72
4:D:50:HIS:HB3	4:D:54:VAL:CB	2.20	0.72
1:A:351:GLU:OE2	1:A:404:ALA:HB3	1.89	0.72
2:B:261:SER:HB3	2:B:320:GLY:HA3	1.70	0.72
6:F:6:VAL:HB	6:F:10:SER:HB2	1.70	0.72
1:A:383:LEU:HD22	1:A:388:ARG:HA	1.70	0.72
6:F:33:ARG:NH2	6:F:91:GLU:OE2	2.23	0.72
3:C:296:PHE:CE1	3:C:300:ILE:HG13	2.25	0.72
4:D:214:LEU:O	4:D:218:LEU:HG	1.90	0.72
5:E:77:LYS:HD2	5:E:98:VAL:HG21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:76:VAL:HG12	9:I:76:VAL:O	1.89	0.72
1:A:15:GLN:O	1:A:26:ALA:HA	1.90	0.72
3:C:81:TYR:OH	4:D:118:ARG:NH2	2.23	0.72
3:C:315:MET:HA	3:C:318:ARG:HG3	1.71	0.71
1:A:392:LEU:CA	1:A:395:TRP:CD1	2.67	0.71
3:C:263:ASN:CG	3:C:264:THR:H	1.98	0.71
1:A:39:VAL:HG11	1:A:117:VAL:HG21	1.72	0.71
1:A:162:PRO:O	1:A:165:GLN:HG2	1.89	0.71
2:B:76:THR:HG21	2:B:133:ARG:CZ	2.21	0.71
3:C:36:LEU:HD22	3:C:235:LEU:HB2	1.71	0.71
3:C:221:HIS:HB3	3:C:222:PRO:HD3	1.71	0.71
3:C:378:LYS:NZ	6:F:91:GLU:OE1	2.24	0.71
5:E:96:LEU:HD21	5:E:195:VAL:HG21	1.71	0.71
1:A:243:HIS:CD2	1:A:425:PHE:CE1	2.79	0.71
3:C:217:LYS:HG3	7:G:7:LEU:HD13	1.72	0.71
3:C:300:ILE:HD13	3:C:362:ILE:HG21	1.72	0.71
1:A:223:TYR:CD2	1:A:224:ASP:N	2.57	0.71
3:C:71:ARG:HH21	4:D:196:PRO:HG3	1.56	0.71
3:C:138:MET:HE1	3:C:269:LYS:H	1.54	0.71
2:B:67:HIS:HD2	2:B:144:LEU:CD2	2.04	0.71
2:B:348:ALA:HB1	2:B:415:LYS:HA	1.73	0.70
5:E:168:SER:OG	5:E:170:ARG:NE	2.20	0.70
3:C:219:PRO:HG2	3:C:222:PRO:HG2	1.73	0.70
4:D:6:HIS:C	4:D:8:PRO:HD2	2.16	0.70
7:G:73:ASN:N	7:G:74:PRO:CD	2.55	0.70
3:C:72:ASP:OD1	4:D:49:ARG:NH1	2.15	0.70
3:C:252:ASP:HB3	3:C:253:PRO:HD3	1.74	0.70
3:C:269:LYS:CD	3:C:340:GLY:HA2	2.21	0.70
1:A:32:GLN:HB3	1:A:33:PRO:HD2	1.73	0.70
1:A:67:THR:CG2	1:A:70:ARG:HB2	2.20	0.70
2:B:366:ALA:O	2:B:370:MET:HG3	1.91	0.70
4:D:48:TYR:OH	4:D:68:VAL:HG11	1.92	0.70
5:E:65:SER:O	5:E:69:LEU:HB2	1.92	0.70
3:C:244:LEU:O	4:D:201:ARG:HD3	1.91	0.70
1:A:75:LEU:HD21	1:A:116:ILE:CD1	2.21	0.70
1:A:111:GLU:HG2	1:A:213:GLN:HE22	1.55	0.70
4:D:113:LEU:HD22	4:D:116:ILE:HD12	1.71	0.70
3:C:92:ILE:O	3:C:96:MET:HG2	1.91	0.70
6:F:73:GLN:HG2	7:G:36:ASN:HD21	1.56	0.70
3:C:206:ASN:ND2	3:C:207:ASN:H	1.90	0.69
4:D:27:ARG:NH1	10:J:58:LYS:HG3	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:187:CYS:O	4:D:190:LEU:HB2	1.92	0.69
5:E:95:PRO:HB2	5:E:137:GLY:HA3	1.73	0.69
1:A:248:LEU:CD1	1:A:425:PHE:CE2	2.74	0.69
4:D:30:PHE:CE1	4:D:50:HIS:CE1	2.80	0.69
3:C:51:LEU:HD11	3:C:80:ARG:HA	1.74	0.69
6:F:73:GLN:HA	7:G:39:ARG:HH21	1.56	0.69
10:J:58:LYS:HG2	10:J:59:TYR:H	1.56	0.69
1:A:291:SER:O	1:A:293:PRO:HD3	1.91	0.69
1:A:317:THR:CG2	1:A:318:GLY:N	2.56	0.69
2:B:124:LEU:HD13	2:B:223:PHE:CG	2.28	0.69
2:B:237:ALA:HB2	2:B:318:ASP:CG	2.17	0.69
4:D:219:VAL:HG22	4:D:222:MET:HE2	1.75	0.69
5:E:33:LYS:HB3	10:J:10:TYR:CE2	2.27	0.69
2:B:89:ILE:HG22	2:B:94:GLY:O	1.92	0.69
2:B:168:TYR:HD1	2:B:238:LYS:O	1.76	0.69
2:B:198:HIS:CE1	2:B:233:SER:HB3	2.28	0.69
3:C:275:LEU:O	3:C:276:PHE:C	2.36	0.69
6:F:59:VAL:HG11	7:G:10:VAL:HG22	1.74	0.69
1:A:39:VAL:HG12	1:A:41:ILE:CD1	2.22	0.69
1:A:248:LEU:CD1	1:A:425:PHE:HE2	2.03	0.69
2:B:53:ALA:HB2	2:B:198:HIS:HB3	1.74	0.69
2:B:58:GLU:OE2	2:B:66:SER:HB3	1.92	0.69
3:C:26:ASN:OD1	6:F:66:LEU:HD22	1.93	0.69
7:G:71:ARG:HH21	8:H:60:ASP:CG	2.00	0.69
9:I:64:LEU:HG	9:I:65:VAL:HG23	1.74	0.69
5:E:102:THR:O	5:E:105:GLU:N	2.26	0.69
1:A:317:THR:HG22	1:A:318:GLY:H	1.58	0.69
2:B:109:VAL:HG22	2:B:119:LEU:CD2	2.22	0.68
3:C:328:LEU:O	3:C:332:LEU:HD12	1.92	0.68
4:D:183:ALA:HA	4:D:186:VAL:HG23	1.75	0.68
9:I:53:GLU:O	9:I:54:SER:C	2.37	0.68
1:A:158:PHE:CE1	1:A:317:THR:CG2	2.65	0.68
1:A:173:ASN:O	1:A:174:VAL:C	2.37	0.68
1:A:42:ASP:CB	1:A:384:LEU:HD22	2.08	0.68
1:A:329:MET:HE2	7:G:2:ARG:HD2	1.76	0.68
2:B:406:ALA:HB3	2:B:409:ASP:HB2	1.74	0.68
3:C:280:ILE:HD13	3:C:355:SER:OG	1.93	0.68
5:E:15:ARG:NH1	7:G:23:GLN:O	2.27	0.68
4:D:82:MET:SD	4:D:86:LYS:HD2	2.33	0.68
2:B:303:VAL:HG12	2:B:304:HIS:N	2.08	0.68
2:B:29:LEU:CD1	2:B:33:LEU:HD21	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:206:ASN:CB	3:C:313:ARG:NH2	2.54	0.68
3:C:237:LEU:HD22	4:D:216:LEU:HD11	1.75	0.68
4:D:117:VAL:HG13	4:D:124:GLU:N	2.08	0.68
9:I:72:VAL:CB	9:I:73:PRO:HD3	2.24	0.68
1:A:328:HIS:CD2	1:A:329:MET:HG2	2.29	0.68
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.29	0.68
5:E:117:LEU:HD13	5:E:121:GLN:H	1.59	0.68
3:C:277:ALA:HB1	3:C:294:LEU:HD11	1.75	0.68
4:D:62:LYS:O	4:D:66:GLU:HG3	1.94	0.68
4:D:165:TYR:CZ	4:D:168:VAL:HG13	2.28	0.68
1:A:192:ALA:HA	1:A:194:ARG:N	2.09	0.67
2:B:156:GLN:NE2	9:I:56:ARG:HD3	2.08	0.67
2:B:183:ILE:HG22	2:B:184:GLY:N	2.08	0.67
4:D:131:LEU:HD13	4:D:164:ILE:HD12	1.75	0.67
1:A:422:VAL:HG21	1:A:437:ILE:HD13	1.75	0.67
3:C:379:TRP:CZ3	6:F:37:ILE:HG23	2.29	0.67
4:D:134:TYR:HE2	4:D:163:PRO:HG2	1.58	0.67
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.10	0.67
2:B:200:THR:HG22	2:B:203:ARG:CD	2.24	0.67
2:B:283:PRO:HG3	9:I:55:LEU:CD2	2.23	0.67
3:C:261:PRO:O	3:C:262:LEU:HD23	1.92	0.67
4:D:50:HIS:HB3	4:D:54:VAL:CG2	2.24	0.67
3:C:296:PHE:HD1	3:C:359:PHE:HE1	1.41	0.67
4:D:64:LEU:O	4:D:68:VAL:HG23	1.94	0.67
4:D:26:ILE:CG2	4:D:54:VAL:HG13	2.25	0.67
4:D:57:THR:HB	4:D:60:GLU:HB2	1.77	0.67
5:E:29:SER:HA	5:E:32:ARG:HD3	1.75	0.67
1:A:287:GLY:O	1:A:290:LEU:HG	1.95	0.67
3:C:47:THR:CG2	3:C:83:HIS:HB2	2.25	0.67
9:I:64:LEU:CD1	9:I:65:VAL:HG23	2.24	0.67
1:A:43:ALA:CB	1:A:189:HIS:HB3	2.25	0.67
1:A:111:GLU:HG2	1:A:213:GLN:NE2	2.10	0.67
3:C:59:THR:HG23	3:C:135:TRP:NE1	2.09	0.67
3:C:67:THR:O	3:C:71:ARG:HG3	1.94	0.67
1:A:120:CYS:O	1:A:122:LEU:HG	1.94	0.67
2:B:204:MET:HE1	2:B:224:LEU:HD22	1.77	0.67
3:C:22:PRO:HG2	7:G:3:GLN:HB3	1.77	0.67
4:D:10:TYR:O	4:D:12:TRP:CD1	2.48	0.67
5:E:80:ASP:OD1	5:E:81:ILE:N	2.28	0.67
6:F:28:LYS:HB3	6:F:74:ILE:HD11	1.77	0.67
7:G:28:HIS:CD2	7:G:31:SER:HB3	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:117:VAL:CG1	4:D:124:GLU:H	2.08	0.67
1:A:38:GLY:HA3	1:A:40:TRP:HZ3	1.58	0.66
5:E:33:LYS:HB3	10:J:10:TYR:HE2	1.60	0.66
1:A:146:ARG:NH2	1:A:308:GLN:HE22	1.92	0.66
2:B:182:ARG:HH12	2:B:185:LYS:HE2	1.60	0.66
2:B:305:GLN:CB	2:B:306:PRO:HD3	2.19	0.66
3:C:44:GLN:HE22	3:C:86:GLY:HA3	1.60	0.66
3:C:137:GLN:HB2	3:C:257:THR:HG22	1.75	0.66
3:C:311:LYS:HD2	3:C:379:TRP:HB3	1.78	0.66
3:C:207:ASN:HD22	3:C:210:GLY:H	1.43	0.66
4:D:50:HIS:O	4:D:54:VAL:N	2.24	0.66
10:J:51:LEU:H	10:J:54:HIS:HD2	1.42	0.66
1:A:198:ALA:HB1	1:A:379:ILE:CG2	2.26	0.66
8:H:35:GLU:O	8:H:39:LEU:HG	1.96	0.66
1:A:27:SER:HB3	1:A:208:LEU:CD2	2.25	0.66
1:A:106:LEU:HD22	1:A:203:LEU:CD1	2.26	0.66
1:A:166:SER:CB	5:E:3:THR:HG22	2.25	0.66
3:C:345:HIS:CB	3:C:346:PRO:CD	2.71	0.66
3:C:357:LEU:HG	3:C:361:LEU:HD11	1.76	0.66
5:E:123:ASP:OD1	5:E:168:SER:HB3	1.95	0.66
2:B:384:SER:HB3	9:I:62:ARG:HG2	1.77	0.66
3:C:310:SER:HB3	3:C:318:ARG:HH12	1.60	0.66
10:J:58:LYS:HG2	10:J:59:TYR:N	2.11	0.66
2:B:309:VAL:HG22	2:B:326:THR:HG22	1.78	0.65
4:D:23:HIS:CD2	10:J:51:LEU:HA	2.31	0.65
4:D:102:ARG:HA	4:D:108:ALA:O	1.96	0.65
1:A:64:PHE:CE2	1:A:88:ALA:HB2	2.30	0.65
1:A:236:PHE:HE2	1:A:258:GLU:HB3	1.57	0.65
4:D:102:ARG:HE	4:D:109:LEU:CD2	2.09	0.65
4:D:113:LEU:O	4:D:114:SER:C	2.39	0.65
4:D:225:HIS:O	4:D:228:SER:OG	2.14	0.65
4:D:150:ASN:OD1	4:D:151:PRO:HD2	1.96	0.65
4:D:161:ALA:O	4:D:163:PRO:HD3	1.95	0.65
1:A:211:LEU:HD12	1:A:211:LEU:O	1.97	0.65
1:A:236:PHE:HD2	1:A:258:GLU:CG	2.08	0.65
2:B:51:ILE:CG2	2:B:199:PHE:HA	2.24	0.65
2:B:62:ASN:C	2:B:62:ASN:HD22	2.01	0.65
3:C:151:SER:HB3	3:C:161:VAL:HG21	1.77	0.65
12:C:380:HEM:HHC	12:C:380:HEM:CBB	2.24	0.65
1:A:67:THR:OG1	1:A:115:ASP:OD1	2.12	0.65
4:D:69:GLU:O	4:D:73:GLY:CA	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:LEU:HD13	2:B:93:GLY:CA	2.26	0.65
2:B:261:SER:HB2	2:B:321:LEU:N	2.12	0.65
3:C:25:SER:HA	3:C:218:ILE:HD12	1.77	0.65
3:C:221:HIS:N	3:C:222:PRO:HD2	2.12	0.65
7:G:28:HIS:O	7:G:29:TYR:C	2.39	0.65
8:H:52:GLU:OE1	8:H:52:GLU:HA	1.96	0.65
9:I:58:GLN:HG2	9:I:78:TYR:CD2	2.32	0.65
1:A:106:LEU:HD22	1:A:203:LEU:HD13	1.78	0.64
2:B:174:ASN:C	2:B:174:ASN:HD22	1.96	0.64
3:C:166:GLY:HA3	3:C:177:ARG:NH2	2.12	0.64
4:D:181:GLN:HA	8:H:77:LEU:CD1	2.25	0.64
6:F:28:LYS:CD	6:F:74:ILE:HD11	2.27	0.64
4:D:231:LYS:HD3	6:F:71:ARG:HG2	1.78	0.64
1:A:86:LEU:HD13	1:A:99:ILE:CD1	2.27	0.64
1:A:351:GLU:OE2	1:A:404:ALA:N	2.30	0.64
2:B:198:HIS:HE1	2:B:233:SER:CB	2.09	0.64
5:E:18:VAL:HG11	5:E:32:ARG:NH1	2.13	0.64
2:B:169:ARG:NH1	2:B:238:LYS:HZ2	1.95	0.64
3:C:214:ASP:HB3	7:G:7:LEU:HB3	1.78	0.64
4:D:50:HIS:O	4:D:51:LEU:C	2.40	0.64
1:A:106:LEU:O	1:A:107:PRO:C	2.40	0.64
3:C:272:TRP:CE2	3:C:273:TYR:HD1	2.15	0.64
8:H:21:ARG:HB3	8:H:65:ARG:NH2	2.12	0.64
1:A:6:GLN:O	1:A:7:ALA:C	2.40	0.64
2:B:361:LYS:O	2:B:365:LYS:HG3	1.97	0.64
1:A:41:ILE:HD12	1:A:41:ILE:H	1.63	0.64
2:B:162:ASN:HD22	2:B:244:ILE:HG22	1.62	0.64
2:B:209:LEU:HG	2:B:209:LEU:O	1.96	0.64
3:C:206:ASN:CB	3:C:313:ARG:HH21	2.08	0.64
5:E:122:HIS:O	5:E:123:ASP:C	2.40	0.64
1:A:417:ASP:OD1	1:A:438:ARG:NH2	2.30	0.64
2:B:378:PHE:O	2:B:382:VAL:HG23	1.98	0.64
3:C:8:HIS:CB	3:C:9:PRO:CD	2.75	0.64
3:C:78:ILE:HD11	5:E:57:GLN:HE22	1.63	0.64
7:G:34:ILE:CB	7:G:35:PRO:HD3	2.28	0.64
9:I:64:LEU:HG	9:I:64:LEU:O	1.97	0.64
1:A:255:ILE:HD13	1:A:342:TRP:CH2	2.33	0.64
2:B:262:ALA:HB2	2:B:272:PHE:CE2	2.32	0.64
5:E:136:ILE:HG22	5:E:138:VAL:HG23	1.80	0.64
6:F:88:SER:HB3	6:F:91:GLU:CD	2.22	0.64
9:I:53:GLU:O	9:I:55:LEU:HG	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:LEU:O	2:B:128:THR:HB	1.98	0.64
2:B:262:ALA:HB3	2:B:269:ALA:HA	1.80	0.64
2:B:322:PHE:CD1	2:B:322:PHE:C	2.76	0.64
4:D:138:PRO:HD2	4:D:141:VAL:HG11	1.80	0.64
5:E:118:ARG:HE	5:E:171:ILE:HG13	1.63	0.64
7:G:54:ALA:O	7:G:58:VAL:HG23	1.98	0.64
10:J:9:LEU:HD12	10:J:13:LEU:HD12	1.80	0.64
1:A:80:GLU:O	1:A:83:GLY:N	2.31	0.63
4:D:115:TYR:HD2	4:D:119:ALA:HB2	1.63	0.63
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.78	0.63
6:F:13:LEU:HA	6:F:16:ILE:HD11	1.79	0.63
6:F:44:LYS:HA	6:F:44:LYS:NZ	2.12	0.63
6:F:101:ARG:HG2	6:F:105:GLU:OE2	1.98	0.63
7:G:33:GLY:O	7:G:34:ILE:C	2.41	0.63
6:F:37:ILE:HD11	6:F:90:LEU:HD23	1.79	0.63
4:D:82:MET:CE	4:D:86:LYS:HD2	2.29	0.63
8:H:62:LEU:HA	8:H:65:ARG:HG2	1.80	0.63
9:I:64:LEU:HD12	9:I:65:VAL:H	1.62	0.63
1:A:236:PHE:HZ	1:A:317:THR:HA	1.63	0.63
6:F:55:TYR:C	6:F:55:TYR:CD1	2.77	0.63
3:C:254:ASP:HB3	4:D:119:ALA:O	1.98	0.63
4:D:7:PRO:HB2	8:H:63:HIS:HE1	1.63	0.63
1:A:70:ARG:HB3	1:A:74:ALA:HB3	1.81	0.63
1:A:75:LEU:HD21	1:A:116:ILE:CG1	2.28	0.63
3:C:306:LEU:N	3:C:306:LEU:HD23	2.14	0.63
4:D:23:HIS:NE2	10:J:51:LEU:HA	2.14	0.63
4:D:119:ALA:O	4:D:120:ARG:C	2.40	0.63
9:I:70:LEU:CD2	9:I:73:PRO:HD2	2.28	0.63
1:A:240:GLN:NE2	1:A:431:LEU:CD2	2.61	0.63
2:B:180:ASP:HA	2:B:183:ILE:HD12	1.79	0.63
2:B:309:VAL:CG2	2:B:326:THR:HG22	2.28	0.63
3:C:47:THR:HG22	3:C:48:GLY:N	2.13	0.63
4:D:211:MET:HA	4:D:211:MET:CE	2.27	0.63
1:A:18:GLN:HE21	1:A:22:GLY:CA	2.00	0.63
2:B:129:ALA:N	2:B:130:PRO:CD	2.61	0.63
3:C:124:MET:HG2	3:C:274:PHE:HE1	1.63	0.63
3:C:298:ILE:HG22	3:C:299:LEU:HD23	1.81	0.63
4:D:3:LEU:HD22	7:G:70:LYS:NZ	2.13	0.63
4:D:34:LYS:O	4:D:34:LYS:HG2	1.99	0.63
1:A:36:THR:CB	1:A:372:THR:HG22	2.29	0.62
2:B:56:ARG:NE	2:B:103:GLU:OE1	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:SER:HA	3:C:272:TRP:HZ2	1.64	0.62
7:G:29:TYR:CD2	7:G:30:PHE:HD2	2.17	0.62
1:A:389:ARG:C	1:A:391:PRO:HD3	2.23	0.62
1:A:392:LEU:HA	1:A:395:TRP:HD1	1.53	0.62
4:D:75:ASN:ND2	4:D:80:MET:O	2.32	0.62
4:D:165:TYR:CD1	4:D:168:VAL:HG22	2.34	0.62
4:D:229:VAL:HG22	7:G:20:PRO:HD3	1.81	0.62
11:K:18:VAL:HB	11:K:19:PRO:HD3	1.81	0.62
1:A:385:THR:CG2	1:A:386:TYR:CD1	2.82	0.62
2:B:264:ILE:HG21	2:B:317:SER:HA	1.81	0.62
2:B:292:THR:HG21	2:B:363:LYS:NZ	2.15	0.62
3:C:320:LEU:HB2	3:C:373:GLU:OE2	1.99	0.62
2:B:102:ARG:HH12	2:B:175:SER:HA	1.63	0.62
3:C:157:GLY:O	3:C:160:LEU:HB3	2.00	0.62
11:K:20:THR:HG23	11:K:24:TRP:CD1	2.35	0.62
1:A:188:ARG:O	1:A:191:LYS:HE2	1.99	0.62
1:A:262:TRP:CG	1:A:385:THR:HG23	2.34	0.62
3:C:327:ALA:O	3:C:331:ASP:N	2.29	0.62
5:E:117:LEU:CD1	5:E:120:PRO:HA	2.30	0.62
7:G:64:GLN:O	7:G:65:GLU:C	2.41	0.62
5:E:122:HIS:O	5:E:125:GLU:HG2	2.00	0.62
7:G:67:GLU:O	7:G:71:ARG:HB3	1.99	0.62
1:A:142:ASP:OD1	5:E:2:HIS:ND1	2.33	0.62
2:B:304:HIS:CD2	2:B:305:GLN:N	2.68	0.62
3:C:190:MET:O	3:C:194:MET:HG3	1.99	0.62
5:E:116:GLN:HA	5:E:116:GLN:HE21	1.65	0.62
5:E:175:PRO:O	5:E:176:ALA:C	2.42	0.62
1:A:159:GLN:HE22	7:G:18:LEU:HD21	1.65	0.61
4:D:126:TYR:OH	13:D:242:HEC:HBA2	2.00	0.61
5:E:29:SER:CB	5:E:32:ARG:HD3	2.30	0.61
1:A:134:ILE:N	1:A:134:ILE:CD1	2.62	0.61
3:C:90:PHE:CE1	3:C:123:VAL:HG11	2.35	0.61
4:D:208:MET:HE3	4:D:209:LEU:N	2.13	0.61
6:F:57:ASP:O	6:F:61:ARG:HG2	2.00	0.61
6:F:91:GLU:O	6:F:95:LYS:HG3	1.98	0.61
1:A:61:HIS:CD2	1:A:134:ILE:CD1	2.81	0.61
1:A:91:THR:CG2	1:A:92:ARG:N	2.63	0.61
1:A:25:VAL:HG12	1:A:205:HIS:CE1	2.35	0.61
1:A:53:ASN:CG	1:A:165:GLN:HB2	2.25	0.61
1:A:308:GLN:HG3	1:A:308:GLN:O	1.98	0.61
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:158:CYS:HB3	5:E:163:SER:HB2	1.83	0.61
1:A:385:THR:HB	1:A:386:TYR:CD1	2.35	0.61
2:B:247:GLN:NE2	2:B:429:ASN:HA	2.15	0.61
3:C:8:HIS:HB3	3:C:9:PRO:CD	2.31	0.61
4:D:176:PRO:HB2	4:D:181:GLN:HE22	1.64	0.61
6:F:96:GLU:OE1	6:F:99:ARG:HD2	2.00	0.61
8:H:21:ARG:CB	8:H:65:ARG:HH21	2.13	0.61
1:A:86:LEU:CD1	1:A:99:ILE:HG12	2.30	0.61
2:B:264:ILE:HG22	2:B:317:SER:HA	1.82	0.61
2:B:270:ASN:O	2:B:274:VAL:HG23	2.00	0.61
3:C:132:VAL:HA	3:C:139:SER:HB2	1.82	0.61
7:G:56:TYR:HD1	7:G:57:LEU:HD23	1.65	0.61
3:C:185:LEU:HB3	3:C:186:PRO:CD	2.27	0.61
4:D:11:PRO:HG2	8:H:74:PHE:CD1	2.35	0.61
4:D:48:TYR:OH	4:D:68:VAL:HG21	2.01	0.61
2:B:174:ASN:O	2:B:174:ASN:ND2	2.26	0.61
3:C:214:ASP:HA	3:C:217:LYS:HE2	1.82	0.61
3:C:234:LEU:HD23	4:D:216:LEU:HD21	1.82	0.61
3:C:269:LYS:HD3	3:C:340:GLY:HA2	1.81	0.61
1:A:4:TYR:O	1:A:7:ALA:HB3	2.00	0.61
1:A:317:THR:CG2	1:A:318:GLY:H	2.14	0.61
1:A:408:ARG:NH2	11:K:15:ARG:HE	1.99	0.61
3:C:27:ILE:O	3:C:27:ILE:HG22	1.99	0.61
3:C:40:CYS:HB3	3:C:90:PHE:CD2	2.36	0.61
3:C:88:SER:O	3:C:92:ILE:HG13	2.01	0.61
3:C:240:MET:O	3:C:244:LEU:HB2	2.01	0.61
4:D:72:ASP:O	4:D:73:GLY:O	2.19	0.61
4:D:76:GLU:O	4:D:76:GLU:HG2	2.01	0.61
4:D:178:THR:HB	4:D:181:GLN:CG	2.28	0.61
7:G:8:THR:CG2	7:G:9:ARG:H	2.03	0.61
3:C:41:LEU:O	3:C:45:ILE:HG13	2.01	0.61
4:D:34:LYS:HD3	4:D:35:GLN:NE2	2.15	0.61
5:E:147:ILE:O	5:E:156:TYR:HA	2.00	0.61
1:A:11:VAL:HG13	1:A:12:PRO:HD2	1.82	0.60
1:A:34:THR:HB	2:B:373:GLU:OE1	1.99	0.60
1:A:166:SER:O	1:A:167:VAL:C	2.43	0.60
1:A:236:PHE:CD2	1:A:258:GLU:HB3	2.35	0.60
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.16	0.60
1:A:106:LEU:HD21	1:A:203:LEU:HD13	1.83	0.60
2:B:275:LEU:HB2	2:B:410:VAL:HG13	1.83	0.60
5:E:34:GLY:CA	10:J:10:TYR:HD2	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ASP:OD1	1:A:430:GLN:NE2	2.34	0.60
5:E:9:ASP:OD1	5:E:11:SER:OG	2.20	0.60
3:C:78:ILE:O	3:C:79:ILE:C	2.43	0.60
3:C:135:TRP:CE3	3:C:175:LEU:HD22	2.36	0.60
4:D:211:MET:HE1	10:J:31:PHE:CZ	2.36	0.60
5:E:6:LYS:H	5:E:6:LYS:HD2	1.65	0.60
5:E:136:ILE:HD11	5:E:183:PRO:HG3	1.84	0.60
6:F:44:LYS:HA	6:F:44:LYS:HZ3	1.64	0.60
8:H:49:GLN:NE2	8:H:52:GLU:OE2	2.34	0.60
1:A:241:ILE:HD12	7:G:16:TYR:HE1	1.65	0.60
2:B:101:THR:HG23	2:B:103:GLU:H	1.67	0.60
2:B:328:SER:OG	2:B:333:ALA:HA	2.02	0.60
5:E:42:THR:O	5:E:45:VAL:N	2.34	0.60
5:E:141:HIS:CE1	5:E:142:LEU:HG	2.36	0.60
2:B:68:LEU:HD22	2:B:186:VAL:HB	1.84	0.60
2:B:304:HIS:CD2	2:B:305:GLN:H	2.19	0.60
5:E:172:ARG:NE	5:E:172:ARG:HA	2.15	0.60
10:J:21:ALA:O	10:J:22:LEU:C	2.43	0.60
1:A:51:LYS:HE2	1:A:177:LEU:HD12	1.83	0.60
1:A:163:LEU:HD21	1:A:314:TYR:CD2	2.37	0.60
3:C:296:PHE:CD1	3:C:359:PHE:HE1	2.20	0.60
4:D:27:ARG:NH2	4:D:60:GLU:OE2	2.35	0.60
4:D:51:LEU:HD22	4:D:58:GLU:HA	1.84	0.60
2:B:384:SER:CB	9:I:62:ARG:HG2	2.32	0.60
4:D:27:ARG:NH1	10:J:58:LYS:CE	2.64	0.60
5:E:29:SER:CA	5:E:32:ARG:HD3	2.31	0.60
5:E:136:ILE:CD1	5:E:183:PRO:HG3	2.31	0.60
1:A:106:LEU:N	1:A:107:PRO:HD2	2.17	0.60
1:A:385:THR:HG22	1:A:386:TYR:N	2.16	0.60
2:B:332:SER:O	2:B:333:ALA:C	2.45	0.60
3:C:329:VAL:O	3:C:332:LEU:HB2	2.01	0.60
5:E:77:LYS:CE	5:E:98:VAL:HG21	2.32	0.60
1:A:91:THR:HG23	1:A:92:ARG:H	1.66	0.60
1:A:198:ALA:CB	1:A:379:ILE:HG22	2.32	0.60
1:A:390:ILE:N	1:A:391:PRO:HD3	2.17	0.60
2:B:262:ALA:HB3	2:B:269:ALA:N	2.17	0.60
4:D:72:ASP:OD1	4:D:76:GLU:OE1	2.20	0.60
4:D:206:LEU:C	4:D:206:LEU:HD22	2.27	0.60
5:E:69:LEU:O	5:E:70:ALA:C	2.45	0.60
5:E:123:ASP:HB2	5:E:170:ARG:NH2	2.16	0.60
2:B:140:LEU:O	2:B:141:GLN:C	2.44	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:161:ALA:HB1	4:D:162:PRO:HD2	1.84	0.59
5:E:77:LYS:CD	5:E:98:VAL:HG21	2.32	0.59
1:A:143:THR:HG23	1:A:143:THR:O	2.02	0.59
1:A:170:PRO:O	1:A:171:SER:C	2.45	0.59
2:B:169:ARG:NH1	2:B:238:LYS:NZ	2.47	0.59
3:C:44:GLN:OE1	3:C:44:GLN:HA	2.01	0.59
4:D:178:THR:CB	4:D:181:GLN:HE21	2.15	0.59
1:A:142:ASP:OD2	5:E:1:SER:HB2	2.02	0.59
1:A:151:ASN:HD22	5:E:2:HIS:CD2	2.20	0.59
2:B:299:VAL:O	2:B:303:VAL:HG23	2.03	0.59
4:D:117:VAL:HG13	4:D:124:GLU:H	1.64	0.59
1:A:442:PHE:O	1:A:443:TRP:CD1	2.56	0.59
4:D:138:PRO:O	4:D:139:THR:C	2.45	0.59
1:A:379:ILE:HD12	1:A:390:ILE:CD1	2.32	0.59
2:B:109:VAL:HG22	2:B:119:LEU:HD21	1.84	0.59
2:B:279:LEU:HD23	2:B:294:SER:HB3	1.84	0.59
3:C:177:ARG:O	3:C:181:PHE:HD2	1.85	0.59
5:E:161:HIS:HB2	14:E:197:FES:S1	2.42	0.59
1:A:328:HIS:NE2	1:A:329:MET:HG2	2.17	0.59
1:A:373:THR:N	1:A:374:PRO:HD2	2.17	0.59
3:C:44:GLN:OE1	3:C:83:HIS:ND1	2.35	0.59
4:D:27:ARG:NH1	10:J:58:LYS:HZ1	1.92	0.59
5:E:77:LYS:HG3	5:E:193:VAL:HG13	1.83	0.59
8:H:22:GLU:O	8:H:25:GLU:HG2	2.02	0.59
1:A:74:ALA:O	1:A:75:LEU:C	2.45	0.59
3:C:41:LEU:CD1	12:C:380:HEM:HBB1	2.33	0.59
5:E:33:LYS:HA	7:G:21:PHE:CE2	2.37	0.59
1:A:49:SER:N	1:A:52:ASN:OD1	2.34	0.59
1:A:171:SER:O	1:A:174:VAL:HB	2.02	0.59
2:B:266:SER:O	2:B:269:ALA:HB3	2.03	0.59
3:C:170:VAL:HG12	3:C:170:VAL:O	2.01	0.59
5:E:119:ASP:OD1	5:E:178:LEU:HA	2.02	0.59
2:B:182:ARG:HH11	2:B:185:LYS:HE2	1.64	0.59
1:A:166:SER:HB3	5:E:3:THR:HG22	1.84	0.59
1:A:428:ILE:CG2	1:A:431:LEU:HB3	2.33	0.59
2:B:207:ILE:HD11	2:B:383:GLY:HA2	1.85	0.59
3:C:292:LEU:N	3:C:292:LEU:HD23	2.17	0.59
4:D:28:ARG:NH1	8:H:78:LYS:OXT	2.35	0.59
5:E:147:ILE:H	5:E:157:TYR:H	1.48	0.59
1:A:86:LEU:HD13	1:A:99:ILE:HG12	1.84	0.58
1:A:255:ILE:HD13	1:A:342:TRP:CZ3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.67	0.58
4:D:56:TYR:HD1	4:D:60:GLU:CD	2.10	0.58
1:A:136:GLN:HE21	9:I:50:LEU:HB3	1.68	0.58
1:A:252:HIS:CD2	1:A:325:VAL:HG22	2.38	0.58
1:A:444:LEU:O	1:A:445:ARG:HG3	2.03	0.58
2:B:49:LEU:HD23	2:B:127:THR:HG21	1.85	0.58
2:B:303:VAL:CG1	2:B:304:HIS:N	2.66	0.58
4:D:5:LEU:CD1	8:H:59:LEU:HB3	2.33	0.58
4:D:5:LEU:C	4:D:7:PRO:HD2	2.28	0.58
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.38	0.58
1:A:294:LEU:HD23	1:A:307:PHE:CZ	2.39	0.58
2:B:95:LYS:NZ	9:I:70:LEU:HD22	2.17	0.58
3:C:107:TYR:C	3:C:107:TYR:CD1	2.81	0.58
1:A:373:THR:N	1:A:374:PRO:CD	2.66	0.58
12:C:381:HEM:O2A	12:C:381:HEM:HHA	2.02	0.58
9:I:58:GLN:HG2	9:I:78:TYR:HD2	1.66	0.58
2:B:175:SER:OG	2:B:176:LEU:N	2.35	0.58
3:C:246:ALA:N	3:C:247:PRO:CD	2.67	0.58
3:C:361:LEU:HD23	3:C:365:LEU:HD12	1.84	0.58
8:H:65:ARG:HG3	8:H:66:ASP:N	2.17	0.58
1:A:11:VAL:CG1	1:A:12:PRO:HD2	2.32	0.58
1:A:73:ASN:ND2	1:A:73:ASN:N	2.52	0.58
1:A:385:THR:HB	1:A:386:TYR:HD1	1.68	0.58
2:B:97:SER:OG	9:I:70:LEU:HB2	2.02	0.58
2:B:132:PHE:HB3	2:B:137:VAL:HG21	1.85	0.58
2:B:147:ASP:O	2:B:150:VAL:HG22	2.04	0.58
2:B:203:ARG:HE	2:B:230:LEU:HD23	1.66	0.58
2:B:304:HIS:CG	2:B:305:GLN:H	2.21	0.58
3:C:27:ILE:O	3:C:27:ILE:CG2	2.51	0.58
10:J:49:GLY:HA2	10:J:54:HIS:CB	2.33	0.58
2:B:24:LEU:HG	2:B:38:LEU:HD11	1.86	0.58
2:B:304:HIS:CG	2:B:305:GLN:N	2.71	0.58
2:B:395:PRO:O	2:B:398:VAL:HB	2.04	0.58
4:D:187:CYS:O	4:D:190:LEU:N	2.36	0.58
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.04	0.58
9:I:58:GLN:HA	9:I:78:TYR:CD2	2.38	0.58
2:B:182:ARG:NH1	2:B:185:LYS:HG2	2.18	0.58
2:B:203:ARG:HH21	2:B:230:LEU:HA	1.69	0.58
2:B:212:SER:OG	2:B:215:VAL:HB	2.03	0.58
2:B:247:GLN:HE22	2:B:429:ASN:ND2	2.00	0.58
4:D:72:ASP:OD2	4:D:92:PRO:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:76:GLU:O	4:D:76:GLU:CG	2.52	0.58
2:B:206:LEU:O	2:B:207:ILE:HD13	2.04	0.58
2:B:300:ALA:HB2	2:B:307:PHE:HZ	1.69	0.58
8:H:37:LEU:HD21	8:H:58:LEU:HA	1.84	0.58
1:A:3:THR:HG23	2:B:114:ASP:OD1	2.03	0.57
1:A:333:ASP:O	1:A:337:VAL:HG23	2.04	0.57
8:H:15:ASP:HB2	8:H:16:PRO:CD	2.33	0.57
2:B:99:THR:CG2	2:B:100:SER:N	2.67	0.57
4:D:94:PRO:HB2	4:D:95:TYR:CE1	2.39	0.57
5:E:185:TYR:HB3	5:E:195:VAL:HA	1.86	0.57
1:A:46:ARG:HG2	1:A:46:ARG:O	2.02	0.57
1:A:343:MET:HE1	1:A:416:TYR:CD2	2.38	0.57
2:B:58:GLU:OE1	2:B:63:LEU:HA	2.04	0.57
3:C:85:ASN:OD1	3:C:243:VAL:HG23	2.04	0.57
3:C:103:TYR:OH	3:C:322:GLN:HG3	2.04	0.57
3:C:153:ILE:CG2	3:C:156:ILE:HG12	2.34	0.57
3:C:272:TRP:NE1	3:C:273:TYR:HD1	2.02	0.57
5:E:67:ASP:OD1	5:E:68:VAL:N	2.36	0.57
2:B:35:ILE:HB	2:B:206:LEU:HB3	1.84	0.57
2:B:177:TYR:O	2:B:178:CYS:C	2.47	0.57
2:B:279:LEU:HD22	2:B:295:LEU:CD1	2.26	0.57
3:C:181:PHE:O	3:C:185:LEU:HB2	2.04	0.57
4:D:6:HIS:N	4:D:7:PRO:HD2	2.19	0.57
8:H:55:THR:O	8:H:56:GLU:C	2.46	0.57
1:A:428:ILE:CG2	1:A:431:LEU:CB	2.80	0.57
3:C:264:THR:O	3:C:266:PRO:CD	2.50	0.57
3:C:313:ARG:HB3	6:F:38:HIS:CD2	2.40	0.57
3:C:355:SER:O	3:C:356:VAL:C	2.43	0.57
4:D:3:LEU:HD11	7:G:71:ARG:HB2	1.85	0.57
5:E:23:LYS:HG3	5:E:24:SER:H	1.70	0.57
5:E:59:VAL:O	5:E:59:VAL:HG12	2.04	0.57
7:G:3:GLN:HA	7:G:3:GLN:OE1	2.04	0.57
9:I:64:LEU:CG	9:I:65:VAL:HG23	2.35	0.57
11:K:23:LEU:HD23	11:K:23:LEU:N	2.19	0.57
2:B:318:ASP:OD1	2:B:318:ASP:N	2.38	0.57
2:B:412:ASN:O	2:B:415:LYS:HB2	2.05	0.57
1:A:76:GLU:HA	1:A:79:VAL:HG23	1.86	0.57
2:B:62:ASN:O	2:B:62:ASN:ND2	2.36	0.57
2:B:166:ALA:HB2	2:B:244:ILE:HD12	1.86	0.57
2:B:239:TYR:OH	2:B:421:ARG:O	2.17	0.57
4:D:23:HIS:CD2	10:J:52:TRP:N	2.73	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:66:ASP:O	8:H:67:HIS:C	2.46	0.57
1:A:224:ASP:OD1	1:A:227:ALA:CB	2.52	0.57
1:A:274:ASN:HD21	1:A:320:LEU:HD11	1.69	0.57
1:A:308:GLN:O	1:A:308:GLN:CG	2.52	0.57
3:C:170:VAL:HG13	3:C:174:THR:CG2	2.32	0.57
4:D:6:HIS:CG	4:D:7:PRO:HD3	2.39	0.57
4:D:23:HIS:CD2	10:J:52:TRP:H	2.23	0.57
2:B:262:ALA:HB3	2:B:269:ALA:CA	2.35	0.57
3:C:19:ILE:HG22	3:C:20:ASP:OD1	2.05	0.57
5:E:114:VAL:HA	5:E:117:LEU:HD11	1.86	0.57
1:A:431:LEU:O	1:A:432:PRO:O	2.22	0.56
1:A:442:PHE:O	1:A:443:TRP:HD1	1.88	0.56
12:C:380:HEM:O2D	12:C:380:HEM:HBA2	2.04	0.56
4:D:182:VAL:O	4:D:186:VAL:HG23	2.04	0.56
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.35	0.56
3:C:218:ILE:HG23	3:C:223:TYR:CD2	2.40	0.56
5:E:91:TRP:CE3	5:E:96:LEU:HD22	2.40	0.56
8:H:34:ARG:O	8:H:38:GLU:HG2	2.04	0.56
2:B:49:LEU:HD11	2:B:204:MET:HB3	1.87	0.56
2:B:362:ASN:HA	2:B:365:LYS:HD2	1.87	0.56
3:C:50:PHE:CE2	5:E:62:MET:HE2	2.41	0.56
3:C:104:TYR:CE1	3:C:208:PRO:HA	2.40	0.56
3:C:215:VAL:HG11	6:F:59:VAL:CG1	2.34	0.56
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.87	0.56
4:D:131:LEU:HD13	4:D:164:ILE:CD1	2.36	0.56
4:D:240:PRO:HD3	7:G:12:HIS:CE1	2.40	0.56
10:J:55:ILE:CG2	10:J:58:LYS:HE2	2.34	0.56
1:A:236:PHE:CZ	1:A:317:THR:HA	2.40	0.56
2:B:71:LEU:HD13	2:B:143:GLN:HG3	1.87	0.56
3:C:51:LEU:O	3:C:53:MET:N	2.38	0.56
1:A:46:ARG:O	1:A:46:ARG:CG	2.53	0.56
1:A:351:GLU:OE2	1:A:404:ALA:CB	2.52	0.56
2:B:192:HIS:O	2:B:193:ASP:C	2.49	0.56
4:D:49:ARG:HG3	4:D:49:ARG:O	2.06	0.56
5:E:127:VAL:HG12	5:E:133:VAL:HA	1.87	0.56
7:G:68:LYS:HD3	7:G:72:LYS:NZ	2.19	0.56
1:A:262:TRP:CE3	1:A:385:THR:CG2	2.87	0.56
3:C:51:LEU:HD13	12:C:380:HEM:O1D	2.05	0.56
5:E:29:SER:OG	5:E:32:ARG:HD3	2.05	0.56
6:F:32:MET:O	6:F:33:ARG:C	2.49	0.56
1:A:351:GLU:OE2	1:A:403:ASP:OD1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLN:HG2	1:A:19:LEU:O	2.06	0.56
1:A:39:VAL:CG1	1:A:41:ILE:HD11	2.36	0.56
1:A:77:LYS:HG2	2:B:291:ALA:CB	2.36	0.56
1:A:294:LEU:HD23	1:A:307:PHE:CE1	2.40	0.56
2:B:213:HIS:N	2:B:214:PRO:CD	2.69	0.56
2:B:375:SER:OG	2:B:376:GLU:N	2.38	0.56
3:C:25:SER:CA	3:C:218:ILE:HD12	2.35	0.56
3:C:130:GLY:HA3	3:C:182:HIS:CE1	2.41	0.56
3:C:307:LEU:HD13	3:C:362:ILE:O	2.06	0.56
3:C:343:VAL:O	3:C:348:ILE:HD11	2.05	0.56
4:D:94:PRO:HB2	4:D:95:TYR:CD1	2.41	0.56
6:F:55:TYR:O	6:F:59:VAL:HG23	2.06	0.56
7:G:68:LYS:O	7:G:69:SER:C	2.46	0.56
1:A:4:TYR:CE2	1:A:396:GLU:HG3	2.39	0.56
3:C:124:MET:CE	3:C:298:ILE:HD13	2.35	0.56
3:C:172:LYS:O	3:C:173:ALA:C	2.47	0.56
4:D:79:GLU:O	4:D:80:MET:C	2.48	0.56
1:A:255:ILE:HG21	1:A:335:MET:HE1	1.88	0.56
3:C:135:TRP:CH2	3:C:170:VAL:HG12	2.40	0.56
4:D:3:LEU:HD22	7:G:70:LYS:HZ3	1.71	0.56
4:D:5:LEU:HD23	4:D:152:TYR:CE1	2.41	0.56
4:D:106:ASN:HD22	4:D:106:ASN:C	2.14	0.56
4:D:228:SER:HB2	7:G:23:GLN:HE22	1.70	0.56
5:E:91:TRP:HZ3	5:E:136:ILE:HD11	1.69	0.56
10:J:17:THR:HA	10:J:20:PHE:HB3	1.87	0.56
2:B:25:GLU:HB3	2:B:213:HIS:ND1	2.20	0.55
5:E:117:LEU:HB2	5:E:120:PRO:HA	1.88	0.55
9:I:70:LEU:HD21	9:I:73:PRO:HD2	1.88	0.55
1:A:39:VAL:HG23	1:A:113:LEU:CD2	2.33	0.55
1:A:54:GLY:HA3	1:A:169:GLY:HA3	1.86	0.55
1:A:322:ALA:HB3	1:A:338:LEU:HD21	1.88	0.55
6:F:7:SER:HA	6:F:11:ARG:HE	1.71	0.55
2:B:33:LEU:HD23	2:B:33:LEU:H	1.70	0.55
7:G:60:THR:O	7:G:61:TRP:C	2.50	0.55
1:A:279:HIS:ND1	1:A:284:TYR:OH	2.38	0.55
3:C:25:SER:HA	3:C:218:ILE:CD1	2.37	0.55
3:C:207:ASN:O	3:C:208:PRO:C	2.48	0.55
3:C:259:ALA:O	3:C:261:PRO:HD3	2.06	0.55
4:D:32:VAL:HG11	4:D:186:VAL:HG22	1.89	0.55
5:E:82:PRO:O	5:E:83:GLU:C	2.48	0.55
5:E:168:SER:HB3	5:E:170:ARG:HH21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:LYS:HG3	2:B:177:TYR:HB3	1.89	0.55
3:C:270:PRO:CB	3:C:274:PHE:HB2	2.32	0.55
1:A:243:HIS:CD2	1:A:425:PHE:HE1	2.24	0.55
2:B:174:ASN:C	2:B:174:ASN:ND2	2.63	0.55
3:C:147:THR:HG22	3:C:161:VAL:HG13	1.88	0.55
3:C:313:ARG:HG3	3:C:313:ARG:O	2.05	0.55
1:A:131:ARG:NH2	1:A:177:LEU:O	2.39	0.55
1:A:262:TRP:CE3	1:A:385:THR:HG23	2.42	0.55
4:D:165:TYR:CG	4:D:168:VAL:HG22	2.41	0.55
5:E:95:PRO:HD2	5:E:138:VAL:HG22	1.88	0.55
6:F:88:SER:HB3	6:F:91:GLU:CG	2.36	0.55
10:J:32:GLU:HG2	10:J:33:ARG:N	2.20	0.55
1:A:224:ASP:O	1:A:227:ALA:N	2.40	0.55
1:A:429:GLU:O	1:A:429:GLU:HG3	2.06	0.55
2:B:162:ASN:HD22	2:B:244:ILE:HG21	1.70	0.55
2:B:345:LYS:HD3	2:B:418:VAL:CG1	2.37	0.55
3:C:303:LEU:O	3:C:304:ILE:C	2.50	0.55
5:E:91:TRP:CE2	5:E:92:ARG:HG3	2.42	0.55
1:A:213:GLN:CB	1:A:215:HIS:CD2	2.90	0.55
2:B:56:ARG:HH21	2:B:103:GLU:CD	2.14	0.55
2:B:304:HIS:CD2	2:B:306:PRO:CD	2.73	0.55
2:B:348:ALA:CB	2:B:415:LYS:HA	2.36	0.55
5:E:53:ASN:N	5:E:53:ASN:OD1	2.40	0.55
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.88	0.55
1:A:276:ILE:HD11	1:A:354:VAL:HA	1.88	0.55
2:B:406:ALA:O	2:B:407:ASP:C	2.49	0.55
4:D:28:ARG:HD2	4:D:185:ASP:OD2	2.07	0.55
7:G:73:ASN:H	7:G:74:PRO:HD2	1.69	0.55
1:A:334:MET:HA	1:A:334:MET:HE3	1.89	0.54
2:B:268:GLU:O	2:B:269:ALA:C	2.51	0.54
2:B:342:ASN:O	2:B:345:LYS:HB2	2.07	0.54
3:C:338:ILE:HD13	3:C:338:ILE:N	2.22	0.54
1:A:163:LEU:HD21	1:A:314:TYR:HD2	1.71	0.54
2:B:299:VAL:CG1	2:B:303:VAL:HG21	2.37	0.54
4:D:153:PHE:CD2	4:D:158:ILE:HD12	2.43	0.54
1:A:240:GLN:HE21	1:A:431:LEU:HD21	1.70	0.54
1:A:243:HIS:CD2	1:A:425:PHE:CD1	2.94	0.54
2:B:203:ARG:CZ	2:B:230:LEU:HD23	2.37	0.54
4:D:69:GLU:O	4:D:73:GLY:HA3	2.08	0.54
4:D:211:MET:SD	5:E:49:TYR:HD2	2.29	0.54
7:G:68:LYS:O	7:G:72:LYS:N	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:ASN:HB2	6:F:69:SER:OG	2.08	0.54
3:C:33:PHE:CE1	3:C:96:MET:HG3	2.42	0.54
2:B:357:VAL:O	2:B:361:LYS:HG3	2.07	0.54
3:C:24:PRO:O	3:C:224:TYR:OH	2.13	0.54
3:C:107:TYR:HB3	3:C:113:TRP:CE3	2.43	0.54
3:C:140:PHE:C	3:C:140:PHE:CD1	2.85	0.54
3:C:271:GLU:O	3:C:272:TRP:C	2.50	0.54
4:D:2:ASP:HB3	4:D:156:GLN:NE2	2.22	0.54
1:A:46:ARG:HH12	1:A:315:ALA:HB3	1.73	0.54
1:A:291:SER:HA	2:B:87:ARG:NH1	2.22	0.54
2:B:169:ARG:HH11	2:B:238:LYS:HZ1	1.49	0.54
3:C:263:ASN:OD1	3:C:264:THR:N	2.33	0.54
4:D:178:THR:HG21	8:H:16:PRO:HG2	1.90	0.54
4:D:178:THR:O	4:D:179:MET:C	2.50	0.54
5:E:166:ASP:C	5:E:166:ASP:OD1	2.50	0.54
1:A:128:GLU:OE2	1:A:131:ARG:NH1	2.40	0.54
1:A:223:TYR:CE2	1:A:224:ASP:HB3	2.42	0.54
1:A:281:ASP:OD1	1:A:282:CYS:N	2.40	0.54
1:A:386:TYR:CD1	1:A:386:TYR:N	2.75	0.54
1:A:406:VAL:O	1:A:410:VAL:HG23	2.08	0.54
2:B:299:VAL:HG13	2:B:303:VAL:HG21	1.89	0.54
3:C:269:LYS:NZ	3:C:340:GLY:CA	2.70	0.54
3:C:328:LEU:HB2	3:C:361:LEU:HD13	1.89	0.54
4:D:123:GLY:O	4:D:125:ASP:N	2.41	0.54
5:E:33:LYS:HA	7:G:21:PHE:CD2	2.43	0.54
1:A:162:PRO:O	1:A:165:GLN:NE2	2.41	0.54
1:A:414:TYR:O	1:A:418:GLN:HG3	2.08	0.54
2:B:168:TYR:CD1	2:B:238:LYS:O	2.60	0.54
2:B:338:LYS:CG	2:B:439:LEU:HD21	2.36	0.54
3:C:91:PHE:HB2	3:C:272:TRP:CZ2	2.43	0.54
3:C:276:PHE:O	3:C:277:ALA:C	2.51	0.54
4:D:82:MET:SD	4:D:86:LYS:HE3	2.47	0.54
5:E:155:GLY:HA3	5:E:165:TYR:O	2.08	0.54
7:G:28:HIS:HD2	7:G:31:SER:H	1.55	0.54
7:G:33:GLY:O	7:G:36:ASN:N	2.40	0.54
4:D:6:HIS:N	4:D:7:PRO:CD	2.71	0.54
4:D:143:LEU:HD22	4:D:147:LEU:O	2.07	0.54
1:A:86:LEU:HD13	1:A:99:ILE:HD13	1.90	0.54
1:A:261:GLY:HA2	1:A:314:TYR:O	2.08	0.54
1:A:301:ASN:O	1:A:302:LYS:C	2.50	0.54
2:B:183:ILE:O	2:B:186:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:THR:O	3:C:110:LEU:N	2.40	0.54
3:C:122:THR:CG2	3:C:185:LEU:HD11	2.38	0.54
3:C:210:GLY:HA3	3:C:314:SER:CB	2.32	0.54
5:E:23:LYS:HG3	5:E:24:SER:N	2.22	0.54
8:H:16:PRO:O	8:H:20:VAL:HG23	2.08	0.54
1:A:5:ALA:O	1:A:8:LEU:HB2	2.08	0.53
1:A:106:LEU:CD2	1:A:203:LEU:HD22	2.35	0.53
1:A:347:THR:HA	11:K:16:ASN:HD22	1.73	0.53
2:B:188:PRO:O	2:B:189:VAL:C	2.49	0.53
6:F:73:GLN:NE2	7:G:32:LYS:NZ	2.55	0.53
6:F:87:LYS:HE2	6:F:89:TYR:HB3	1.90	0.53
6:F:95:LYS:O	6:F:96:GLU:C	2.49	0.53
2:B:95:LYS:HG2	2:B:96:LEU:N	2.21	0.53
4:D:102:ARG:HG2	4:D:108:ALA:O	2.07	0.53
5:E:112:VAL:CG1	5:E:117:LEU:HD21	2.39	0.53
7:G:34:ILE:HB	7:G:35:PRO:CD	2.36	0.53
4:D:211:MET:HE1	10:J:31:PHE:HZ	1.73	0.53
2:B:393:THR:HG22	2:B:394:PRO:O	2.09	0.53
4:D:120:ARG:HG2	4:D:120:ARG:HH11	1.73	0.53
4:D:128:PHE:HB2	4:D:187:CYS:SG	2.48	0.53
5:E:34:GLY:HA2	10:J:10:TYR:HD2	1.71	0.53
5:E:45:VAL:HG23	10:J:24:ILE:HG23	1.90	0.53
5:E:121:GLN:HG2	5:E:125:GLU:OE2	2.08	0.53
5:E:192:MET:HA	5:E:192:MET:HE3	1.91	0.53
6:F:106:GLU:OE1	6:F:109:LYS:HE2	2.09	0.53
1:A:27:SER:HB3	1:A:208:LEU:HD22	1.90	0.53
1:A:51:LYS:O	1:A:53:ASN:N	2.42	0.53
2:B:213:HIS:O	2:B:213:HIS:HD2	1.90	0.53
3:C:79:ILE:HA	3:C:82:MET:HE3	1.89	0.53
4:D:116:ILE:HD13	13:D:242:HEC:HMA1	1.90	0.53
4:D:118:ARG:HG3	4:D:194:ALA:HB1	1.91	0.53
5:E:137:GLY:O	5:E:145:VAL:HG22	2.08	0.53
1:A:29:GLN:HG3	1:A:203:LEU:O	2.09	0.53
1:A:429:GLU:OE2	7:G:4:PHE:O	2.26	0.53
2:B:38:LEU:CD1	2:B:378:PHE:CE2	2.92	0.53
3:C:177:ARG:O	3:C:181:PHE:CD2	2.61	0.53
3:C:309:THR:HG21	3:C:370:GLY:HA3	1.90	0.53
5:E:32:ARG:HH12	7:G:22:GLU:CD	2.16	0.53
5:E:157:TYR:O	5:E:159:PRO:HD3	2.08	0.53
9:I:72:VAL:CB	9:I:73:PRO:CD	2.78	0.53
3:C:300:ILE:HD13	3:C:362:ILE:CG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:ARG:CB	5:E:16:PRO:HD2	2.38	0.53
5:E:191:ASP:N	5:E:191:ASP:OD1	2.41	0.53
7:G:56:TYR:CD1	7:G:57:LEU:HD23	2.43	0.53
1:A:48:GLU:OE1	1:A:52:ASN:O	2.27	0.53
2:B:59:ASN:O	2:B:63:LEU:HG	2.09	0.53
2:B:258:VAL:HG11	2:B:321:LEU:HB3	1.91	0.53
3:C:91:PHE:CB	3:C:272:TRP:CH2	2.92	0.53
3:C:304:ILE:O	3:C:305:PRO:C	2.50	0.53
5:E:91:TRP:NE1	5:E:92:ARG:HG3	2.23	0.53
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.44	0.53
1:A:156:THR:HG23	1:A:239:SER:OG	2.08	0.53
1:A:227:ALA:O	1:A:229:PRO:HD3	2.09	0.53
1:A:426:GLY:HA2	1:A:427:PRO:C	2.33	0.53
2:B:155:PRO:O	2:B:156:GLN:C	2.52	0.53
3:C:89:MET:HE2	3:C:238:ALA:HB3	1.91	0.53
12:C:380:HEM:CMC	12:C:380:HEM:HBC2	2.39	0.53
4:D:233:ARG:HG2	7:G:17:SER:CB	2.20	0.53
9:I:64:LEU:HD12	9:I:64:LEU:C	2.31	0.53
1:A:78:GLU:HG2	1:A:112:LEU:HD21	1.91	0.53
1:A:394:GLU:O	1:A:395:TRP:C	2.49	0.53
2:B:248:ASN:CB	2:B:428:GLY:HA2	2.31	0.53
3:C:4:ILE:O	3:C:5:ARG:C	2.52	0.53
4:D:136:GLU:O	4:D:137:PRO:C	2.50	0.53
6:F:73:GLN:HA	7:G:39:ARG:NH2	2.21	0.53
7:G:29:TYR:HD2	7:G:30:PHE:HD2	1.46	0.53
1:A:159:GLN:HE22	7:G:18:LEU:CD2	2.22	0.52
2:B:135:TRP:NE1	2:B:136:GLU:HG3	2.24	0.52
2:B:379:LEU:HG	2:B:379:LEU:O	2.09	0.52
4:D:176:PRO:HB2	4:D:181:GLN:NE2	2.24	0.52
5:E:6:LYS:HD2	5:E:6:LYS:N	2.24	0.52
1:A:307:PHE:CD1	1:A:307:PHE:C	2.86	0.52
3:C:65:SER:OG	3:C:66:VAL:N	2.42	0.52
4:D:98:PRO:O	4:D:101:ALA:HB3	2.10	0.52
10:J:49:GLY:HA2	10:J:54:HIS:HB3	1.90	0.52
1:A:174:VAL:HG12	1:A:175:ARG:N	2.19	0.52
1:A:240:GLN:HE22	1:A:431:LEU:CD2	2.21	0.52
1:A:371:GLY:O	1:A:375:VAL:HG22	2.09	0.52
1:A:391:PRO:HB2	1:A:395:TRP:CZ2	2.44	0.52
1:A:395:TRP:O	1:A:396:GLU:C	2.51	0.52
3:C:37:LEU:HD23	3:C:93:CYS:HB3	1.91	0.52
5:E:191:ASP:OD1	5:E:192:MET:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:32:GLU:HG2	10:J:33:ARG:H	1.74	0.52
1:A:157:ALA:HB1	1:A:319:LEU:HD21	1.92	0.52
1:A:343:MET:HE2	1:A:442:PHE:HA	1.91	0.52
1:A:383:LEU:HD22	1:A:388:ARG:C	2.34	0.52
1:A:431:LEU:O	1:A:432:PRO:C	2.53	0.52
2:B:187:THR:O	2:B:190:GLU:HB2	2.08	0.52
2:B:303:VAL:CG1	2:B:307:PHE:CD2	2.92	0.52
1:A:171:SER:OG	1:A:172:GLU:N	2.41	0.52
2:B:67:HIS:CD2	2:B:144:LEU:HD22	2.37	0.52
2:B:261:SER:HB2	2:B:321:LEU:C	2.35	0.52
2:B:300:ALA:CB	2:B:307:PHE:HZ	2.22	0.52
3:C:47:THR:HG23	3:C:83:HIS:HB2	1.92	0.52
3:C:121:LEU:HD23	3:C:124:MET:CE	2.39	0.52
12:C:380:HEM:HBC2	12:C:380:HEM:HMC1	1.92	0.52
4:D:82:MET:HE1	4:D:86:LYS:HD2	1.91	0.52
1:A:136:GLN:CD	9:I:51:CYS:HB3	2.35	0.52
1:A:158:PHE:CZ	1:A:317:THR:HG21	2.38	0.52
1:A:180:ALA:O	1:A:183:THR:HB	2.10	0.52
1:A:350:THR:HB	1:A:353:GLU:CG	2.39	0.52
2:B:352:LEU:HD21	2:B:357:VAL:HG23	1.90	0.52
3:C:207:ASN:ND2	3:C:210:GLY:H	2.07	0.52
4:D:46:VAL:HG12	4:D:47:ALA:O	2.10	0.52
2:B:408:ALA:HA	2:B:411:ILE:HG13	1.92	0.52
3:C:223:TYR:HB3	4:D:227:TRP:CE2	2.45	0.52
3:C:299:LEU:O	3:C:300:ILE:C	2.52	0.52
4:D:6:HIS:O	4:D:8:PRO:HD2	2.10	0.52
4:D:137:PRO:HG3	4:D:143:LEU:HD11	1.92	0.52
10:J:32:GLU:CG	10:J:33:ARG:N	2.73	0.52
1:A:21:ASN:CB	1:A:217:SER:CB	2.64	0.52
2:B:169:ARG:HD3	2:B:238:LYS:NZ	2.22	0.52
3:C:178:PHE:O	3:C:179:PHE:C	2.52	0.52
4:D:10:TYR:H	4:D:125:ASP:CG	2.18	0.52
4:D:10:TYR:CB	4:D:125:ASP:OD1	2.54	0.52
1:A:50:GLU:O	1:A:173:ASN:ND2	2.42	0.52
2:B:196:GLN:HG2	2:B:197:ASN:OD1	2.09	0.52
2:B:262:ALA:HB2	2:B:268:GLU:HB3	1.92	0.52
3:C:107:TYR:C	3:C:107:TYR:HD1	2.17	0.52
4:D:183:ALA:O	4:D:184:LYS:C	2.53	0.52
4:D:239:PRO:HB2	4:D:241:LYS:HB3	1.92	0.52
8:H:59:LEU:O	8:H:60:ASP:C	2.52	0.52
1:A:75:LEU:CD2	1:A:116:ILE:HD11	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:THR:CG2	1:A:92:ARG:H	2.23	0.52
1:A:270:LEU:O	1:A:273:ALA:N	2.43	0.52
2:B:68:LEU:HB2	2:B:144:LEU:HD21	1.91	0.52
4:D:23:HIS:CD2	10:J:50:LYS:O	2.63	0.52
4:D:228:SER:HB2	7:G:23:GLN:HE21	1.74	0.52
5:E:20:ASP:O	5:E:21:SER:C	2.53	0.52
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.92	0.52
9:I:78:TYR:CD1	9:I:78:TYR:C	2.88	0.52
3:C:269:LYS:NZ	3:C:340:GLY:HA3	2.24	0.51
3:C:362:ILE:HA	3:C:366:MET:HE2	1.92	0.51
7:G:18:LEU:HB2	7:G:23:GLN:OE1	2.09	0.51
8:H:27:LEU:O	8:H:30:CYS:N	2.36	0.51
2:B:24:LEU:H	2:B:24:LEU:CD1	1.98	0.51
3:C:243:VAL:HG12	3:C:244:LEU:N	2.25	0.51
3:C:310:SER:HB3	3:C:318:ARG:HH11	1.72	0.51
3:C:338:ILE:HA	3:C:341:GLN:HG2	1.90	0.51
4:D:5:LEU:HD13	8:H:59:LEU:HB3	1.92	0.51
4:D:220:TYR:O	4:D:224:ARG:HG2	2.09	0.51
11:K:32:LEU:O	11:K:33:VAL:C	2.53	0.51
1:A:381:ARG:HA	1:A:384:LEU:HD12	1.92	0.51
1:A:428:ILE:O	1:A:431:LEU:N	2.39	0.51
2:B:197:ASN:HB2	2:B:198:HIS:CD2	2.45	0.51
2:B:354:ASN:N	2:B:355:PRO:HD2	2.25	0.51
4:D:76:GLU:OE2	4:D:93:LYS:O	2.28	0.51
6:F:7:SER:O	6:F:11:ARG:HB2	2.11	0.51
7:G:39:ARG:HA	7:G:42:ARG:HD2	1.92	0.51
10:J:43:TYR:O	10:J:46:ILE:HG13	2.10	0.51
1:A:239:SER:HB2	7:G:18:LEU:HD23	1.92	0.51
2:B:46:ARG:HH12	2:B:376:GLU:HG3	1.75	0.51
4:D:11:PRO:CD	8:H:70:ALA:HB1	2.39	0.51
10:J:9:LEU:HD12	10:J:13:LEU:CD1	2.40	0.51
1:A:48:GLU:OE1	1:A:53:ASN:O	2.28	0.51
4:D:120:ARG:HH11	4:D:120:ARG:CG	2.24	0.51
4:D:127:VAL:HG12	4:D:187:CYS:SG	2.50	0.51
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.26	0.51
5:E:94:LYS:HB3	5:E:95:PRO:CD	2.41	0.51
1:A:51:LYS:HE2	1:A:177:LEU:CD1	2.41	0.51
1:A:123:GLU:O	1:A:124:ASP:C	2.52	0.51
3:C:91:PHE:HB3	3:C:272:TRP:CH2	2.46	0.51
4:D:138:PRO:O	4:D:141:VAL:HB	2.11	0.51
4:D:161:ALA:O	4:D:163:PRO:CD	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:O	1:A:128:GLU:HG2	2.11	0.51
1:A:192:ALA:HB2	1:A:195:MET:HB2	1.92	0.51
1:A:408:ARG:HH22	11:K:15:ARG:HE	1.59	0.51
2:B:58:GLU:HB3	2:B:62:ASN:HB3	1.92	0.51
2:B:385:GLN:O	2:B:386:ALA:C	2.53	0.51
3:C:138:MET:HE1	3:C:269:LYS:N	2.25	0.51
3:C:153:ILE:HG21	3:C:156:ILE:HD11	1.91	0.51
3:C:186:PRO:HA	3:C:189:ILE:HG13	1.93	0.51
3:C:240:MET:HE3	3:C:244:LEU:HD22	1.91	0.51
6:F:87:LYS:HG3	6:F:89:TYR:HB3	1.91	0.51
1:A:176:LYS:O	1:A:177:LEU:C	2.52	0.51
1:A:327:ASP:OD1	1:A:328:HIS:N	2.43	0.51
1:A:390:ILE:N	1:A:391:PRO:CD	2.74	0.51
2:B:433:THR:O	2:B:434:PRO:C	2.53	0.51
3:C:341:GLN:HA	3:C:341:GLN:NE2	2.25	0.51
4:D:4:GLU:HG3	4:D:6:HIS:ND1	2.26	0.51
4:D:46:VAL:HG11	4:D:91:PHE:CE2	2.46	0.51
1:A:158:PHE:O	1:A:159:GLN:C	2.53	0.51
1:A:172:GLU:O	1:A:173:ASN:C	2.53	0.51
1:A:233:PRO:HA	1:A:316:ASP:HB3	1.92	0.51
2:B:47:ILE:HB	2:B:109:VAL:HG12	1.93	0.51
3:C:119:LEU:HG	12:C:381:HEM:CAB	2.40	0.51
3:C:250:LEU:O	3:C:252:ASP:N	2.44	0.51
3:C:328:LEU:HG	3:C:332:LEU:HD12	1.93	0.51
4:D:27:ARG:NH1	10:J:58:LYS:HE3	2.25	0.51
5:E:147:ILE:N	5:E:157:TYR:H	2.09	0.51
1:A:99:ILE:HG13	1:A:113:LEU:HD13	1.93	0.51
1:A:260:PRO:HG3	1:A:414:TYR:CZ	2.46	0.51
1:A:355:LEU:HD22	1:A:358:LYS:HZ3	1.75	0.51
2:B:237:ALA:CB	2:B:318:ASP:HB2	2.40	0.51
2:B:383:GLY:O	2:B:386:ALA:HB3	2.11	0.51
3:C:353:LEU:HD23	3:C:353:LEU:N	2.25	0.51
5:E:129:LYS:HG3	5:E:187:PHE:CE1	2.46	0.51
1:A:86:LEU:HD13	1:A:99:ILE:CG1	2.40	0.50
1:A:179:ARG:HG3	1:A:180:ALA:N	2.25	0.50
1:A:204:GLU:HG2	1:A:206:ARG:HB3	1.93	0.50
1:A:207:GLN:O	1:A:208:LEU:C	2.55	0.50
2:B:98:VAL:HG13	2:B:107:TYR:CE2	2.47	0.50
3:C:206:ASN:ND2	3:C:207:ASN:N	2.59	0.50
10:J:31:PHE:O	10:J:32:GLU:C	2.51	0.50
1:A:136:GLN:HE21	9:I:50:LEU:HG	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PHE:CD2	1:A:258:GLU:CB	2.93	0.50
2:B:255:ALA:HA	2:B:425:ALA:O	2.11	0.50
3:C:279:ALA:O	3:C:280:ILE:C	2.54	0.50
4:D:212:MET:HG3	4:D:216:LEU:HD12	1.93	0.50
5:E:123:ASP:O	5:E:125:GLU:N	2.44	0.50
1:A:236:PHE:CD2	1:A:258:GLU:CG	2.89	0.50
2:B:300:ALA:HA	2:B:307:PHE:HZ	1.75	0.50
4:D:33:TYR:HA	4:D:37:CYS:HB2	1.93	0.50
4:D:44:ASP:OD1	4:D:93:LYS:NZ	2.40	0.50
4:D:211:MET:SD	5:E:49:TYR:CD2	3.05	0.50
5:E:123:ASP:OD1	5:E:168:SER:CB	2.59	0.50
1:A:383:LEU:HD22	1:A:388:ARG:CA	2.40	0.50
2:B:122:PHE:O	2:B:126:VAL:HG23	2.11	0.50
4:D:6:HIS:O	4:D:8:PRO:CD	2.60	0.50
1:A:166:SER:O	1:A:169:GLY:N	2.41	0.50
1:A:289:HIS:O	1:A:290:LEU:C	2.54	0.50
5:E:188:THR:OG1	5:E:192:MET:HB2	2.11	0.50
6:F:25:GLY:O	6:F:26:PHE:C	2.54	0.50
10:J:55:ILE:O	10:J:58:LYS:HD3	2.12	0.50
1:A:136:GLN:NE2	9:I:50:LEU:HG	2.27	0.50
2:B:49:LEU:HD21	2:B:204:MET:SD	2.50	0.50
2:B:62:ASN:ND2	2:B:65:THR:OG1	2.45	0.50
2:B:262:ALA:CB	2:B:272:PHE:CE2	2.95	0.50
3:C:257:THR:O	3:C:258:PRO:C	2.52	0.50
3:C:263:ASN:CG	3:C:264:THR:N	2.69	0.50
3:C:309:THR:HG21	3:C:367:PRO:O	2.11	0.50
4:D:29:GLY:HA3	4:D:185:ASP:O	2.11	0.50
6:F:71:ARG:HH11	6:F:71:ARG:HB3	1.76	0.50
11:K:20:THR:HG23	11:K:24:TRP:HD1	1.76	0.50
1:A:42:ASP:HB2	1:A:94:HIS:ND1	2.26	0.50
2:B:71:LEU:HD21	2:B:147:ASP:OD2	2.11	0.50
2:B:198:HIS:O	2:B:203:ARG:HD3	2.12	0.50
4:D:35:GLN:OE1	4:D:35:GLN:HA	2.11	0.50
1:A:252:HIS:O	1:A:424:GLY:HA2	2.11	0.50
3:C:39:ILE:O	3:C:40:CYS:C	2.53	0.50
5:E:96:LEU:HD21	5:E:195:VAL:HG11	1.94	0.50
6:F:75:LEU:C	6:F:80:TRP:HE1	2.18	0.50
8:H:68:CYS:O	8:H:69:VAL:C	2.52	0.50
9:I:64:LEU:HD11	9:I:65:VAL:HG23	1.93	0.50
1:A:111:GLU:O	1:A:115:ASP:HB2	2.12	0.50
2:B:56:ARG:HA	2:B:174:ASN:HD21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:ILE:HG23	3:C:221:HIS:HB2	1.94	0.50
3:C:310:SER:OG	3:C:311:LYS:N	2.43	0.50
5:E:76:ILE:HA	5:E:193:VAL:O	2.12	0.50
11:K:32:LEU:HD12	11:K:36:THR:OG1	2.11	0.50
1:A:262:TRP:CE3	1:A:385:THR:HG21	2.47	0.49
1:A:329:MET:HA	1:A:430:GLN:OE1	2.12	0.49
2:B:133:ARG:O	2:B:134:ARG:C	2.54	0.49
3:C:26:ASN:ND2	3:C:26:ASN:C	2.70	0.49
3:C:46:LEU:O	3:C:47:THR:C	2.55	0.49
3:C:164:ILE:O	3:C:177:ARG:NH1	2.44	0.49
3:C:186:PRO:HG2	12:C:380:HEM:HMC3	1.94	0.49
3:C:376:LEU:HD12	6:F:20:TYR:CD2	2.47	0.49
6:F:13:LEU:HB3	6:F:16:ILE:HD11	1.93	0.49
6:F:76:PRO:O	6:F:80:TRP:CD1	2.64	0.49
8:H:53:ASP:C	8:H:53:ASP:OD1	2.53	0.49
1:A:30:SER:OG	1:A:32:GLN:HG2	2.12	0.49
1:A:192:ALA:HB1	1:A:193:PRO:HA	1.94	0.49
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.42	0.49
7:G:45:ILE:O	7:G:49:ALA:HB3	2.13	0.49
10:J:23:THR:HG22	10:J:24:ILE:N	2.25	0.49
2:B:217:LYS:HE3	2:B:221:GLU:OE2	2.11	0.49
3:C:40:CYS:HB3	3:C:90:PHE:HD2	1.77	0.49
5:E:116:GLN:HA	5:E:116:GLN:NE2	2.27	0.49
5:E:145:VAL:HG12	5:E:146:PRO:O	2.12	0.49
2:B:306:PRO:HB2	2:B:329:GLN:HE22	1.74	0.49
3:C:26:ASN:HA	6:F:70:MET:HA	1.94	0.49
3:C:51:LEU:O	3:C:52:ALA:C	2.54	0.49
3:C:129:MET:O	3:C:132:VAL:HB	2.12	0.49
4:D:187:CYS:O	4:D:188:THR:C	2.55	0.49
1:A:26:ALA:O	1:A:27:SER:HB3	2.12	0.49
1:A:53:ASN:HB3	1:A:170:PRO:HD2	1.95	0.49
1:A:322:ALA:HB2	1:A:338:LEU:HD11	1.95	0.49
1:A:433:ASP:O	1:A:437:ILE:HG13	2.13	0.49
2:B:286:LYS:HD3	2:B:287:ARG:NH1	2.28	0.49
2:B:367:GLY:O	2:B:371:SER:OG	2.28	0.49
3:C:345:HIS:HB3	3:C:346:PRO:HD2	1.89	0.49
4:D:7:PRO:N	4:D:8:PRO:HD2	2.27	0.49
6:F:28:LYS:HB3	6:F:74:ILE:CG1	2.42	0.49
10:J:3:PRO:HG2	10:J:8:ARG:HG2	1.94	0.49
1:A:379:ILE:HD12	1:A:390:ILE:HD12	1.94	0.49
1:A:433:ASP:OD2	3:C:223:TYR:OH	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:ALA:O	2:B:411:ILE:N	2.45	0.49
3:C:153:ILE:HG21	3:C:156:ILE:CG1	2.42	0.49
5:E:37:TYR:CZ	7:G:21:PHE:HZ	2.31	0.49
2:B:100:SER:HB2	2:B:105:MET:HG3	1.94	0.49
2:B:182:ARG:HH12	2:B:185:LYS:HG2	1.78	0.49
2:B:219:VAL:HG12	2:B:220:ALA:N	2.27	0.49
3:C:78:ILE:O	3:C:82:MET:HB2	2.13	0.49
3:C:163:TRP:O	3:C:177:ARG:NH1	2.38	0.49
3:C:344:GLU:OE1	7:G:66:PHE:CE1	2.65	0.49
1:A:51:LYS:O	1:A:173:ASN:ND2	2.46	0.49
1:A:144:SER:OG	1:A:147:ASP:HB2	2.13	0.49
1:A:232:SER:O	1:A:233:PRO:C	2.54	0.49
1:A:297:ILE:HD12	1:A:337:VAL:CG1	2.43	0.49
2:B:283:PRO:HG3	9:I:55:LEU:CG	2.43	0.49
9:I:54:SER:O	9:I:55:LEU:HD23	2.13	0.49
1:A:58:PHE:O	1:A:59:VAL:C	2.54	0.49
2:B:257:LEU:HD13	2:B:424:MET:CE	2.41	0.49
4:D:165:TYR:CE1	4:D:168:VAL:HG22	2.47	0.49
5:E:129:LYS:HD2	5:E:187:PHE:CE2	2.48	0.49
7:G:36:ASN:HA	7:G:39:ARG:CD	2.33	0.49
1:A:4:TYR:HE2	1:A:396:GLU:HG3	1.78	0.49
1:A:309:THR:HA	1:A:322:ALA:HA	1.94	0.49
1:A:379:ILE:HD12	1:A:390:ILE:HD11	1.95	0.49
2:B:276:GLN:HG2	2:B:277:HIS:N	2.28	0.49
2:B:393:THR:HG22	2:B:398:VAL:HG23	1.94	0.49
3:C:345:HIS:O	3:C:346:PRO:C	2.55	0.49
5:E:81:ILE:HG22	5:E:100:HIS:CB	2.42	0.49
5:E:148:ALA:O	5:E:149:ASN:C	2.56	0.49
11:K:34:SER:O	11:K:35:ALA:C	2.55	0.49
1:A:369:LEU:HD21	1:A:378:ASP:OD2	2.13	0.48
2:B:295:LEU:O	2:B:299:VAL:HG23	2.13	0.48
2:B:434:PRO:HB3	2:B:438:GLU:HB3	1.95	0.48
3:C:71:ARG:NH2	4:D:193:ALA:O	2.46	0.48
3:C:88:SER:HA	3:C:272:TRP:CZ2	2.45	0.48
3:C:257:THR:HG22	3:C:257:THR:O	2.13	0.48
3:C:379:TRP:CH2	6:F:37:ILE:HG23	2.48	0.48
4:D:30:PHE:CD1	4:D:189:PHE:CE2	2.92	0.48
5:E:53:ASN:O	5:E:54:VAL:C	2.54	0.48
8:H:15:ASP:CB	8:H:16:PRO:CD	2.91	0.48
1:A:67:THR:HG22	1:A:70:ARG:CB	2.30	0.48
2:B:262:ALA:CB	2:B:269:ALA:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:SER:HB3	9:I:62:ARG:HD2	1.94	0.48
3:C:153:ILE:HG21	3:C:156:ILE:HG12	1.95	0.48
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.46	0.48
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.48	0.48
1:A:36:THR:HA	1:A:99:ILE:O	2.13	0.48
2:B:99:THR:HG22	2:B:100:SER:N	2.27	0.48
4:D:210:LEU:O	4:D:211:MET:C	2.57	0.48
9:I:58:GLN:HB3	9:I:78:TYR:HB2	1.95	0.48
2:B:303:VAL:HG11	2:B:307:PHE:CD2	2.48	0.48
3:C:77:TRP:O	3:C:81:TYR:HD2	1.97	0.48
3:C:296:PHE:O	3:C:300:ILE:HB	2.14	0.48
3:C:304:ILE:HB	3:C:305:PRO:HD3	1.94	0.48
2:B:135:TRP:CD1	2:B:136:GLU:HG3	2.48	0.48
4:D:48:TYR:OH	4:D:68:VAL:CB	2.61	0.48
4:D:48:TYR:HH	4:D:68:VAL:HG11	1.77	0.48
1:A:19:LEU:HG	1:A:23:LEU:HB3	1.96	0.48
1:A:34:THR:HG22	1:A:101:ALA:O	2.14	0.48
1:A:245:GLU:O	1:A:247:GLY:N	2.47	0.48
1:A:279:HIS:CE1	1:A:284:TYR:HH	2.29	0.48
1:A:365:LEU:O	1:A:369:LEU:HD12	2.13	0.48
2:B:69:LEU:O	2:B:72:ALA:N	2.44	0.48
2:B:276:GLN:OE1	2:B:313:ASN:HB3	2.13	0.48
2:B:289:SER:OG	2:B:290:ASN:N	2.46	0.48
3:C:8:HIS:O	3:C:9:PRO:C	2.56	0.48
3:C:36:LEU:HD22	3:C:235:LEU:CB	2.42	0.48
3:C:47:THR:HG21	3:C:83:HIS:CB	2.43	0.48
8:H:21:ARG:O	8:H:24:CYS:HB2	2.14	0.48
2:B:258:VAL:CG1	2:B:321:LEU:HB3	2.43	0.48
3:C:3:ASN:CA	3:C:8:HIS:NE2	2.77	0.48
3:C:73:VAL:HG12	3:C:76:GLY:HA3	1.93	0.48
4:D:43:MET:HA	4:D:112:ASP:OD1	2.14	0.48
4:D:102:ARG:HH21	4:D:109:LEU:HD23	1.78	0.48
5:E:12:ASP:O	7:G:24:ARG:NH2	2.39	0.48
8:H:52:GLU:O	8:H:53:ASP:C	2.57	0.48
1:A:408:ARG:HH22	11:K:15:ARG:NE	2.11	0.48
1:A:417:ASP:OD1	1:A:438:ARG:NH1	2.46	0.48
2:B:140:LEU:O	2:B:143:GLN:N	2.46	0.48
2:B:231:GLY:C	2:B:233:SER:N	2.67	0.48
4:D:35:GLN:HB2	4:D:169:LEU:CD1	2.43	0.48
4:D:138:PRO:HD2	4:D:141:VAL:CG1	2.43	0.48
6:F:28:LYS:HB3	6:F:74:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:ASN:CG	6:F:41:ASP:H	2.21	0.48
8:H:22:GLU:O	8:H:23:GLN:C	2.54	0.48
1:A:240:GLN:HG3	1:A:422:VAL:CB	2.38	0.48
1:A:343:MET:HE2	1:A:442:PHE:CA	2.44	0.48
1:A:343:MET:CE	1:A:416:TYR:CD2	2.97	0.48
1:A:381:ARG:HA	1:A:384:LEU:CD1	2.44	0.48
2:B:46:ARG:CZ	2:B:376:GLU:HB2	2.43	0.48
2:B:46:ARG:NH1	2:B:376:GLU:HB2	2.29	0.48
2:B:46:ARG:NH2	2:B:376:GLU:HB2	2.28	0.48
2:B:203:ARG:HG2	2:B:230:LEU:HD21	1.95	0.48
2:B:322:PHE:CD1	2:B:323:GLY:N	2.82	0.48
2:B:333:ALA:O	2:B:337:ILE:HD12	2.14	0.48
3:C:192:ILE:O	3:C:193:ALA:C	2.54	0.48
3:C:218:ILE:CG2	3:C:223:TYR:CD2	2.96	0.48
3:C:366:MET:HB2	3:C:367:PRO:HD3	1.95	0.48
4:D:199:ASP:O	4:D:200:HIS:C	2.55	0.48
4:D:206:LEU:C	4:D:206:LEU:CD2	2.87	0.48
5:E:101:ARG:HG3	5:E:131:GLU:O	2.12	0.48
1:A:36:THR:HG21	1:A:373:THR:HA	1.96	0.48
1:A:45:SER:HA	1:A:48:GLU:HG3	1.95	0.48
2:B:156:GLN:OE1	9:I:58:GLN:NE2	2.33	0.48
2:B:306:PRO:HB2	2:B:329:GLN:HE21	1.77	0.48
2:B:348:ALA:HB3	2:B:418:VAL:HG21	1.95	0.48
3:C:3:ASN:HA	3:C:8:HIS:CD2	2.49	0.48
3:C:124:MET:HE3	3:C:298:ILE:HD13	1.96	0.48
3:C:171:ASP:O	3:C:172:LYS:C	2.56	0.48
3:C:182:HIS:O	3:C:186:PRO:HD2	2.14	0.48
3:C:197:LEU:HD12	3:C:197:LEU:HA	1.80	0.48
3:C:358:TYR:CD1	3:C:358:TYR:C	2.92	0.48
4:D:72:ASP:O	4:D:72:ASP:OD1	2.32	0.48
4:D:79:GLU:OE1	4:D:82:MET:HG3	2.13	0.48
4:D:100:ALA:O	4:D:101:ALA:C	2.56	0.48
5:E:106:ILE:HD11	5:E:131:GLU:HA	1.96	0.48
1:A:61:HIS:CB	1:A:130:GLU:HG3	2.44	0.47
1:A:223:TYR:CE2	1:A:224:ASP:CB	2.97	0.47
1:A:399:ILE:O	1:A:402:VAL:HG23	2.14	0.47
2:B:163:LEU:O	2:B:164:HIS:C	2.54	0.47
2:B:258:VAL:CG1	2:B:321:LEU:HD22	2.44	0.47
3:C:163:TRP:O	3:C:164:ILE:C	2.57	0.47
5:E:171:ILE:O	5:E:172:ARG:HD2	2.14	0.47
1:A:34:THR:CG2	2:B:370:MET:HG2	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLN:O	1:A:342:TRP:C	2.56	0.47
1:A:377:GLU:O	1:A:378:ASP:C	2.57	0.47
2:B:308:ASP:HB2	9:I:54:SER:HB2	1.96	0.47
3:C:47:THR:HG21	3:C:83:HIS:HB2	1.96	0.47
3:C:149:LEU:HD21	3:C:281:LEU:CD2	2.44	0.47
4:D:26:ILE:HG22	4:D:27:ARG:N	2.29	0.47
5:E:168:SER:CB	5:E:170:ARG:HH21	2.26	0.47
2:B:341:TYR:CD2	2:B:345:LYS:HE3	2.48	0.47
3:C:44:GLN:HE22	3:C:86:GLY:CA	2.24	0.47
3:C:90:PHE:O	3:C:94:LEU:HB2	2.15	0.47
3:C:317:PHE:CD1	6:F:26:PHE:HB3	2.49	0.47
6:F:50:LEU:N	6:F:50:LEU:HD23	2.30	0.47
6:F:91:GLU:N	6:F:92:PRO:CD	2.77	0.47
2:B:283:PRO:CG	9:I:55:LEU:HD13	2.44	0.47
2:B:303:VAL:HG11	2:B:307:PHE:CG	2.50	0.47
3:C:313:ARG:CB	6:F:38:HIS:CD2	2.98	0.47
4:D:162:PRO:O	4:D:163:PRO:C	2.57	0.47
4:D:165:TYR:O	4:D:168:VAL:CG2	2.55	0.47
9:I:58:GLN:O	9:I:59:ALA:HB2	2.14	0.47
1:A:52:ASN:HB2	1:A:55:ALA:CB	2.38	0.47
2:B:213:HIS:O	2:B:213:HIS:CD2	2.67	0.47
3:C:70:CYS:SG	3:C:80:ARG:HD2	2.55	0.47
3:C:342:PRO:HG2	7:G:66:PHE:CZ	2.50	0.47
4:D:69:GLU:O	4:D:73:GLY:HA2	2.15	0.47
5:E:81:ILE:CD1	5:E:87:MET:HB2	2.44	0.47
9:I:57:GLY:O	9:I:78:TYR:CE2	2.68	0.47
9:I:72:VAL:HB	9:I:73:PRO:HD2	1.92	0.47
1:A:167:VAL:O	1:A:168:GLU:C	2.55	0.47
1:A:186:LEU:O	1:A:187:SER:C	2.58	0.47
1:A:272:VAL:O	1:A:275:ALA:HB3	2.14	0.47
2:B:37:SER:HB3	2:B:213:HIS:HB2	1.95	0.47
3:C:131:TYR:O	3:C:134:PRO:HD2	2.13	0.47
4:D:48:TYR:OH	4:D:68:VAL:CG1	2.61	0.47
4:D:165:TYR:CE1	4:D:168:VAL:HA	2.49	0.47
8:H:70:ALA:HA	8:H:73:LEU:CD2	2.37	0.47
1:A:257:VAL:O	1:A:257:VAL:HG23	2.15	0.47
2:B:219:VAL:O	2:B:220:ALA:C	2.56	0.47
3:C:137:GLN:NE2	3:C:263:ASN:HB3	2.29	0.47
3:C:156:ILE:HG12	3:C:157:GLY:H	1.79	0.47
3:C:221:HIS:HB3	3:C:222:PRO:CD	2.41	0.47
4:D:3:LEU:N	4:D:3:LEU:HD23	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:208:MET:HE3	4:D:209:LEU:CA	2.45	0.47
4:D:224:ARG:O	4:D:225:HIS:C	2.54	0.47
5:E:16:PRO:HB2	5:E:17:GLU:HG2	1.96	0.47
6:F:91:GLU:HB2	6:F:92:PRO:HD3	1.96	0.47
7:G:50:PRO:CB	7:G:51:PRO:HD3	2.44	0.47
1:A:46:ARG:HB3	1:A:92:ARG:O	2.14	0.47
1:A:334:MET:O	1:A:336:PHE:N	2.47	0.47
3:C:4:ILE:O	3:C:4:ILE:HG22	2.15	0.47
3:C:32:ASN:HD21	3:C:228:ASP:HA	1.79	0.47
3:C:120:LEU:HB2	12:C:381:HEM:CMC	2.45	0.47
3:C:156:ILE:O	3:C:157:GLY:C	2.57	0.47
4:D:23:HIS:HA	4:D:26:ILE:HB	1.97	0.47
5:E:33:LYS:CB	10:J:10:TYR:CE2	2.97	0.47
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.96	0.47
6:F:67:ASP:O	6:F:70:MET:HE3	2.14	0.47
1:A:95:THR:HG21	1:A:190:TYR:OH	2.15	0.47
1:A:422:VAL:HG21	1:A:437:ILE:CD1	2.44	0.47
2:B:170:ASN:CG	2:B:171:ALA:N	2.73	0.47
3:C:7:SER:O	3:C:8:HIS:O	2.32	0.47
3:C:106:SER:C	3:C:108:THR:H	2.23	0.47
3:C:160:LEU:O	3:C:161:VAL:C	2.58	0.47
3:C:186:PRO:HB3	12:C:380:HEM:CBB	2.45	0.47
6:F:33:ARG:O	6:F:35:ASP:N	2.48	0.47
8:H:66:ASP:HA	8:H:69:VAL:HG23	1.96	0.47
1:A:131:ARG:O	1:A:132:ASP:C	2.58	0.47
3:C:183:PHE:CE1	3:C:187:PHE:HE2	2.33	0.47
3:C:272:TRP:NE1	3:C:273:TYR:CD1	2.82	0.47
3:C:291:VAL:O	3:C:294:LEU:HB3	2.15	0.47
4:D:70:VAL:CG2	4:D:84:PRO:HD3	2.29	0.47
4:D:120:ARG:HG2	4:D:120:ARG:NH1	2.30	0.47
4:D:165:TYR:H	4:D:168:VAL:CG2	2.28	0.47
1:A:241:ILE:HD12	7:G:16:TYR:CE1	2.48	0.46
3:C:153:ILE:HG22	3:C:156:ILE:HG12	1.97	0.46
5:E:74:ILE:HG23	5:E:74:ILE:O	2.15	0.46
5:E:163:SER:HA	5:E:173:LYS:O	2.15	0.46
8:H:21:ARG:NH1	8:H:66:ASP:OD1	2.47	0.46
1:A:141:ASN:HD22	1:A:168:GLU:CD	2.22	0.46
1:A:154:HIS:O	1:A:155:ALA:C	2.57	0.46
1:A:243:HIS:NE2	1:A:425:PHE:HE1	2.14	0.46
1:A:426:GLY:HA2	1:A:428:ILE:H	1.79	0.46
2:B:285:VAL:CG1	2:B:288:GLY:HA3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:TYR:OH	4:D:118:ARG:CZ	2.63	0.46
4:D:31:GLN:OE1	4:D:31:GLN:HA	2.15	0.46
6:F:96:GLU:O	6:F:97:VAL:C	2.58	0.46
7:G:45:ILE:HD12	7:G:45:ILE:HA	1.74	0.46
1:A:53:ASN:OD1	1:A:170:PRO:CD	2.64	0.46
1:A:64:PHE:HA	1:A:75:LEU:CD2	2.46	0.46
1:A:106:LEU:HB3	1:A:107:PRO:CD	2.45	0.46
1:A:426:GLY:HA2	1:A:428:ILE:HG13	1.97	0.46
2:B:300:ALA:CA	2:B:307:PHE:HZ	2.28	0.46
4:D:206:LEU:HD12	10:J:43:TYR:HB2	1.97	0.46
10:J:18:SER:HB3	11:K:23:LEU:HD12	1.97	0.46
11:K:18:VAL:HB	11:K:19:PRO:CD	2.45	0.46
1:A:18:GLN:HA	1:A:23:LEU:O	2.14	0.46
1:A:143:THR:O	1:A:143:THR:CG2	2.64	0.46
1:A:379:ILE:N	1:A:379:ILE:HD13	2.31	0.46
2:B:101:THR:CG2	2:B:104:ASN:H	2.28	0.46
2:B:283:PRO:HG3	9:I:55:LEU:HB3	1.98	0.46
3:C:166:GLY:HA3	3:C:177:ARG:CZ	2.45	0.46
3:C:304:ILE:HB	3:C:305:PRO:CD	2.45	0.46
4:D:189:PHE:CD1	4:D:189:PHE:C	2.92	0.46
5:E:77:LYS:HZ1	5:E:193:VAL:HG21	1.81	0.46
7:G:67:GLU:O	7:G:71:ARG:CB	2.61	0.46
1:A:61:HIS:CD2	2:B:287:ARG:HD3	2.51	0.46
2:B:155:PRO:HB2	2:B:254:HIS:CE1	2.50	0.46
2:B:314:ALA:CB	9:I:64:LEU:HD22	2.46	0.46
2:B:408:ALA:O	2:B:411:ILE:HB	2.16	0.46
3:C:280:ILE:O	3:C:283:SER:OG	2.32	0.46
3:C:328:LEU:HG	3:C:332:LEU:CD1	2.46	0.46
5:E:89:PHE:N	5:E:89:PHE:CD1	2.84	0.46
8:H:43:ARG:HG2	8:H:43:ARG:O	2.14	0.46
9:I:62:ARG:HB3	9:I:63:PRO:CD	2.35	0.46
1:A:55:ALA:O	1:A:56:GLY:C	2.57	0.46
1:A:157:ALA:CB	1:A:319:LEU:HD21	2.46	0.46
2:B:33:LEU:HB3	2:B:201:SER:O	2.16	0.46
2:B:154:ASN:O	2:B:155:PRO:C	2.59	0.46
2:B:308:ASP:OD1	2:B:308:ASP:C	2.56	0.46
4:D:137:PRO:HG3	4:D:143:LEU:CD1	2.46	0.46
5:E:59:VAL:O	5:E:59:VAL:CG1	2.64	0.46
7:G:33:GLY:O	7:G:37:VAL:N	2.35	0.46
9:I:64:LEU:CD1	9:I:64:LEU:C	2.85	0.46
1:A:279:HIS:CE1	1:A:284:TYR:OH	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:GLY:CA	3:C:177:ARG:NH2	2.79	0.46
3:C:272:TRP:CE2	3:C:273:TYR:CD1	3.00	0.46
4:D:165:TYR:OH	4:D:168:VAL:HG13	2.15	0.46
4:D:218:LEU:O	4:D:221:ALA:HB3	2.16	0.46
10:J:56:LYS:HG2	10:J:60:GLU:OE1	2.15	0.46
1:A:19:LEU:HB2	1:A:23:LEU:HB3	1.98	0.46
1:A:130:GLU:OE2	9:I:52:ARG:NH2	2.49	0.46
1:A:385:THR:HG22	1:A:386:TYR:CD1	2.50	0.46
2:B:191:LEU:O	2:B:192:HIS:C	2.58	0.46
3:C:276:PHE:CG	3:C:277:ALA:N	2.83	0.46
4:D:21:LEU:CD1	4:D:192:TRP:HB2	2.46	0.46
4:D:31:GLN:O	4:D:32:VAL:C	2.58	0.46
4:D:39:SER:O	4:D:94:PRO:HB3	2.15	0.46
4:D:147:LEU:O	4:D:148:TYR:C	2.58	0.46
4:D:160:MET:HE2	4:D:163:PRO:HG3	1.96	0.46
4:D:200:HIS:CD2	4:D:204:MET:HG3	2.51	0.46
5:E:173:LYS:HG3	5:E:174:GLY:N	2.30	0.46
6:F:106:GLU:O	6:F:109:LYS:HG2	2.16	0.46
7:G:3:GLN:O	7:G:7:LEU:HG	2.15	0.46
1:A:146:ARG:HH21	1:A:308:GLN:HE22	1.62	0.46
1:A:276:ILE:O	1:A:292:SER:HB2	2.16	0.46
1:A:310:PHE:C	1:A:310:PHE:CD1	2.94	0.46
2:B:65:THR:O	2:B:66:SER:C	2.59	0.46
4:D:23:HIS:O	4:D:24:THR:C	2.55	0.46
4:D:183:ALA:CA	4:D:186:VAL:HG23	2.45	0.46
4:D:208:MET:C	4:D:208:MET:CE	2.84	0.46
8:H:65:ARG:O	8:H:69:VAL:HG23	2.16	0.46
10:J:4:THR:HG22	10:J:6:THR:N	2.31	0.46
1:A:39:VAL:HG11	1:A:117:VAL:CG2	2.43	0.46
1:A:52:ASN:O	1:A:53:ASN:C	2.59	0.46
1:A:281:ASP:HB3	1:A:284:TYR:CD1	2.51	0.46
3:C:263:ASN:O	3:C:265:PRO:HD3	2.16	0.46
3:C:296:PHE:HE1	3:C:300:ILE:HG13	1.74	0.46
3:C:318:ARG:HB3	3:C:373:GLU:OE1	2.16	0.46
4:D:6:HIS:ND1	4:D:7:PRO:HD3	2.30	0.46
6:F:10:SER:HA	6:F:13:LEU:HG	1.97	0.46
1:A:70:ARG:HB3	1:A:74:ALA:CB	2.45	0.45
2:B:67:HIS:CD2	2:B:144:LEU:CD2	2.93	0.45
2:B:83:PHE:CZ	2:B:87:ARG:HG3	2.52	0.45
2:B:162:ASN:ND2	2:B:244:ILE:HG21	2.31	0.45
2:B:292:THR:CG2	2:B:363:LYS:NZ	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:THR:CG2	3:C:83:HIS:CB	2.94	0.45
3:C:130:GLY:O	3:C:131:TYR:C	2.56	0.45
1:A:5:ALA:O	1:A:6:GLN:C	2.59	0.45
1:A:64:PHE:HA	1:A:75:LEU:HD22	1.98	0.45
1:A:310:PHE:CD1	1:A:310:PHE:O	2.69	0.45
2:B:79:GLY:HA3	2:B:125:ASN:HD21	1.81	0.45
2:B:431:GLY:O	2:B:432:HIS:HD2	1.98	0.45
3:C:221:HIS:CB	3:C:222:PRO:CD	2.94	0.45
3:C:237:LEU:O	3:C:241:LEU:HB2	2.16	0.45
5:E:10:PHE:O	5:E:11:SER:C	2.58	0.45
5:E:68:VAL:O	5:E:69:LEU:C	2.57	0.45
6:F:73:GLN:HG2	7:G:36:ASN:ND2	2.29	0.45
1:A:89:TYR:CD1	1:A:89:TYR:C	2.95	0.45
1:A:243:HIS:O	1:A:425:PHE:HA	2.17	0.45
2:B:316:TYR:OH	9:I:64:LEU:HD23	2.15	0.45
4:D:181:GLN:CA	8:H:77:LEU:HD13	2.39	0.45
5:E:77:LYS:HZ3	5:E:98:VAL:HG22	1.81	0.45
1:A:51:LYS:CG	1:A:52:ASN:N	2.78	0.45
1:A:136:GLN:HE21	9:I:50:LEU:CB	2.28	0.45
2:B:161:GLU:OE1	2:B:175:SER:HB2	2.16	0.45
3:C:378:LYS:HD3	6:F:33:ARG:HH12	1.80	0.45
4:D:30:PHE:HE2	4:D:64:LEU:HD21	1.81	0.45
4:D:50:HIS:HB3	4:D:54:VAL:HG21	1.96	0.45
4:D:69:GLU:HA	4:D:73:GLY:HA2	1.99	0.45
5:E:77:LYS:HG3	5:E:193:VAL:CG1	2.46	0.45
1:A:428:ILE:HG22	1:A:431:LEU:HB3	1.98	0.45
2:B:352:LEU:O	2:B:352:LEU:HG	2.16	0.45
3:C:260:ASN:O	3:C:262:LEU:N	2.49	0.45
3:C:341:GLN:NE2	3:C:341:GLN:CA	2.79	0.45
5:E:71:MET:HA	5:E:74:ILE:HG22	1.98	0.45
5:E:127:VAL:CG1	5:E:133:VAL:HG23	2.47	0.45
6:F:75:LEU:HD12	6:F:75:LEU:HA	1.78	0.45
1:A:3:THR:O	1:A:4:TYR:C	2.58	0.45
1:A:248:LEU:HD12	1:A:425:PHE:CD2	2.51	0.45
1:A:446:PHE:CZ	3:C:6:LYS:HE3	2.51	0.45
2:B:157:ALA:O	2:B:161:GLU:CG	2.65	0.45
2:B:170:ASN:OD1	2:B:171:ALA:N	2.47	0.45
3:C:124:MET:HE1	3:C:298:ILE:HD13	1.97	0.45
3:C:310:SER:CB	3:C:318:ARG:HH11	2.30	0.45
4:D:14:HIS:HA	4:D:19:SER:HB3	1.99	0.45
4:D:27:ARG:CZ	10:J:58:LYS:HE3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:49:ARG:NH1	6:F:97:VAL:CG2	2.80	0.45
1:A:79:VAL:HG12	1:A:84:ALA:HB3	1.99	0.45
1:A:343:MET:CE	1:A:416:TYR:CE2	3.00	0.45
2:B:124:LEU:HD13	2:B:223:PHE:CB	2.47	0.45
3:C:44:GLN:NE2	3:C:86:GLY:C	2.75	0.45
5:E:15:ARG:HD3	7:G:23:GLN:C	2.42	0.45
5:E:43:THR:O	5:E:47:VAL:HG23	2.17	0.45
5:E:77:LYS:CE	5:E:98:VAL:CG2	2.94	0.45
10:J:25:VAL:HG12	11:K:30:VAL:HG12	1.99	0.45
1:A:85:HIS:CD2	2:B:370:MET:HE1	2.51	0.45
2:B:303:VAL:CG1	2:B:304:HIS:H	2.30	0.45
2:B:433:THR:HA	2:B:434:PRO:HD2	1.71	0.45
3:C:133:LEU:HD23	3:C:133:LEU:HA	1.79	0.45
3:C:138:MET:HG2	3:C:253:PRO:HB3	1.97	0.45
3:C:269:LYS:HZ2	3:C:340:GLY:HA3	1.80	0.45
3:C:373:GLU:O	3:C:377:LEU:HD12	2.17	0.45
6:F:44:LYS:HA	6:F:44:LYS:CE	2.47	0.45
6:F:102:LYS:O	6:F:103:GLU:C	2.58	0.45
3:C:122:THR:HG23	3:C:185:LEU:HD11	1.97	0.45
3:C:221:HIS:N	3:C:222:PRO:CD	2.78	0.45
3:C:275:LEU:HB3	3:C:339:GLY:HA3	1.99	0.45
4:D:137:PRO:HA	4:D:138:PRO:HD3	1.85	0.45
4:D:200:HIS:HD2	4:D:204:MET:HG3	1.81	0.45
5:E:137:GLY:O	5:E:146:PRO:HD2	2.17	0.45
1:A:31:SER:N	1:A:202:GLY:HA2	2.31	0.45
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.98	0.45
4:D:44:ASP:O	4:D:90:TYR:CD2	2.70	0.45
4:D:146:GLY:O	4:D:159:GLY:HA2	2.17	0.45
4:D:189:PHE:O	4:D:189:PHE:CG	2.69	0.45
6:F:71:ARG:O	6:F:73:GLN:HG3	2.17	0.45
6:F:91:GLU:N	6:F:92:PRO:HD2	2.32	0.45
7:G:34:ILE:CB	7:G:35:PRO:CD	2.93	0.45
1:A:16:VAL:HG11	1:A:388:ARG:HB2	1.98	0.44
1:A:257:VAL:HG21	1:A:414:TYR:O	2.17	0.44
1:A:436:ARG:HE	3:C:222:PRO:CD	2.26	0.44
2:B:307:PHE:CD1	2:B:307:PHE:C	2.95	0.44
3:C:82:MET:HA	3:C:243:VAL:HG21	1.98	0.44
3:C:101:GLY:HA2	3:C:106:SER:HB2	1.97	0.44
4:D:34:LYS:O	4:D:38:SER:OG	2.26	0.44
4:D:54:VAL:O	4:D:54:VAL:CG1	2.59	0.44
5:E:72:SER:C	5:E:92:ARG:HH21	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:71:ARG:O	7:G:73:ASN:N	2.50	0.44
7:G:72:LYS:HB3	7:G:75:ALA:CB	2.24	0.44
8:H:49:GLN:O	8:H:51:GLU:N	2.50	0.44
1:A:61:HIS:NE2	1:A:134:ILE:HD12	2.32	0.44
1:A:280:TYR:CD1	1:A:280:TYR:C	2.96	0.44
1:A:375:VAL:O	1:A:376:CYS:C	2.58	0.44
1:A:394:GLU:O	1:A:397:SER:N	2.50	0.44
2:B:47:ILE:CD1	2:B:211:VAL:HG21	2.36	0.44
2:B:217:LYS:O	2:B:218:GLN:C	2.60	0.44
2:B:381:GLU:O	2:B:381:GLU:HG3	2.16	0.44
2:B:392:TYR:O	2:B:392:TYR:CG	2.66	0.44
3:C:97:HIS:HD2	12:C:381:HEM:C1C	2.35	0.44
3:C:243:VAL:CG1	3:C:244:LEU:N	2.75	0.44
5:E:71:MET:HA	5:E:74:ILE:CG2	2.48	0.44
9:I:54:SER:O	9:I:55:LEU:HG	2.17	0.44
1:A:145:MET:SD	1:A:248:LEU:HD13	2.57	0.44
2:B:51:ILE:HD13	2:B:199:PHE:CG	2.52	0.44
2:B:101:THR:HG23	2:B:104:ASN:H	1.82	0.44
2:B:261:SER:HB2	2:B:321:LEU:CA	2.47	0.44
4:D:43:MET:CE	4:D:91:PHE:CE2	3.01	0.44
4:D:82:MET:SD	4:D:86:LYS:CD	3.05	0.44
6:F:29:LEU:HD23	6:F:29:LEU:HA	1.72	0.44
10:J:14:PHE:O	10:J:15:ARG:C	2.59	0.44
10:J:52:TRP:O	10:J:53:LYS:C	2.60	0.44
1:A:38:GLY:HA3	1:A:40:TRP:CZ3	2.46	0.44
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.75	0.44
1:A:200:ALA:CB	1:A:375:VAL:HG23	2.48	0.44
2:B:211:VAL:HG12	2:B:212:SER:N	2.33	0.44
2:B:314:ALA:CB	9:I:64:LEU:CD2	2.95	0.44
3:C:288:LEU:HD12	3:C:288:LEU:O	2.17	0.44
4:D:117:VAL:O	4:D:123:GLY:HA2	2.17	0.44
5:E:65:SER:O	5:E:66:ALA:C	2.58	0.44
5:E:81:ILE:HD13	5:E:98:VAL:O	2.17	0.44
1:A:31:SER:H	1:A:202:GLY:HA2	1.82	0.44
1:A:32:GLN:HB3	1:A:33:PRO:CD	2.44	0.44
1:A:116:ILE:HG22	1:A:117:VAL:N	2.32	0.44
1:A:162:PRO:O	1:A:165:GLN:CG	2.63	0.44
1:A:370:ASP:O	1:A:374:PRO:HG2	2.17	0.44
3:C:5:ARG:O	3:C:9:PRO:HD2	2.17	0.44
3:C:71:ARG:HH21	4:D:196:PRO:CG	2.29	0.44
3:C:207:ASN:ND2	3:C:209:THR:OG1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:367:PRO:O	3:C:368:THR:C	2.59	0.44
1:A:277:ILE:O	1:A:292:SER:OG	2.33	0.44
1:A:350:THR:HB	1:A:353:GLU:HG3	1.99	0.44
1:A:351:GLU:O	1:A:352:SER:C	2.60	0.44
2:B:53:ALA:O	2:B:105:MET:HB2	2.17	0.44
2:B:283:PRO:CG	9:I:55:LEU:HB3	2.48	0.44
2:B:345:LYS:HD3	2:B:418:VAL:HG11	1.99	0.44
4:D:24:THR:O	4:D:27:ARG:HB3	2.17	0.44
5:E:25:SER:HA	5:E:28:SER:OG	2.17	0.44
5:E:109:GLU:HG3	5:E:167:ALA:HB3	2.00	0.44
5:E:165:TYR:HD1	5:E:169:GLY:O	2.01	0.44
6:F:13:LEU:HA	6:F:16:ILE:CD1	2.47	0.44
1:A:45:SER:HB3	1:A:92:ARG:HG3	2.00	0.44
1:A:53:ASN:ND2	1:A:165:GLN:HG3	2.32	0.44
1:A:416:TYR:O	1:A:418:GLN:HG2	2.18	0.44
2:B:69:LEU:O	2:B:72:ALA:HB3	2.18	0.44
2:B:343:GLN:O	2:B:343:GLN:HG3	2.17	0.44
2:B:351:ASN:C	2:B:351:ASN:OD1	2.61	0.44
5:E:55:VAL:O	5:E:59:VAL:HG23	2.18	0.44
5:E:118:ARG:HE	5:E:171:ILE:CG1	2.28	0.44
1:A:62:LEU:HB3	1:A:122:LEU:HD22	1.99	0.44
1:A:248:LEU:CD1	1:A:425:PHE:CD2	3.01	0.44
1:A:264:HIS:O	1:A:265:PRO:C	2.60	0.44
1:A:347:THR:O	11:K:16:ASN:HB2	2.18	0.44
2:B:62:ASN:O	2:B:63:LEU:C	2.57	0.44
3:C:91:PHE:HB2	3:C:272:TRP:CH2	2.52	0.44
3:C:341:GLN:CA	3:C:341:GLN:HE21	2.29	0.44
8:H:49:GLN:H	8:H:49:GLN:HG3	1.61	0.44
10:J:31:PHE:CD1	10:J:31:PHE:C	2.95	0.44
1:A:61:HIS:HB3	1:A:130:GLU:HG3	1.99	0.44
1:A:166:SER:CB	5:E:3:THR:CG2	2.95	0.44
1:A:172:GLU:O	1:A:175:ARG:N	2.51	0.44
1:A:191:LYS:C	1:A:192:ALA:O	2.58	0.44
2:B:200:THR:HG22	2:B:203:ARG:CG	2.48	0.44
2:B:209:LEU:CD2	2:B:375:SER:HB2	2.42	0.44
2:B:264:ILE:HB	2:B:316:TYR:O	2.18	0.44
2:B:436:ILE:H	2:B:436:ILE:HG13	1.16	0.44
3:C:44:GLN:HE22	3:C:86:GLY:C	2.26	0.44
4:D:3:LEU:CD2	7:G:70:LYS:HZ3	2.31	0.44
5:E:15:ARG:O	5:E:16:PRO:C	2.61	0.44
5:E:35:PHE:O	5:E:38:LEU:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:43:THR:HG22	5:E:44:THR:N	2.31	0.44
8:H:73:LEU:HD21	8:H:74:PHE:HD1	1.83	0.44
11:K:18:VAL:O	11:K:19:PRO:C	2.61	0.44
1:A:45:SER:HB2	1:A:167:VAL:HG22	2.00	0.43
1:A:53:ASN:OD1	1:A:170:PRO:HD3	2.18	0.43
1:A:355:LEU:HD22	1:A:358:LYS:NZ	2.32	0.43
2:B:42:ALA:HB1	2:B:43:PRO:CD	2.44	0.43
2:B:294:SER:OG	2:B:343:GLN:NE2	2.46	0.43
2:B:308:ASP:CB	9:I:54:SER:HB2	2.48	0.43
2:B:312:PHE:CD1	9:I:58:GLN:O	2.71	0.43
3:C:50:PHE:HA	3:C:53:MET:HE3	2.00	0.43
3:C:72:ASP:HB3	5:E:67:ASP:H	1.83	0.43
3:C:286:ASN:C	3:C:286:ASN:OD1	2.60	0.43
3:C:345:HIS:CB	3:C:346:PRO:HD3	2.37	0.43
12:C:381:HEM:HMC2	12:C:381:HEM:CBC	2.32	0.43
4:D:115:TYR:O	4:D:118:ARG:N	2.51	0.43
5:E:19:LEU:O	5:E:19:LEU:CD1	2.54	0.43
10:J:62:LYS:HD3	10:J:62:LYS:HA	1.49	0.43
1:A:86:LEU:HD12	1:A:98:TYR:O	2.18	0.43
2:B:372:VAL:O	2:B:372:VAL:HG12	2.18	0.43
3:C:268:ILE:H	3:C:268:ILE:HG13	1.59	0.43
3:C:342:PRO:HD2	3:C:347:TYR:CE2	2.53	0.43
5:E:127:VAL:HG13	5:E:133:VAL:HG23	2.00	0.43
8:H:49:GLN:O	8:H:52:GLU:N	2.32	0.43
1:A:19:LEU:HD11	1:A:212:ALA:HB3	2.00	0.43
1:A:51:LYS:C	1:A:53:ASN:H	2.26	0.43
1:A:112:LEU:HD13	1:A:112:LEU:HA	1.72	0.43
1:A:405:ARG:O	1:A:409:GLU:HG3	2.17	0.43
1:A:428:ILE:O	1:A:428:ILE:HG22	2.18	0.43
2:B:90:GLU:O	2:B:91:ALA:C	2.61	0.43
2:B:269:ALA:O	2:B:272:PHE:HB2	2.18	0.43
2:B:308:ASP:OD2	9:I:54:SER:O	2.36	0.43
3:C:252:ASP:CB	3:C:253:PRO:HD3	2.46	0.43
3:C:315:MET:HG2	3:C:321:SER:HB2	1.99	0.43
4:D:83:ARG:CB	4:D:84:PRO:CD	2.62	0.43
10:J:60:GLU:HG3	10:J:60:GLU:O	2.17	0.43
1:A:61:HIS:NE2	1:A:134:ILE:CD1	2.81	0.43
1:A:252:HIS:HD2	1:A:323:HIS:HE1	1.66	0.43
1:A:293:PRO:O	1:A:294:LEU:C	2.61	0.43
1:A:434:TYR:CD1	1:A:434:TYR:C	2.96	0.43
2:B:97:SER:OG	9:I:70:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:THR:HB	2:B:188:PRO:HD2	2.01	0.43
3:C:33:PHE:O	3:C:37:LEU:N	2.48	0.43
4:D:56:TYR:CD1	4:D:60:GLU:CD	2.95	0.43
5:E:18:VAL:HG12	5:E:25:SER:HB3	2.01	0.43
5:E:69:LEU:HA	5:E:69:LEU:HD12	1.66	0.43
1:A:46:ARG:HB2	1:A:163:LEU:HD13	2.00	0.43
1:A:191:LYS:O	1:A:192:ALA:C	2.59	0.43
1:A:243:HIS:ND1	7:G:14:ILE:HG13	2.33	0.43
1:A:324:PHE:CD2	1:A:334:MET:HG2	2.53	0.43
2:B:227:ARG:N	2:B:227:ARG:HD2	2.33	0.43
3:C:153:ILE:HG21	3:C:156:ILE:CD1	2.48	0.43
3:C:304:ILE:O	3:C:307:LEU:N	2.40	0.43
4:D:136:GLU:O	4:D:137:PRO:O	2.37	0.43
5:E:23:LYS:CG	5:E:24:SER:H	2.29	0.43
10:J:40:ASP:O	10:J:41:ALA:C	2.61	0.43
1:A:106:LEU:HD12	1:A:110:VAL:HG23	1.99	0.43
2:B:119:LEU:HD12	2:B:119:LEU:HA	1.80	0.43
2:B:206:LEU:HD12	2:B:206:LEU:HA	1.72	0.43
2:B:280:GLY:HA2	2:B:311:ALA:HB3	2.01	0.43
3:C:121:LEU:HD23	3:C:124:MET:HE1	2.01	0.43
3:C:121:LEU:HD21	3:C:298:ILE:HG21	2.00	0.43
3:C:269:LYS:NZ	3:C:340:GLY:HA2	2.32	0.43
4:D:79:GLU:HB3	4:D:82:MET:HB2	2.01	0.43
5:E:29:SER:O	5:E:30:GLU:C	2.58	0.43
5:E:116:GLN:HE21	5:E:116:GLN:CA	2.29	0.43
6:F:42:ASP:CG	6:F:101:ARG:NH1	2.74	0.43
7:G:35:PRO:O	7:G:39:ARG:HB3	2.18	0.43
7:G:44:CYS:O	7:G:47:ARG:N	2.48	0.43
1:A:40:TRP:O	1:A:384:LEU:HD21	2.19	0.43
1:A:57:TYR:CE2	1:A:61:HIS:HE1	2.37	0.43
1:A:145:MET:SD	1:A:248:LEU:CD1	3.06	0.43
2:B:97:SER:HG	9:I:70:LEU:HB2	1.82	0.43
2:B:235:ALA:O	2:B:236:LYS:CB	2.66	0.43
2:B:332:SER:O	2:B:335:ASP:N	2.52	0.43
3:C:8:HIS:CB	3:C:9:PRO:HD3	2.38	0.43
3:C:37:LEU:CD2	3:C:93:CYS:HB3	2.48	0.43
3:C:151:SER:OG	3:C:287:LYS:NZ	2.51	0.43
3:C:278:TYR:O	3:C:281:LEU:N	2.50	0.43
4:D:32:VAL:HG11	4:D:186:VAL:CG2	2.48	0.43
4:D:160:MET:O	4:D:161:ALA:O	2.37	0.43
4:D:188:THR:O	4:D:189:PHE:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:206:LEU:HD22	4:D:206:LEU:O	2.18	0.43
5:E:86:ASN:HD22	5:E:148:ALA:HB2	1.82	0.43
10:J:18:SER:CB	11:K:23:LEU:HB2	2.48	0.43
2:B:166:ALA:HB2	2:B:244:ILE:CD1	2.48	0.43
2:B:381:GLU:O	2:B:385:GLN:HG3	2.19	0.43
3:C:3:ASN:CA	3:C:8:HIS:CD2	3.02	0.43
3:C:109:PHE:O	3:C:110:LEU:C	2.61	0.43
3:C:134:PRO:O	3:C:135:TRP:CB	2.65	0.43
3:C:246:ALA:N	3:C:247:PRO:HD3	2.34	0.43
3:C:304:ILE:H	3:C:304:ILE:HG12	1.66	0.43
3:C:361:LEU:O	3:C:366:MET:HG3	2.18	0.43
4:D:174:GLY:O	4:D:175:THR:C	2.61	0.43
4:D:208:MET:HE3	4:D:208:MET:O	2.19	0.43
2:B:31:ASN:ND2	2:B:225:ASN:OD1	2.52	0.43
2:B:46:ARG:NE	2:B:375:SER:OG	2.52	0.43
2:B:304:HIS:NE2	2:B:306:PRO:HD2	2.27	0.43
2:B:347:ILE:O	2:B:411:ILE:HG23	2.19	0.43
2:B:378:PHE:CE2	2:B:382:VAL:HG21	2.53	0.43
4:D:28:ARG:CD	4:D:185:ASP:OD2	2.66	0.43
4:D:36:VAL:HG23	4:D:169:LEU:HD11	2.01	0.43
4:D:160:MET:HE3	13:D:242:HEC:C1C	2.48	0.43
4:D:180:SER:HB3	8:H:17:LEU:HB2	2.00	0.43
5:E:77:LYS:NZ	5:E:98:VAL:CG2	2.82	0.43
10:J:56:LYS:NZ	10:J:60:GLU:OE1	2.49	0.43
1:A:194:ARG:O	1:A:384:LEU:HD23	2.18	0.43
2:B:137:VAL:O	2:B:137:VAL:HG12	2.19	0.43
2:B:272:PHE:O	2:B:273:SER:C	2.59	0.43
3:C:135:TRP:CD2	3:C:175:LEU:HD22	2.53	0.43
3:C:357:LEU:HG	3:C:361:LEU:CD1	2.45	0.43
4:D:93:LYS:O	4:D:94:PRO:C	2.61	0.43
4:D:195:GLU:HG3	4:D:198:HIS:HB2	2.01	0.43
4:D:212:MET:HE3	4:D:212:MET:HB2	1.89	0.43
10:J:4:THR:O	10:J:5:LEU:C	2.61	0.43
10:J:22:LEU:O	10:J:23:THR:C	2.62	0.43
1:A:244:ARG:CZ	7:G:10:VAL:HB	2.49	0.42
1:A:277:ILE:H	1:A:277:ILE:HG12	1.64	0.42
2:B:207:ILE:CD1	2:B:383:GLY:HA2	2.47	0.42
2:B:402:ILE:O	2:B:405:VAL:HG23	2.19	0.42
5:E:15:ARG:H	5:E:15:ARG:HG2	1.50	0.42
5:E:34:GLY:N	10:J:10:TYR:CD2	2.87	0.42
5:E:73:LYS:O	5:E:73:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:GLY:H	2:B:125:ASN:ND2	2.17	0.42
3:C:37:LEU:HD12	3:C:97:HIS:CD2	2.54	0.42
3:C:251:GLY:O	3:C:252:ASP:C	2.61	0.42
4:D:167:GLU:HG2	4:D:167:GLU:O	2.19	0.42
7:G:65:GLU:HA	7:G:65:GLU:OE1	2.19	0.42
11:K:20:THR:O	11:K:24:TRP:CD1	2.72	0.42
1:A:24:ARG:HB2	1:A:196:VAL:HG22	2.01	0.42
1:A:169:GLY:HA2	1:A:170:PRO:HD2	1.77	0.42
1:A:244:ARG:CZ	1:A:429:GLU:HB2	2.49	0.42
2:B:90:GLU:O	2:B:92:VAL:N	2.52	0.42
2:B:109:VAL:HG13	2:B:109:VAL:O	2.19	0.42
2:B:126:VAL:O	2:B:130:PRO:HG3	2.19	0.42
2:B:261:SER:H	2:B:320:GLY:C	2.27	0.42
3:C:37:LEU:HD23	3:C:37:LEU:HA	1.81	0.42
3:C:45:ILE:O	3:C:46:LEU:C	2.61	0.42
3:C:246:ALA:O	3:C:247:PRO:C	2.62	0.42
12:C:381:HEM:HBC2	12:C:381:HEM:CMC	2.26	0.42
4:D:203:ARG:HA	10:J:43:TYR:CE1	2.55	0.42
8:H:39:LEU:O	8:H:40:CYS:C	2.63	0.42
10:J:52:TRP:CG	10:J:53:LYS:N	2.86	0.42
1:A:53:ASN:O	1:A:53:ASN:ND2	2.51	0.42
1:A:287:GLY:O	1:A:289:HIS:N	2.53	0.42
2:B:346:THR:HG23	2:B:351:ASN:HB3	2.01	0.42
3:C:25:SER:HB3	3:C:218:ILE:HD11	2.01	0.42
3:C:122:THR:O	3:C:122:THR:HG22	2.18	0.42
3:C:248:ASP:O	3:C:251:GLY:N	2.52	0.42
1:A:4:TYR:O	1:A:5:ALA:C	2.62	0.42
1:A:270:LEU:O	1:A:271:GLN:C	2.62	0.42
1:A:385:THR:CB	1:A:386:TYR:CD1	3.02	0.42
2:B:181:TYR:CD2	2:B:181:TYR:C	2.96	0.42
2:B:201:SER:OG	2:B:226:ILE:N	2.51	0.42
2:B:312:PHE:HD1	9:I:58:GLN:O	2.02	0.42
2:B:353:SER:C	2:B:355:PRO:HD2	2.44	0.42
3:C:221:HIS:HA	3:C:225:THR:HG23	2.00	0.42
3:C:321:SER:O	3:C:322:GLN:C	2.62	0.42
4:D:43:MET:HE3	4:D:46:VAL:HG21	2.01	0.42
4:D:48:TYR:OH	4:D:68:VAL:CG2	2.67	0.42
4:D:117:VAL:CG2	4:D:190:LEU:HB3	2.50	0.42
4:D:227:TRP:CE3	4:D:230:LEU:HD12	2.53	0.42
6:F:16:ILE:H	6:F:16:ILE:HG13	1.34	0.42
7:G:63:THR:O	7:G:64:GLN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:GLY:O	2:B:89:ILE:C	2.62	0.42
2:B:348:ALA:CB	2:B:418:VAL:HG21	2.49	0.42
2:B:396:SER:O	2:B:400:GLN:HG3	2.20	0.42
3:C:90:PHE:C	3:C:90:PHE:CD1	2.98	0.42
4:D:190:LEU:O	4:D:191:ARG:C	2.61	0.42
5:E:75:GLU:O	5:E:194:ILE:HA	2.20	0.42
5:E:112:VAL:HG12	5:E:117:LEU:HD21	2.01	0.42
6:F:46:ALA:O	6:F:50:LEU:HD23	2.20	0.42
8:H:27:LEU:O	8:H:29:LYS:N	2.52	0.42
1:A:56:GLY:O	1:A:59:VAL:N	2.52	0.42
1:A:235:ARG:O	1:A:235:ARG:HG2	2.20	0.42
2:B:63:LEU:HD22	2:B:174:ASN:HB2	2.02	0.42
3:C:25:SER:HB3	3:C:218:ILE:CD1	2.50	0.42
3:C:121:LEU:HD23	3:C:124:MET:HE2	2.01	0.42
3:C:249:LEU:C	3:C:249:LEU:CD2	2.92	0.42
3:C:257:THR:C	3:C:258:PRO:O	2.59	0.42
4:D:5:LEU:HD23	4:D:152:TYR:HE1	1.82	0.42
4:D:153:PHE:CE2	4:D:158:ILE:HD12	2.55	0.42
5:E:86:ASN:HB2	5:E:99:ARG:HD2	2.01	0.42
1:A:235:ARG:HB3	5:E:21:SER:O	2.20	0.42
1:A:264:HIS:CE1	1:A:266:ASP:OD1	2.72	0.42
1:A:322:ALA:HB3	1:A:338:LEU:CD2	2.50	0.42
1:A:429:GLU:CG	7:G:4:PHE:O	2.67	0.42
2:B:180:ASP:HA	2:B:183:ILE:CD1	2.46	0.42
2:B:182:ARG:O	2:B:183:ILE:C	2.61	0.42
3:C:85:ASN:O	3:C:86:GLY:C	2.63	0.42
3:C:115:ILE:H	3:C:115:ILE:HG12	1.47	0.42
3:C:310:SER:CB	3:C:318:ARG:NH1	2.73	0.42
3:C:319:PRO:O	3:C:320:LEU:C	2.62	0.42
4:D:160:MET:C	4:D:161:ALA:O	2.62	0.42
4:D:216:LEU:N	4:D:217:PRO:CD	2.83	0.42
5:E:18:VAL:HG11	5:E:32:ARG:HH12	1.85	0.42
5:E:171:ILE:HD13	5:E:176:ALA:HB3	2.02	0.42
6:F:75:LEU:HB3	6:F:80:TRP:HE1	1.84	0.42
1:A:33:PRO:O	1:A:103:SER:N	2.47	0.42
1:A:134:ILE:HD13	1:A:134:ILE:H	1.79	0.42
1:A:197:LEU:C	1:A:197:LEU:HD12	2.44	0.42
1:A:243:HIS:NE2	1:A:425:PHE:CE1	2.87	0.42
2:B:283:PRO:HG3	9:I:55:LEU:HD13	2.02	0.42
2:B:368:TYR:HA	2:B:371:SER:OG	2.20	0.42
3:C:156:ILE:CG1	3:C:157:GLY:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:380:HEM:CBB	12:C:380:HEM:CHC	2.92	0.42
4:D:57:THR:N	4:D:60:GLU:HB3	2.35	0.42
4:D:74:PRO:HB3	4:D:79:GLU:HB2	1.95	0.42
4:D:220:TYR:CE2	4:D:224:ARG:HD3	2.55	0.42
6:F:7:SER:O	6:F:11:ARG:HD2	2.20	0.42
7:G:61:TRP:O	7:G:64:GLN:HB2	2.20	0.42
10:J:55:ILE:O	10:J:55:ILE:HG22	2.20	0.42
1:A:37:VAL:HA	1:A:199:ALA:CB	2.44	0.42
1:A:198:ALA:O	1:A:199:ALA:HB2	2.20	0.42
2:B:25:GLU:O	2:B:213:HIS:CE1	2.73	0.42
2:B:57:TYR:HB3	2:B:198:HIS:CE1	2.55	0.42
2:B:100:SER:CB	2:B:105:MET:HG3	2.50	0.42
2:B:109:VAL:O	2:B:109:VAL:CG1	2.67	0.42
3:C:46:LEU:HB3	3:C:47:THR:H	1.54	0.42
3:C:217:LYS:HG3	7:G:7:LEU:CD1	2.45	0.42
4:D:51:LEU:HD23	4:D:61:ALA:HB3	2.02	0.42
8:H:77:LEU:N	8:H:77:LEU:HD23	2.35	0.42
1:A:5:ALA:O	1:A:6:GLN:O	2.38	0.41
2:B:282:GLY:HA2	2:B:283:PRO:HD2	1.79	0.41
2:B:292:THR:HG21	2:B:363:LYS:HZ1	1.85	0.41
2:B:381:GLU:OE2	9:I:62:ARG:NH2	2.53	0.41
2:B:414:ALA:O	2:B:418:VAL:HG23	2.19	0.41
3:C:27:ILE:O	3:C:28:SER:C	2.63	0.41
3:C:131:TYR:OH	3:C:253:PRO:HG2	2.20	0.41
6:F:13:LEU:CA	6:F:16:ILE:HD11	2.47	0.41
6:F:96:GLU:OE1	6:F:96:GLU:HA	2.20	0.41
8:H:73:LEU:HD23	8:H:74:PHE:N	2.34	0.41
1:A:80:GLU:HG2	2:B:284:HIS:HD2	1.85	0.41
1:A:106:LEU:O	1:A:107:PRO:O	2.37	0.41
1:A:223:TYR:CD2	1:A:224:ASP:HB3	2.55	0.41
2:B:148:LYS:HE2	2:B:152:LEU:HD11	2.03	0.41
3:C:218:ILE:HG23	3:C:219:PRO:HD2	2.02	0.41
3:C:366:MET:O	3:C:367:PRO:C	2.61	0.41
4:D:56:TYR:CD1	4:D:60:GLU:OE2	2.73	0.41
4:D:118:ARG:CG	4:D:194:ALA:HB1	2.50	0.41
5:E:185:TYR:CB	5:E:195:VAL:HA	2.50	0.41
6:F:33:ARG:O	6:F:34:ASP:C	2.61	0.41
7:G:48:VAL:O	7:G:51:PRO:HD2	2.20	0.41
8:H:73:LEU:CD2	8:H:74:PHE:HD1	2.33	0.41
10:J:20:PHE:O	10:J:23:THR:HB	2.20	0.41
1:A:381:ARG:O	1:A:384:LEU:HD12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:LYS:HZ3	9:I:70:LEU:HD22	1.83	0.41
2:B:435:PHE:O	2:B:436:ILE:C	2.61	0.41
3:C:91:PHE:O	3:C:92:ILE:C	2.62	0.41
3:C:103:TYR:HA	3:C:315:MET:HE3	2.03	0.41
4:D:30:PHE:CE1	4:D:50:HIS:HE1	2.34	0.41
4:D:150:ASN:OD1	4:D:151:PRO:CD	2.68	0.41
5:E:158:CYS:HA	5:E:159:PRO:HD2	1.93	0.41
5:E:170:ARG:HA	5:E:179:ASN:CG	2.45	0.41
1:A:45:SER:HB3	1:A:92:ARG:CA	2.36	0.41
2:B:79:GLY:CA	2:B:125:ASN:HD21	2.33	0.41
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.35	0.41
2:B:303:VAL:HG12	2:B:307:PHE:CD2	2.55	0.41
3:C:51:LEU:HD12	3:C:83:HIS:CD2	2.56	0.41
3:C:81:TYR:CZ	4:D:118:ARG:NH2	2.85	0.41
3:C:140:PHE:HD1	3:C:141:TRP:CD1	2.38	0.41
3:C:312:GLN:C	3:C:314:SER:H	2.28	0.41
5:E:129:LYS:HD2	5:E:187:PHE:CD2	2.55	0.41
6:F:88:SER:HB3	6:F:91:GLU:HG3	2.01	0.41
7:G:71:ARG:NH2	8:H:60:ASP:OD1	2.37	0.41
1:A:106:LEU:CD1	1:A:110:VAL:HG23	2.51	0.41
1:A:282:CYS:SG	1:A:305:GLN:OE1	2.79	0.41
1:A:341:GLN:OE1	1:A:344:ARG:NH1	2.53	0.41
1:A:359:ASN:O	1:A:360:LEU:C	2.63	0.41
1:A:376:CYS:O	1:A:379:ILE:HB	2.21	0.41
2:B:35:ILE:HG13	2:B:216:LEU:HD23	2.02	0.41
2:B:195:VAL:HG13	2:B:199:PHE:CD2	2.54	0.41
2:B:308:ASP:O	2:B:309:VAL:HG23	2.20	0.41
2:B:331:ALA:CA	2:B:432:HIS:ND1	2.73	0.41
3:C:87:ALA:O	3:C:91:PHE:HD2	2.03	0.41
3:C:173:ALA:O	3:C:174:THR:C	2.58	0.41
4:D:28:ARG:HD2	4:D:185:ASP:CG	2.46	0.41
4:D:79:GLU:O	4:D:80:MET:O	2.39	0.41
5:E:102:THR:OG1	5:E:105:GLU:HB2	2.20	0.41
7:G:50:PRO:HB2	7:G:51:PRO:HD3	2.03	0.41
8:H:45:SER:OG	8:H:46:SER:N	2.43	0.41
1:A:37:VAL:HG13	1:A:199:ALA:CB	2.51	0.41
1:A:240:GLN:CG	1:A:422:VAL:HB	2.45	0.41
1:A:292:SER:O	1:A:295:ALA:N	2.53	0.41
1:A:336:PHE:HE2	1:A:446:PHE:HD2	1.68	0.41
1:A:428:ILE:O	1:A:429:GLU:C	2.63	0.41
2:B:41:TYR:CG	2:B:42:ALA:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:ARG:HD2	3:C:80:ARG:HH11	1.43	0.41
3:C:282:ARG:O	3:C:283:SER:C	2.60	0.41
3:C:299:LEU:HD23	3:C:299:LEU:N	2.35	0.41
3:C:304:ILE:N	3:C:305:PRO:HD2	2.36	0.41
4:D:52:VAL:HG13	10:J:52:TRP:CD1	2.56	0.41
4:D:126:TYR:CD1	4:D:126:TYR:C	2.98	0.41
5:E:38:LEU:O	5:E:42:THR:OG1	2.38	0.41
5:E:81:ILE:HD11	5:E:87:MET:HB2	2.03	0.41
6:F:16:ILE:O	6:F:17:ARG:C	2.63	0.41
7:G:1:GLY:O	7:G:2:ARG:C	2.63	0.41
7:G:11:ARG:O	7:G:12:HIS:HB2	2.19	0.41
7:G:49:ALA:N	7:G:50:PRO:HD2	2.36	0.41
7:G:71:ARG:O	7:G:73:ASN:ND2	2.54	0.41
11:K:17:TRP:O	11:K:21:ALA:N	2.36	0.41
1:A:53:ASN:C	1:A:53:ASN:HD22	2.27	0.41
1:A:223:TYR:CD2	1:A:224:ASP:CB	3.03	0.41
3:C:107:TYR:HB3	3:C:113:TRP:CZ3	2.55	0.41
3:C:147:THR:HG21	3:C:165:TRP:NE1	2.36	0.41
3:C:172:LYS:H	3:C:172:LYS:HG2	1.35	0.41
3:C:338:ILE:HA	3:C:338:ILE:HD12	1.87	0.41
4:D:74:PRO:HG2	4:D:82:MET:CE	2.49	0.41
4:D:81:PHE:O	4:D:81:PHE:CD2	2.74	0.41
8:H:49:GLN:O	8:H:50:THR:C	2.63	0.41
10:J:36:ASP:O	10:J:37:GLN:C	2.64	0.41
10:J:51:LEU:HB3	10:J:52:TRP:HZ3	1.82	0.41
1:A:136:GLN:HE21	9:I:50:LEU:CG	2.34	0.41
2:B:47:ILE:HB	2:B:109:VAL:CG1	2.51	0.41
3:C:30:TRP:HA	3:C:33:PHE:HE2	1.86	0.41
3:C:341:GLN:HA	3:C:341:GLN:HE21	1.86	0.41
4:D:36:VAL:O	4:D:36:VAL:HG12	2.20	0.41
7:G:80:ASP:O	7:G:81:ARG:HB2	2.20	0.41
10:J:52:TRP:CE3	10:J:52:TRP:N	2.89	0.41
1:A:46:ARG:HB2	1:A:163:LEU:CD1	2.51	0.41
1:A:286:GLY:O	1:A:287:GLY:O	2.38	0.41
1:A:313:CYS:O	1:A:314:TYR:CD1	2.74	0.41
1:A:313:CYS:O	1:A:314:TYR:HD1	2.03	0.41
2:B:51:ILE:CD1	2:B:199:PHE:CG	3.04	0.41
2:B:122:PHE:HD1	2:B:122:PHE:HA	1.73	0.41
2:B:145:ARG:O	2:B:149:ALA:HB2	2.21	0.41
2:B:245:ARG:HH21	2:B:433:THR:HB	1.86	0.41
2:B:352:LEU:HD21	2:B:357:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.86	0.41
3:C:272:TRP:CG	3:C:273:TYR:N	2.88	0.41
3:C:360:LEU:HG	3:C:365:LEU:HD21	2.02	0.41
3:C:376:LEU:O	6:F:17:ARG:HG2	2.20	0.41
4:D:26:ILE:HG21	4:D:54:VAL:HG22	2.03	0.41
4:D:165:TYR:CD2	4:D:168:VAL:HG22	2.56	0.41
6:F:37:ILE:HD13	6:F:37:ILE:HG21	1.87	0.41
7:G:65:GLU:O	7:G:66:PHE:C	2.63	0.41
8:H:15:ASP:N	8:H:16:PRO:HD2	2.35	0.41
1:A:93:GLU:O	1:A:94:HIS:ND1	2.54	0.41
1:A:106:LEU:HD22	1:A:203:LEU:CG	2.50	0.41
1:A:133:VAL:HG12	1:A:134:ILE:HD13	2.03	0.41
1:A:284:TYR:CD1	9:I:72:VAL:O	2.74	0.41
2:B:148:LYS:O	2:B:152:LEU:HG	2.21	0.41
2:B:211:VAL:HG11	2:B:216:LEU:HD13	2.03	0.41
2:B:211:VAL:CG1	2:B:212:SER:N	2.84	0.41
4:D:72:ASP:OD2	4:D:92:PRO:CB	2.68	0.41
5:E:42:THR:O	5:E:43:THR:C	2.64	0.41
5:E:94:LYS:HB3	5:E:95:PRO:HD2	2.02	0.41
5:E:119:ASP:CG	5:E:178:LEU:HA	2.45	0.41
8:H:15:ASP:HB2	8:H:16:PRO:HD2	2.00	0.41
10:J:56:LYS:CE	10:J:60:GLU:OE1	2.69	0.41
1:A:329:MET:HE2	7:G:2:ARG:CD	2.49	0.40
1:A:428:ILE:O	1:A:430:GLN:N	2.55	0.40
2:B:294:SER:O	2:B:295:LEU:C	2.64	0.40
2:B:431:GLY:C	2:B:432:HIS:HD2	2.29	0.40
3:C:149:LEU:HD21	3:C:281:LEU:HD22	2.02	0.40
4:D:61:ALA:O	4:D:62:LYS:C	2.64	0.40
4:D:208:MET:CE	4:D:209:LEU:HG	2.51	0.40
5:E:3:THR:C	5:E:5:ILE:H	2.29	0.40
5:E:23:LYS:CG	5:E:24:SER:N	2.83	0.40
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.51	0.40
6:F:49:ARG:NH1	6:F:97:VAL:HG22	2.36	0.40
10:J:41:ALA:O	10:J:42:ILE:C	2.63	0.40
10:J:57:HIS:O	10:J:58:LYS:C	2.64	0.40
1:A:53:ASN:C	1:A:53:ASN:ND2	2.79	0.40
1:A:159:GLN:NE2	7:G:18:LEU:HD21	2.33	0.40
1:A:240:GLN:HE22	1:A:431:LEU:HD21	1.80	0.40
2:B:68:LEU:CD2	2:B:186:VAL:HB	2.50	0.40
3:C:150:LEU:HD12	3:C:150:LEU:HA	1.87	0.40
3:C:228:ASP:O	3:C:229:ILE:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:338:ILE:O	3:C:341:GLN:HB2	2.20	0.40
3:C:341:GLN:HE21	3:C:341:GLN:N	2.19	0.40
5:E:129:LYS:O	5:E:130:PRO:C	2.63	0.40
6:F:43:VAL:O	6:F:47:ILE:HG13	2.22	0.40
8:H:66:ASP:O	8:H:67:HIS:O	2.39	0.40
1:A:22:GLY:O	1:A:24:ARG:HG2	2.21	0.40
1:A:24:ARG:HH11	1:A:24:ARG:HD2	1.72	0.40
1:A:168:GLU:H	1:A:168:GLU:HG3	1.60	0.40
2:B:163:LEU:HD22	2:B:256:ALA:CB	2.51	0.40
2:B:198:HIS:HE1	2:B:233:SER:OG	2.03	0.40
3:C:130:GLY:O	3:C:133:LEU:HB2	2.21	0.40
3:C:372:ILE:O	3:C:376:LEU:HG	2.21	0.40
4:D:102:ARG:CG	4:D:109:LEU:HB2	2.50	0.40
5:E:15:ARG:HB2	5:E:16:PRO:CD	2.51	0.40
6:F:66:LEU:O	6:F:67:ASP:C	2.64	0.40
1:A:200:ALA:HB3	1:A:375:VAL:HG23	2.02	0.40
1:A:385:THR:HG21	1:A:386:TYR:CE1	2.56	0.40
2:B:34:VAL:O	2:B:205:ALA:HA	2.20	0.40
2:B:38:LEU:CD1	2:B:378:PHE:HE2	2.34	0.40
2:B:394:PRO:O	2:B:398:VAL:HG23	2.21	0.40
3:C:138:MET:HE1	3:C:268:ILE:CA	2.42	0.40
4:D:126:TYR:O	4:D:127:VAL:C	2.63	0.40
6:F:80:TRP:O	6:F:81:THR:C	2.63	0.40
7:G:37:VAL:O	7:G:41:THR:HG23	2.21	0.40
1:A:61:HIS:HB3	1:A:130:GLU:CG	2.52	0.40
2:B:24:LEU:N	2:B:24:LEU:CD1	2.68	0.40
2:B:109:VAL:CG2	2:B:119:LEU:HG	2.51	0.40
2:B:309:VAL:CG1	2:B:310:SER:N	2.83	0.40
4:D:131:LEU:HD22	4:D:163:PRO:HB3	2.03	0.40
4:D:139:THR:OG1	8:H:41:ASP:OD1	2.34	0.40
4:D:222:MET:CE	5:E:43:THR:HG21	2.51	0.40
5:E:15:ARG:CB	5:E:16:PRO:CD	2.98	0.40
5:E:33:LYS:HB2	5:E:33:LYS:HE3	1.91	0.40
5:E:100:HIS:HD2	5:E:101:ARG:N	2.19	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:264:THR:OG1	5:E:141:HIS:O[10_665]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ARG:NH2	2:B:438:GLU:OE2[10_665]	1.99	0.21
3:C:177:ARG:NH2	5:E:62:MET:O[10_665]	2.12	0.08

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	444/446 (100%)	359 (81%)	65 (15%)	20 (4%)	2 12
2	B	417/439 (95%)	360 (86%)	43 (10%)	14 (3%)	3 17
3	C	377/379 (100%)	300 (80%)	55 (15%)	22 (6%)	1 8
4	D	239/241 (99%)	188 (79%)	32 (13%)	19 (8%)	1 3
5	E	194/196 (99%)	144 (74%)	40 (21%)	10 (5%)	1 9
6	F	104/110 (94%)	89 (86%)	14 (14%)	1 (1%)	12 45
7	G	79/81 (98%)	57 (72%)	18 (23%)	4 (5%)	1 10
8	H	62/78 (80%)	46 (74%)	11 (18%)	5 (8%)	1 3
9	I	31/78 (40%)	17 (55%)	9 (29%)	5 (16%)	0 0
10	J	60/62 (97%)	47 (78%)	13 (22%)	0	100 100
11	K	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	0 2
All	All	2027/2166 (94%)	1622 (80%)	303 (15%)	102 (5%)	1 10

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	PRO
1	A	432	PRO
2	B	183	ILE
3	C	8	HIS
3	C	27	ILE
3	C	46	LEU

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Mol	Chain	Res	Type
3	C	157	GLY
3	C	223	TYR
3	C	224	TYR
3	C	272	TRP
4	D	73	GLY
4	D	124	GLU
5	E	16	PRO
5	E	70	ALA
5	E	177	PRO
7	G	27	PRO
9	I	72	VAL
1	A	52	ASN
1	A	171	SER
1	A	246	ASP
1	A	287	GLY
1	A	288	ALA
1	A	315	ALA
1	A	385	THR
1	A	429	GLU
2	B	333	ALA
2	B	351	ASN
3	C	28	SER
3	C	52	ALA
3	C	109	PHE
3	C	255	ASN
4	D	38	SER
4	D	51	LEU
4	D	101	ALA
5	E	71	MET
5	E	87	MET
5	E	124	LEU
7	G	29	TYR
11	K	33	VAL
1	A	233	PRO
1	A	290	LEU
1	A	391	PRO
2	B	236	LYS
2	B	269	ALA
2	B	283	PRO
2	B	305	GLN
3	C	172	LYS
3	C	278	TYR

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Mol	Chain	Res	Type
3	C	279	ALA
4	D	98	PRO
4	D	119	ALA
4	D	123	GLY
5	E	69	LEU
6	F	97	VAL
7	G	45	ILE
8	H	49	GLN
8	H	50	THR
9	I	54	SER
9	I	59	ALA
1	A	109	ALA
1	A	395	TRP
2	B	52	LYS
2	B	88	GLY
3	C	345	HIS
4	D	139	THR
4	D	162	PRO
11	K	32	LEU
1	A	6	GLN
1	A	7	ALA
1	A	227	ALA
2	B	330	ALA
3	C	110	LEU
3	C	208	PRO
3	C	222	PRO
3	C	247	PRO
3	C	261	PRO
3	C	270	PRO
4	D	8	PRO
4	D	80	MET
4	D	100	ALA
4	D	120	ARG
4	D	137	PRO
4	D	161	ALA
5	E	8	PRO
5	E	152	ASP
7	G	34	ILE
8	H	39	LEU
8	H	53	ASP
2	B	192	HIS
2	B	307	PHE

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Mol	Chain	Res	Type
3	C	251	GLY
5	E	106	ILE
1	A	174	VAL
4	D	83	ARG
4	D	154	PRO
8	H	69	VAL
1	A	426	GLY
9	I	65	VAL
2	B	434	PRO
4	D	176	PRO
9	I	73	PRO
2	B	141	GLN

5.3.2 Protein sidechains (i)

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	370/370 (100%)	277 (75%)	93 (25%)	0 3
2	B	328/343 (96%)	254 (77%)	74 (23%)	1 5
3	C	327/327 (100%)	257 (79%)	70 (21%)	1 6
4	D	206/206 (100%)	170 (82%)	36 (18%)	2 10
5	E	168/168 (100%)	117 (70%)	51 (30%)	0 1
6	F	96/98 (98%)	71 (74%)	25 (26%)	0 3
7	G	71/71 (100%)	54 (76%)	17 (24%)	1 4
8	H	61/74 (82%)	49 (80%)	12 (20%)	1 8
9	I	27/60 (45%)	20 (74%)	7 (26%)	0 3
10	J	52/52 (100%)	42 (81%)	10 (19%)	1 8
11	K	15/46 (33%)	11 (73%)	4 (27%)	0 3
All	All	1721/1815 (95%)	1322 (77%)	399 (23%)	1 4

All (399) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	24	ARG
1	A	25	VAL
1	A	30	SER
1	A	34	THR
1	A	37	VAL
1	A	42	ASP
1	A	46	ARG
1	A	49	SER
1	A	51	LYS
1	A	59	VAL
1	A	65	LYS
1	A	73	ASN
1	A	75	LEU
1	A	77	LYS
1	A	79	VAL
1	A	81	SER
1	A	82	MET
1	A	86	LEU
1	A	89	TYR
1	A	91	THR
1	A	92	ARG
1	A	97	TYR
1	A	99	ILE
1	A	100	LYS
1	A	108	LYS
1	A	112	LEU
1	A	116	ILE
1	A	121	SER
1	A	122	LEU
1	A	125	SER
1	A	127	ILE
1	A	128	GLU
1	A	130	GLU
1	A	133	VAL
1	A	134	ILE
1	A	137	GLU
1	A	138	LEU
1	A	143	THR
1	A	144	SER
1	A	149	VAL
1	A	156	THR
1	A	171	SER

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Mol	Chain	Res	Type
1	A	175	ARG
1	A	176	LYS
1	A	178	SER
1	A	179	ARG
1	A	191	LYS
1	A	197	LEU
1	A	206	ARG
1	A	211	LEU
1	A	213	GLN
1	A	216	PHE
1	A	217	SER
1	A	220	SER
1	A	231	LEU
1	A	232	SER
1	A	239	SER
1	A	245	GLU
1	A	246	ASP
1	A	255	ILE
1	A	283	THR
1	A	292	SER
1	A	296	SER
1	A	302	LYS
1	A	312	ILE
1	A	323	HIS
1	A	330	SER
1	A	331	ILE
1	A	334	MET
1	A	337	VAL
1	A	341	GLN
1	A	344	ARG
1	A	346	CYS
1	A	350	THR
1	A	351	GLU
1	A	352	SER
1	A	353	GLU
1	A	356	ARG
1	A	358	LYS
1	A	360	LEU
1	A	366	VAL
1	A	370	ASP
1	A	379	ILE
1	A	382	SER

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Mol	Chain	Res	Type
1	A	383	LEU
1	A	384	LEU
1	A	386	TYR
1	A	388	ARG
1	A	402	VAL
1	A	407	VAL
1	A	412	SER
1	A	431	LEU
2	B	23	ASP
2	B	24	LEU
2	B	35	ILE
2	B	37	SER
2	B	38	LEU
2	B	46	ARG
2	B	47	ILE
2	B	52	LYS
2	B	56	ARG
2	B	58	GLU
2	B	66	SER
2	B	70	ARG
2	B	73	SER
2	B	74	SER
2	B	78	LYS
2	B	86	THR
2	B	95	LYS
2	B	99	THR
2	B	108	THR
2	B	109	VAL
2	B	112	LEU
2	B	113	ARG
2	B	117	ASP
2	B	127	THR
2	B	134	ARG
2	B	145	ARG
2	B	146	ILE
2	B	160	ILE
2	B	174	ASN
2	B	175	SER
2	B	182	ARG
2	B	183	ILE
2	B	185	LYS
2	B	186	VAL

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Mol	Chain	Res	Type
2	B	190	GLU
2	B	196	GLN
2	B	203	ARG
2	B	209	LEU
2	B	212	SER
2	B	215	VAL
2	B	219	VAL
2	B	221	GLU
2	B	222	GLN
2	B	233	SER
2	B	236	LYS
2	B	240	HIS
2	B	253	VAL
2	B	258	VAL
2	B	264	ILE
2	B	266	SER
2	B	273	SER
2	B	276	GLN
2	B	293	SER
2	B	295	LEU
2	B	297	GLN
2	B	315	SER
2	B	318	ASP
2	B	322	PHE
2	B	338	LYS
2	B	345	LYS
2	B	346	THR
2	B	354	ASN
2	B	365	LYS
2	B	371	SER
2	B	396	SER
2	B	402	ILE
2	B	411	ILE
2	B	418	VAL
2	B	419	SER
2	B	422	LYS
2	B	427	SER
2	B	436	ILE
2	B	437	ASP
2	B	438	GLU
3	C	4	ILE
3	C	5	ARG

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Mol	Chain	Res	Type
3	C	6	LYS
3	C	11	MET
3	C	25	SER
3	C	27	ILE
3	C	32	ASN
3	C	35	SER
3	C	43	LEU
3	C	47	THR
3	C	56	THR
3	C	60	THR
3	C	61	THR
3	C	65	SER
3	C	69	ILE
3	C	70	CYS
3	C	73	VAL
3	C	78	ILE
3	C	89	MET
3	C	92	ILE
3	C	94	LEU
3	C	102	LEU
3	C	108	THR
3	C	110	LEU
3	C	111	GLU
3	C	112	THR
3	C	115	ILE
3	C	118	ILE
3	C	119	LEU
3	C	124	MET
3	C	126	THR
3	C	138	MET
3	C	144	THR
3	C	156	ILE
3	C	158	THR
3	C	172	LYS
3	C	174	THR
3	C	175	LEU
3	C	176	THR
3	C	189	ILE
3	C	190	MET
3	C	195	VAL
3	C	197	LEU
3	C	207	ASN

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Mol	Chain	Res	Type
3	C	226	ILE
3	C	227	LYS
3	C	236	ILE
3	C	243	VAL
3	C	244	LEU
3	C	249	LEU
3	C	257	THR
3	C	271	GLU
3	C	288	LEU
3	C	299	LEU
3	C	300	ILE
3	C	304	ILE
3	C	306	LEU
3	C	311	LYS
3	C	313	ARG
3	C	316	MET
3	C	318	ARG
3	C	324	LEU
3	C	328	LEU
3	C	338	ILE
3	C	341	GLN
3	C	343	VAL
3	C	349	THR
3	C	353	LEU
3	C	363	LEU
3	C	377	LEU
4	D	1	SER
4	D	3	LEU
4	D	5	LEU
4	D	17	LEU
4	D	20	SER
4	D	26	ILE
4	D	40	CYS
4	D	42	SER
4	D	51	LEU
4	D	55	CYS
4	D	70	VAL
4	D	80	MET
4	D	82	MET
4	D	83	ARG
4	D	95	TYR
4	D	106	ASN

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Mol	Chain	Res	Type
4	D	109	LEU
4	D	114	SER
4	D	116	ILE
4	D	120	ARG
4	D	124	GLU
4	D	126	TYR
4	D	127	VAL
4	D	132	THR
4	D	141	VAL
4	D	160	MET
4	D	179	MET
4	D	180	SER
4	D	182	VAL
4	D	186	VAL
4	D	206	LEU
4	D	208	MET
4	D	211	MET
4	D	212	MET
4	D	222	MET
4	D	224	ARG
5	E	1	SER
5	E	3	THR
5	E	5	ILE
5	E	6	LYS
5	E	11	SER
5	E	15	ARG
5	E	17	GLU
5	E	18	VAL
5	E	19	LEU
5	E	23	LYS
5	E	28	SER
5	E	32	ARG
5	E	33	LYS
5	E	36	SER
5	E	42	THR
5	E	43	THR
5	E	45	VAL
5	E	52	LYS
5	E	56	SER
5	E	58	PHE
5	E	67	ASP
5	E	68	VAL

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Mol	Chain	Res	Type
5	E	71	MET
5	E	74	ILE
5	E	76	ILE
5	E	77	LYS
5	E	78	LEU
5	E	79	SER
5	E	83	GLU
5	E	85	LYS
5	E	86	ASN
5	E	87	MET
5	E	101	ARG
5	E	105	GLU
5	E	112	VAL
5	E	114	VAL
5	E	115	SER
5	E	116	GLN
5	E	119	ASP
5	E	124	LEU
5	E	126	ARG
5	E	138	VAL
5	E	166	ASP
5	E	173	LYS
5	E	178	LEU
5	E	182	VAL
5	E	184	SER
5	E	186	GLU
5	E	188	THR
5	E	190	ASP
5	E	193	VAL
6	F	9	SER
6	F	11	ARG
6	F	13	LEU
6	F	16	ILE
6	F	18	LYS
6	F	37	ILE
6	F	44	LYS
6	F	48	ARG
6	F	50	LEU
6	F	53	ASN
6	F	54	LEU
6	F	59	VAL
6	F	63	LYS

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Mol	Chain	Res	Type
6	F	69	SER
6	F	70	MET
6	F	75	LEU
6	F	76	PRO
6	F	77	LYS
6	F	82	LYS
6	F	85	GLU
6	F	87	LYS
6	F	98	ILE
6	F	100	GLU
6	F	105	GLU
6	F	110	LYS
7	G	4	PHE
7	G	9	ARG
7	G	10	VAL
7	G	15	THR
7	G	17	SER
7	G	24	ARG
7	G	28	HIS
7	G	38	LEU
7	G	39	ARG
7	G	40	ARG
7	G	42	ARG
7	G	44	CYS
7	G	45	ILE
7	G	46	LEU
7	G	60	THR
7	G	63	THR
7	G	70	LYS
8	H	19	THR
8	H	20	VAL
8	H	29	LYS
8	H	30	CYS
8	H	31	VAL
8	H	46	SER
8	H	47	ARG
8	H	60	ASP
8	H	73	LEU
8	H	74	PHE
8	H	76	SER
8	H	77	LEU
9	I	46	LYS

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Mol	Chain	Res	Type
9	I	49	VAL
9	I	62	ARG
9	I	70	LEU
9	I	76	VAL
9	I	77	ARG
9	I	78	TYR
10	J	4	THR
10	J	18	SER
10	J	24	ILE
10	J	33	ARG
10	J	42	ILE
10	J	46	ILE
10	J	51	LEU
10	J	52	TRP
10	J	58	LYS
10	J	62	LYS
11	K	20	THR
11	K	23	LEU
11	K	34	SER
11	K	36	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	85	HIS
1	A	136	GLN
1	A	151	ASN
1	A	154	HIS
1	A	159	GLN
1	A	189	HIS
1	A	213	GLN
1	A	240	GLN
1	A	243	HIS
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	323	HIS
2	B	62	ASN
2	B	67	HIS
2	B	125	ASN
2	B	156	GLN

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Mol	Chain	Res	Type
2	B	158	HIS
2	B	162	ASN
2	B	174	ASN
2	B	198	HIS
2	B	247	GLN
2	B	304	HIS
2	B	313	ASN
2	B	329	GLN
2	B	343	GLN
2	B	429	ASN
3	C	3	ASN
3	C	15	ASN
3	C	26	ASN
3	C	32	ASN
3	C	201	HIS
3	C	206	ASN
3	C	267	HIS
3	C	312	GLN
3	C	341	GLN
3	C	374	ASN
4	D	50	HIS
4	D	75	ASN
4	D	106	ASN
4	D	156	GLN
4	D	181	GLN
4	D	200	HIS
5	E	57	GLN
5	E	86	ASN
5	E	116	GLN
5	E	122	HIS
6	F	38	HIS
6	F	73	GLN
7	G	12	HIS
7	G	28	HIS
7	G	36	ASN
8	H	49	GLN
8	H	63	HIS
9	I	58	GLN
10	J	54	HIS
11	K	16	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
12	HEM	C	381	3	50,50,50	1.17	4 (8%)	67,82,82	1.51	14 (20%)
12	HEM	C	380	3	50,50,50	1.27	6 (12%)	67,82,82	1.26	6 (8%)
14	FES	E	197	5	0,4,4	-	-	-		
13	HEC	D	242	4	50,50,50	1.36	5 (10%)	68,82,82	1.17	7 (10%)

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
12	HEM	C	381	3	-	5/14/54/54	-
12	HEM	C	380	3	-	5/14/54/54	-
14	FES	E	197	5	-	-	0/1/1/1
13	HEC	D	242	4	-	9/14/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	242	HEC	CBB-CAB	-4.01	1.34	1.51
13	D	242	HEC	CBC-CAC	-3.70	1.35	1.51
12	C	380	HEM	FE-NB	3.39	2.05	1.94
12	C	380	HEM	CAB-C3B	2.95	1.55	1.47
12	C	380	HEM	CAC-C3C	2.68	1.54	1.47
12	C	381	HEM	CAB-C3B	2.49	1.54	1.47
12	C	380	HEM	CMA-C3A	2.41	1.55	1.50
12	C	381	HEM	C3B-C2B	-2.36	1.32	1.37
12	C	380	HEM	FE-NC	2.36	2.02	1.95
12	C	381	HEM	C2A-C3A	-2.32	1.32	1.38
13	D	242	HEC	FE-ND	2.24	2.01	1.94
12	C	381	HEM	FE-NB	2.21	2.01	1.94
13	D	242	HEC	FE-NA	2.14	2.02	1.95
13	D	242	HEC	CMC-C2C	2.07	1.55	1.50
12	C	380	HEM	C3B-C2B	-2.06	1.33	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	380	HEM	CBD-CAD-C3D	3.97	123.52	112.53
12	C	381	HEM	C4C-C3C-C2C	3.50	109.85	106.81
12	C	381	HEM	C3D-C4D-ND	-3.48	106.35	110.17
12	C	381	HEM	C4D-C3D-C2D	3.48	111.95	106.89
13	D	242	HEC	O2A-CGA-O1A	3.46	132.23	123.33
12	C	380	HEM	CMA-C3A-C2A	3.25	132.53	125.62
12	C	381	HEM	O1D-CGD-CBD	-3.18	113.01	123.09
12	C	381	HEM	CHD-C4C-NC	3.16	127.90	124.45
12	C	380	HEM	CMA-C3A-C4A	-3.01	120.83	125.42
12	C	381	HEM	O2D-CGD-O1D	2.91	130.83	123.33
13	D	242	HEC	CBB-CAB-C3B	2.57	119.39	112.42
12	C	381	HEM	C3B-C2B-C1B	2.50	108.28	106.41
12	C	381	HEM	CBC-CAC-C3C	-2.46	115.23	127.53
12	C	381	HEM	CHA-C4D-C3D	2.45	129.75	125.23
12	C	381	HEM	CBD-CAD-C3D	2.39	119.14	112.53
12	C	380	HEM	O2A-CGA-O1A	2.36	129.41	123.33
12	C	381	HEM	CHC-C1C-NC	2.34	127.01	124.45
12	C	381	HEM	CAD-C3D-C4D	-2.30	120.69	124.70
13	D	242	HEC	CAB-C3B-C4B	-2.27	121.83	124.79
12	C	381	HEM	CHA-C1A-C2A	2.25	130.22	125.30
13	D	242	HEC	CBD-CAD-C3D	2.22	118.68	112.53
13	D	242	HEC	O1A-CGA-CBA	-2.19	116.14	123.09
13	D	242	HEC	CBA-CAA-C2A	2.17	118.53	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	381	HEM	C1D-C2D-C3D	-2.16	104.71	106.98
13	D	242	HEC	CAD-CBD-CGD	2.14	119.34	113.67
12	C	380	HEM	O1A-CGA-CBA	-2.07	116.51	123.09
12	C	380	HEM	O1D-CGD-CBD	-2.06	116.57	123.09

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	242	HEC	C2B-C3B-CAB-CBB
13	D	242	HEC	C1A-C2A-CAA-CBA
13	D	242	HEC	C3A-C2A-CAA-CBA
13	D	242	HEC	C4B-C3B-CAB-CBB
13	D	242	HEC	C2A-CAA-CBA-CGA
12	C	381	HEM	C2D-C3D-CAD-CBD
12	C	380	HEM	CAD-CBD-CGD-O2D
12	C	380	HEM	CAD-CBD-CGD-O1D
12	C	380	HEM	C2A-CAA-CBA-CGA
12	C	381	HEM	CAD-CBD-CGD-O2D
13	D	242	HEC	CAA-CBA-CGA-O2A
12	C	381	HEM	CAA-CBA-CGA-O1A
13	D	242	HEC	CAA-CBA-CGA-O1A
12	C	380	HEM	CAA-CBA-CGA-O2A
12	C	381	HEM	CAD-CBD-CGD-O1D
12	C	380	HEM	CAA-CBA-CGA-O1A
12	C	381	HEM	CAA-CBA-CGA-O2A
13	D	242	HEC	CAD-CBD-CGD-O2D
13	D	242	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

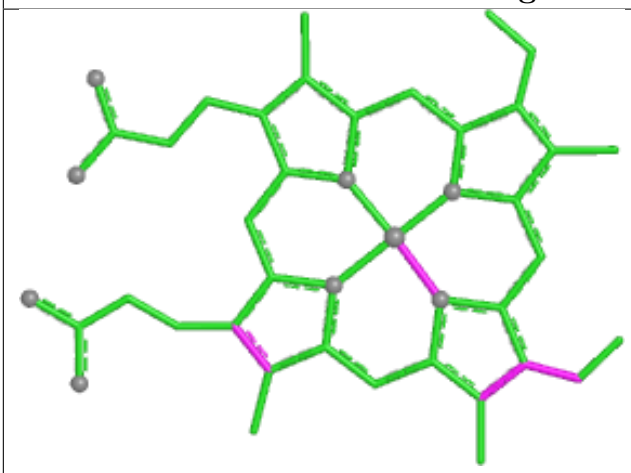
4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	381	HEM	9	0
12	C	380	HEM	10	0
14	E	197	FES	1	0
13	D	242	HEC	3	0

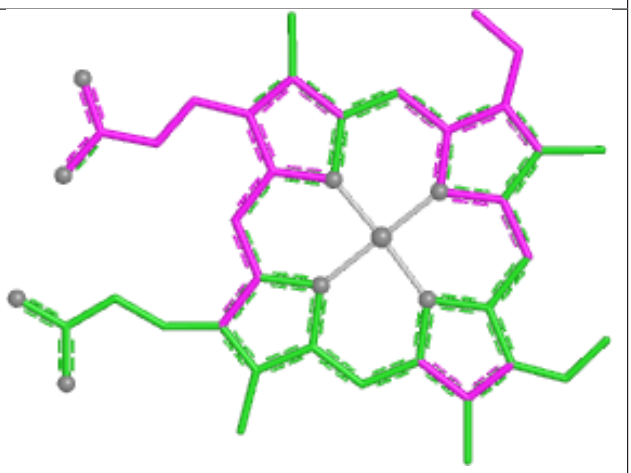
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

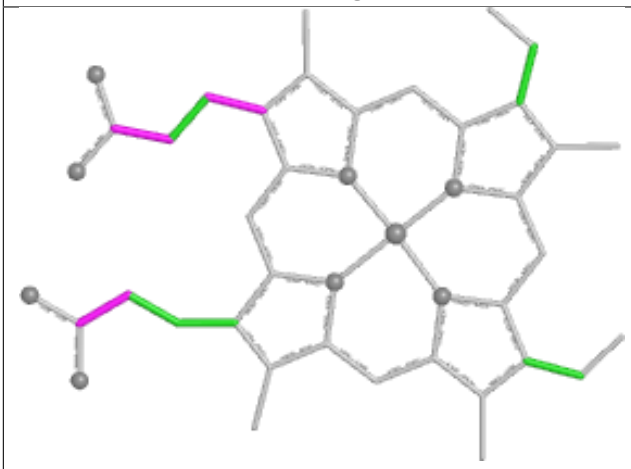
Ligand HEM C 381



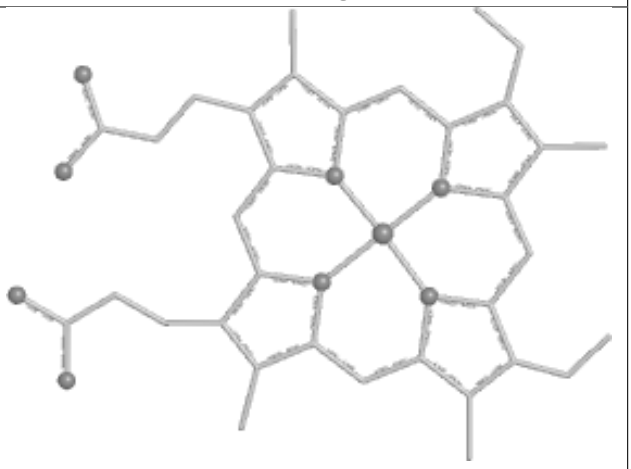
Bond lengths



Bond angles

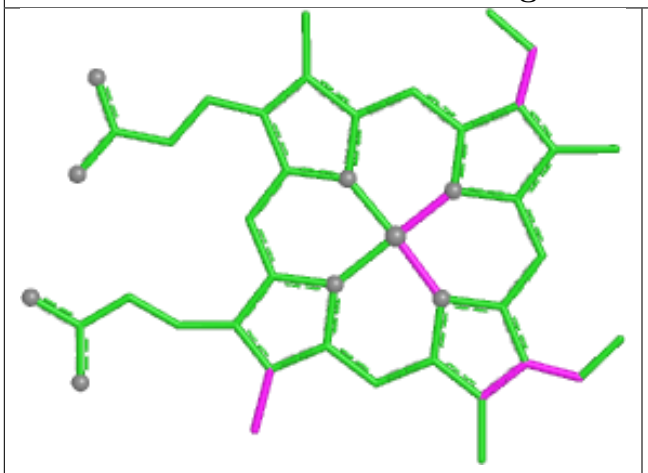


Torsions

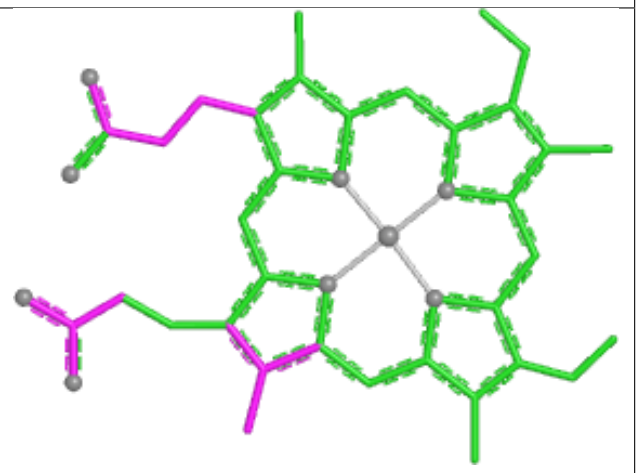


Rings

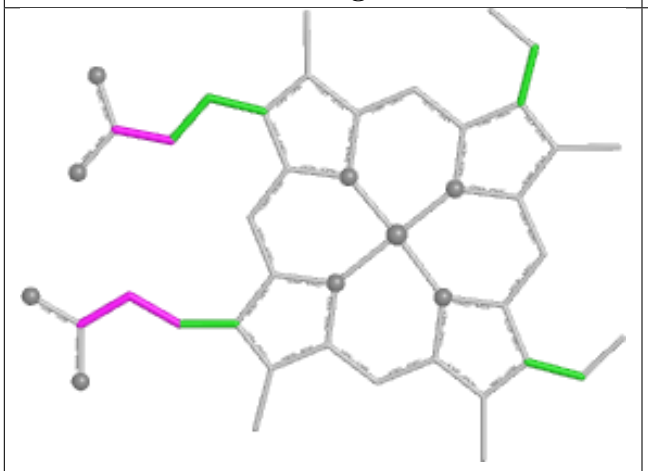
Ligand HEM C 380



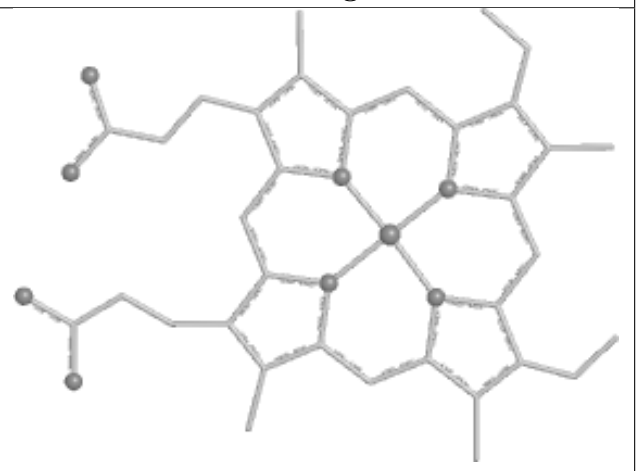
Bond lengths



Bond angles

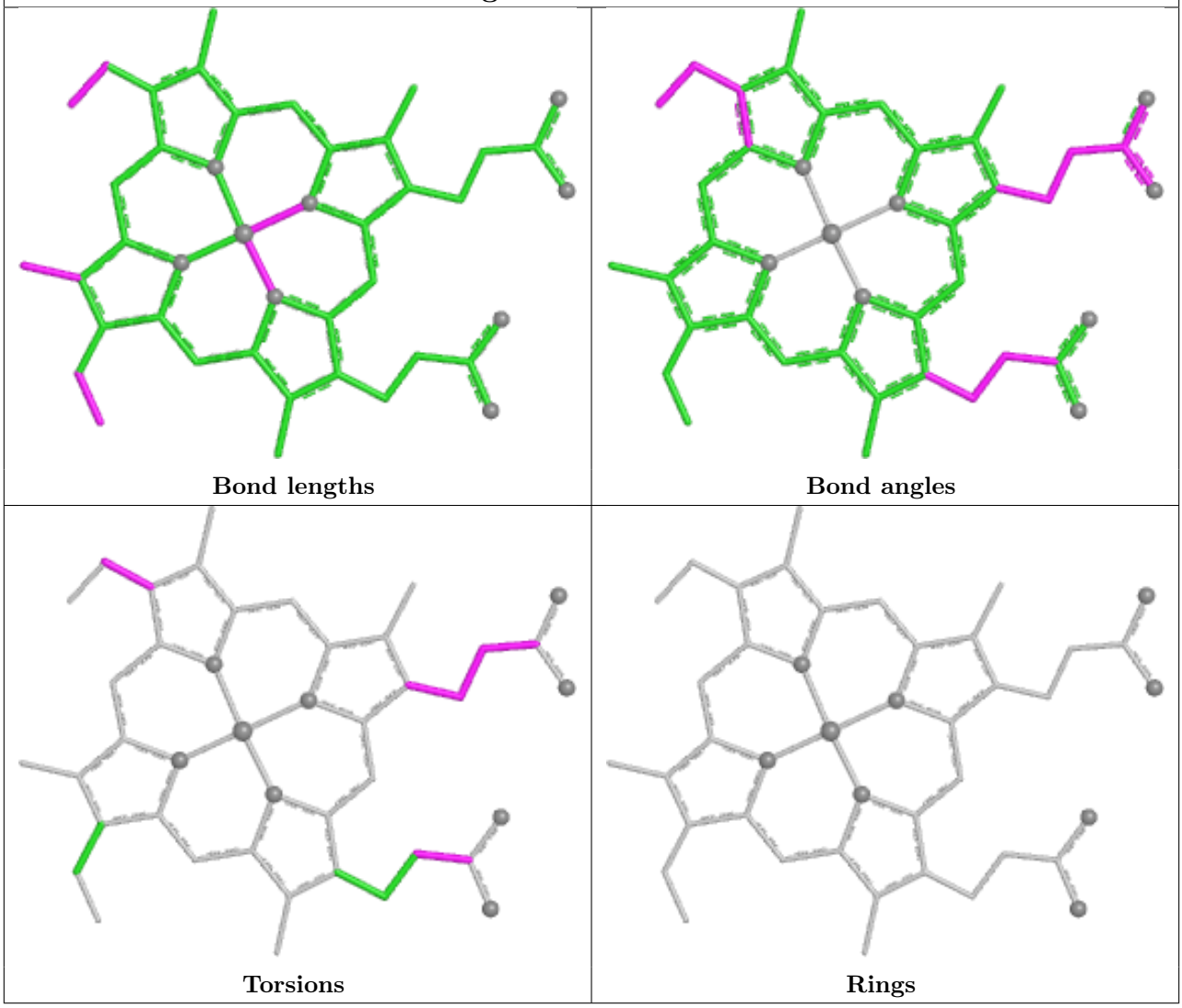


Torsions



Rings

Ligand HEC D 242



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.