Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 08:22 PM JST

PDB ID	:	8IC3 / pdb_00008ic3
EMDB ID	:	EMD-35353
Title	:	Respiratory complex Peripheral Arm of CI, focus-refined map of type I, PERK -/- mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-10
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

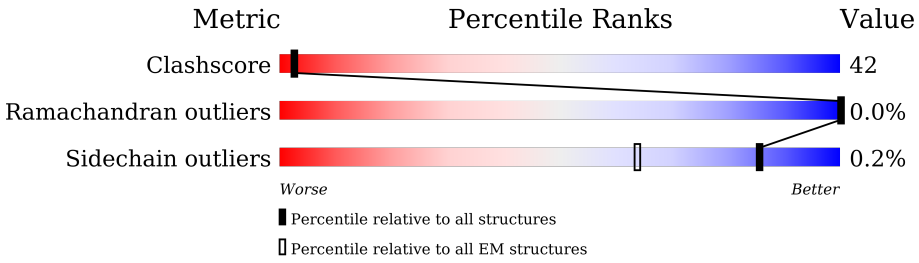
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

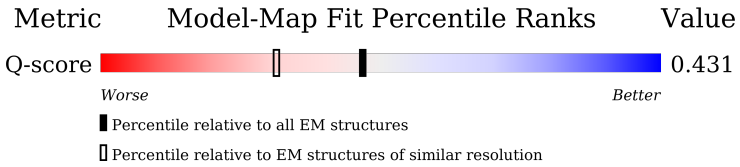
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	15%, 20%, 58%, 21%
2	B	224	31%, 34%, 30%
3	C	263	40%, 33%, 25%
4	D	463	32%, 48%, 17%

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Mol	Chain	Length	Quality of chain
5	E	248	18% 29% 52% 15%
6	F	464	11% 36% 51% 5% 9%
7	G	727	38% 51% 5% 6%
8	H	318	33% 61% 6%
9	I	212	39% 38% 5% 18%
10	P	377	17% 33% 54% 10%
11	Q	175	34% 30% 33%
12	R	116	41% 22% 40% 9% 28%
13	S	99	8% 26% 49% 8% 16%
14	T	156	19% 16% 26% 6% 52%
15	V	116	49% 41% 6%
16	W	131	7% 46% 39% 13%
17	X	172	15% 32% 48% 17%
18	Z	144	19% 45% 47%
19	a	70	33% 59%
20	b	84	12% 33% 60% 6%
21	q	145	67% 36% 41% 7% 16%
22	r	113	25% 18% 22% 5% 55%
23	s	104	19% 14% 12% 72%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	SF4	B	301	-	-	X	-
24	SF4	F	502	-	-	X	-
24	SF4	G	802	-	-	X	-
24	SF4	I	303	-	-	X	-
27	FES	E	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	FES	G	803	-	-	X	-
29	UQ9	H	401	-	-	X	-
34	CDL	q	201	-	-	X	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 33934 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	91	737	511	102	118	6	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	156	1247	796	223	214	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	198	1641	1060	279	299	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	385	3088	1970	533	562	23	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1635	1039	275	310	11	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	424	Total	C	N	O	S	0	0
			3273	2062	586	603	22		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total	C	N	O	S	0	0
			5287	3316	918	1012	41		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	317	Total	C	N	O	S	0	0
			2531	1701	383	425	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	173	Total	C	N	O	S	0	0
			1389	875	239	263	12		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	339	Total	C	N	O	S	0	0
			2720	1759	476	478	7		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	118	Total	C	N	O	S	0	0
			957	608	165	180	4		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	83	Total	C	N	O	S	0	0
			660	411	120	126	3		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	83	Total	C	N	O	S	0	0
			667	419	126	119	3		

- Molecule 14 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	142	Total	C	N	O	S	0	0
			1164	736	209	209	10		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	79	Total	C	N	O	S	0	0
			620	408	98	110	4		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	122	Total	C	N	O	S	0	0
			1020	655	180	181	4		

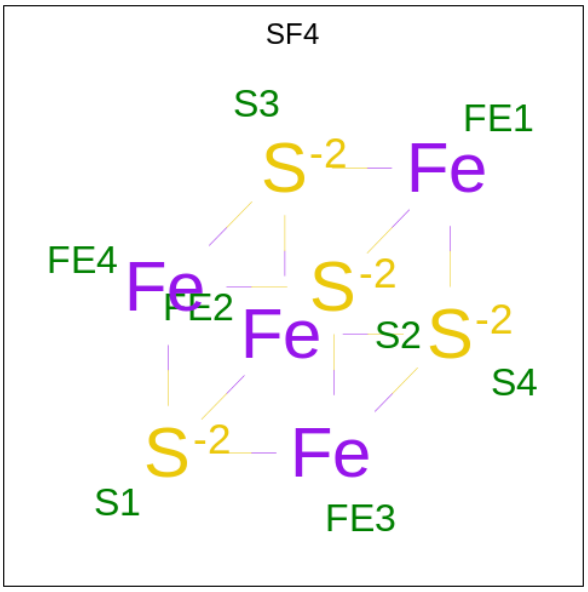
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	51	Total	C	N	O	S	0	0
			418	266	78	73	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

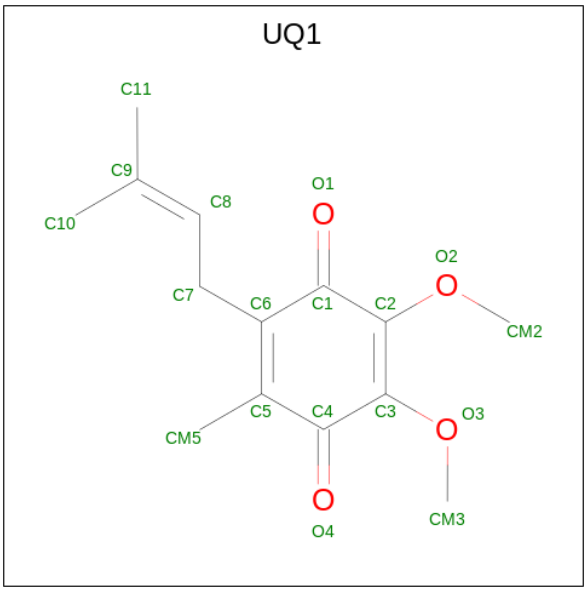
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	29	Total	C	N	O	0	0
			238	151	39	48		

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



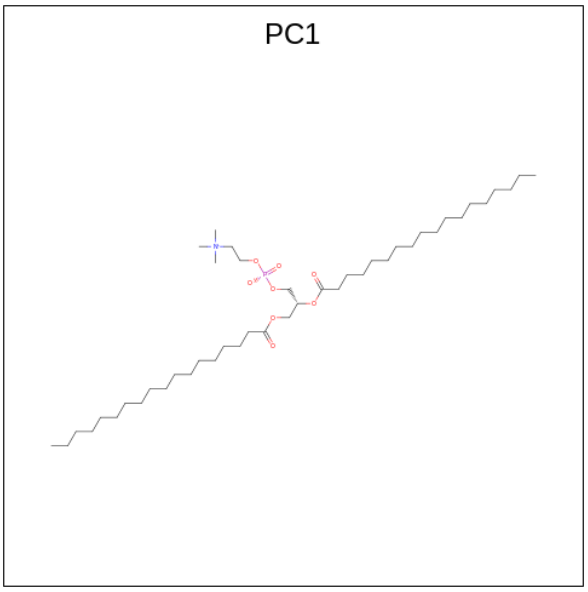
Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total Fe S 8 4 4	0
24	F	1	Total Fe S 8 4 4	0
24	G	1	Total Fe S 8 4 4	0
24	G	1	Total Fe S 8 4 4	0
24	I	1	Total Fe S 8 4 4	0
24	I	1	Total Fe S 8 4 4	0

- Molecule 25 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



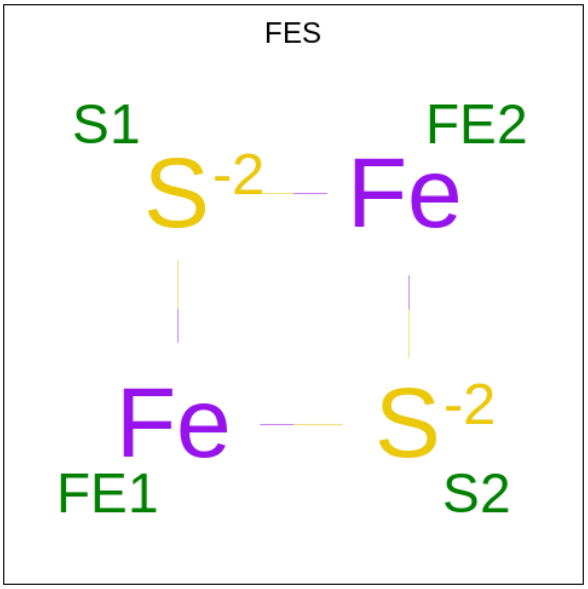
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			18	14	4	

- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



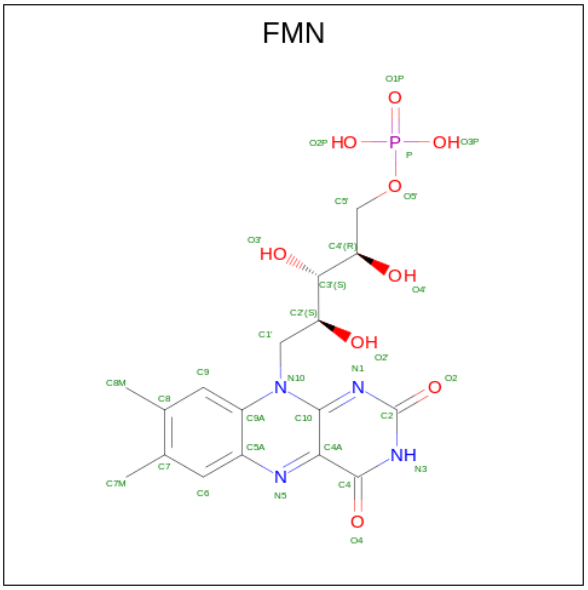
Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
26	I	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 27 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



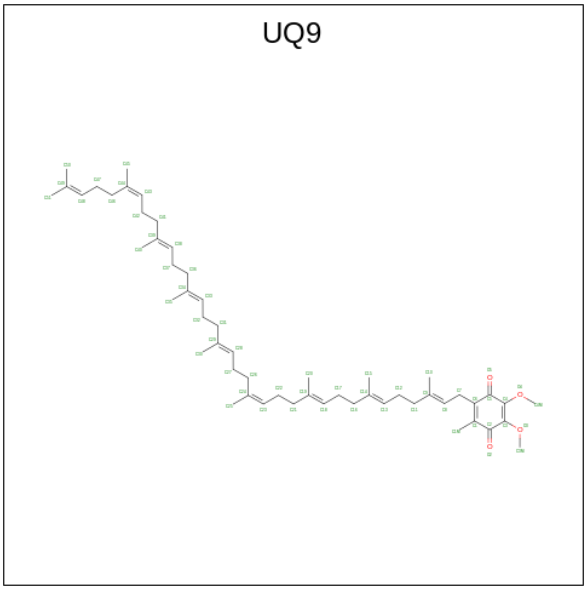
Mol	Chain	Residues	Atoms	AltConf
27	E	1	Total Fe S 4 2 2	0
27	G	1	Total Fe S 4 2 2	0

- Molecule 28 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



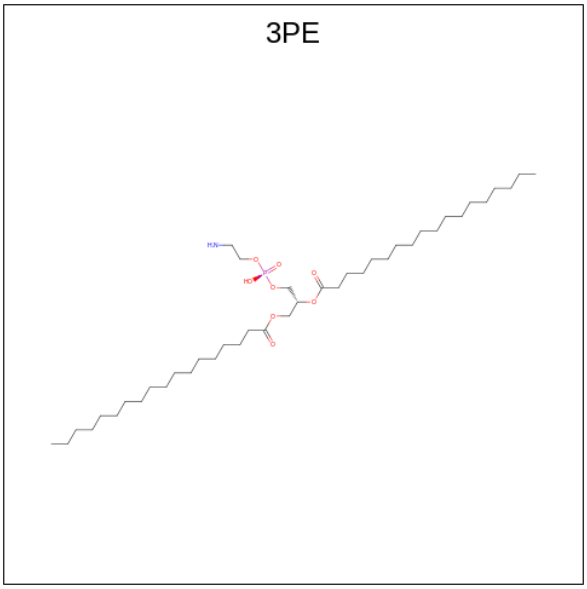
Mol	Chain	Residues	Atoms					AltConf
28	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 29 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



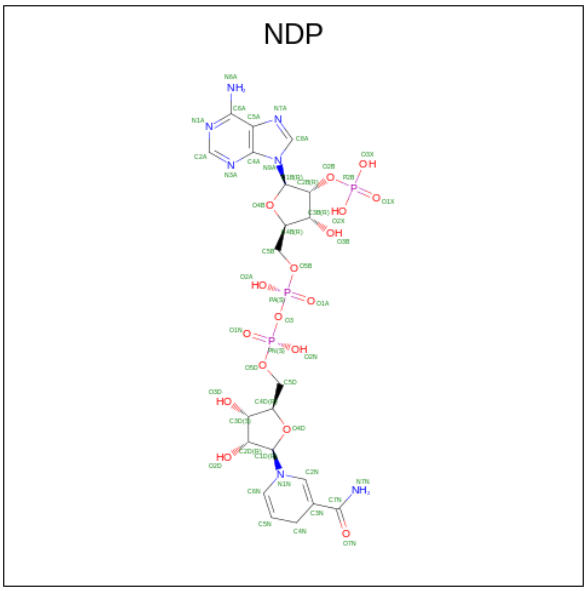
Mol	Chain	Residues	Atoms			AltConf
29	H	1	Total	C	O	0
			35	31	4	

- Molecule 30 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
30	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	H	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 31 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

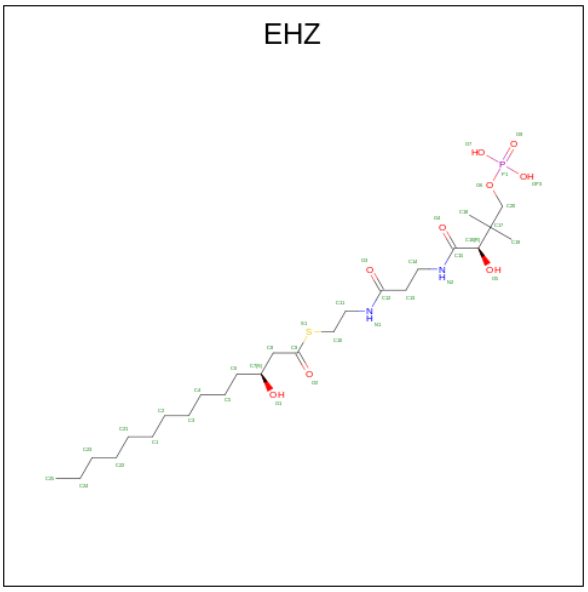


Mol	Chain	Residues	Atoms					AltConf
31	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

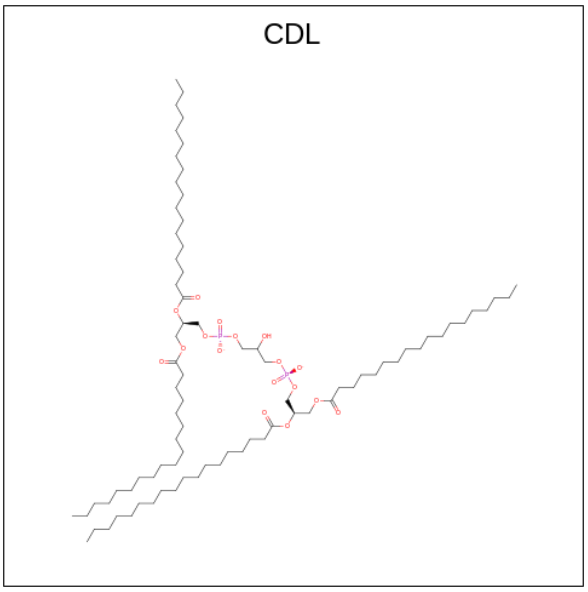
Mol	Chain	Residues	Atoms		AltConf
32	R	1	Total	Zn	0
			1	1	

- Molecule 33 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
33	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

- Molecule 34 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

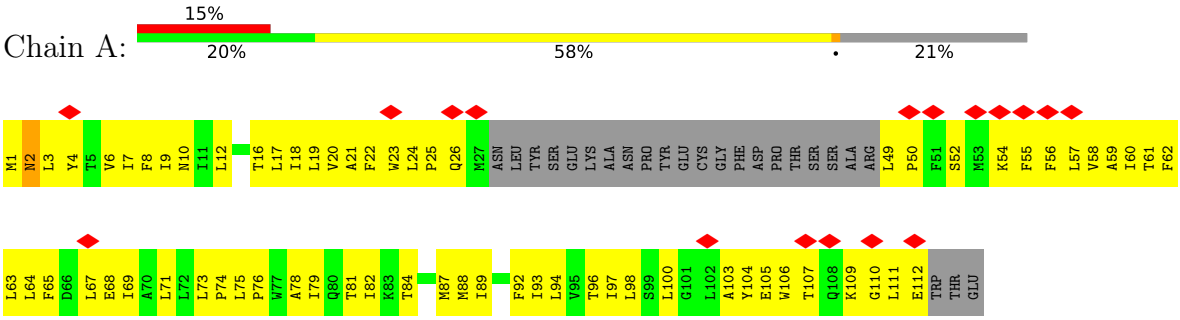


Mol	Chain	Residues	Atoms				AltConf
34	q	1	Total	C	O	P	0
			57	38	17	2	

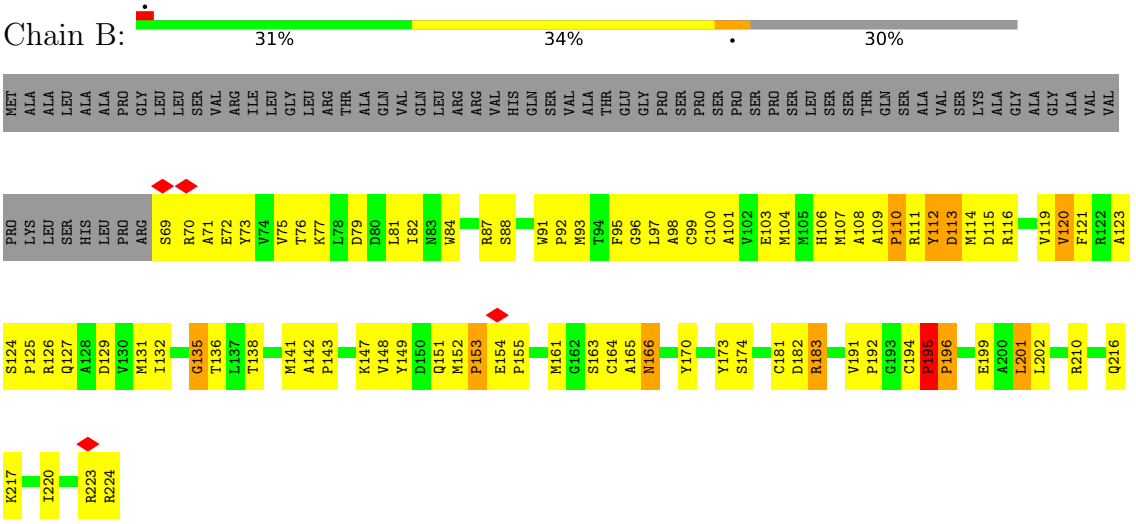
3 Residue-property plots (i)

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

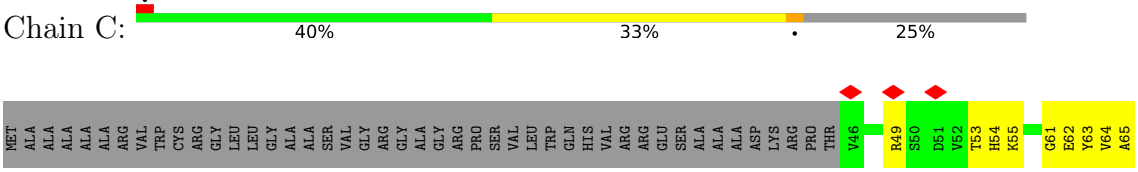
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

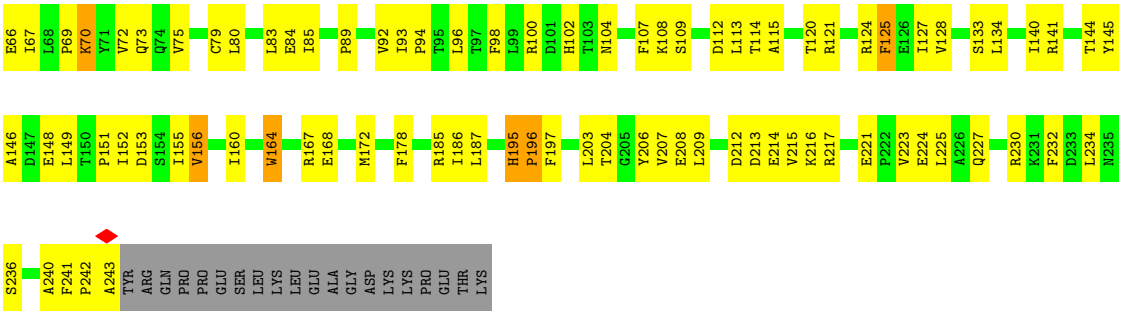


• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

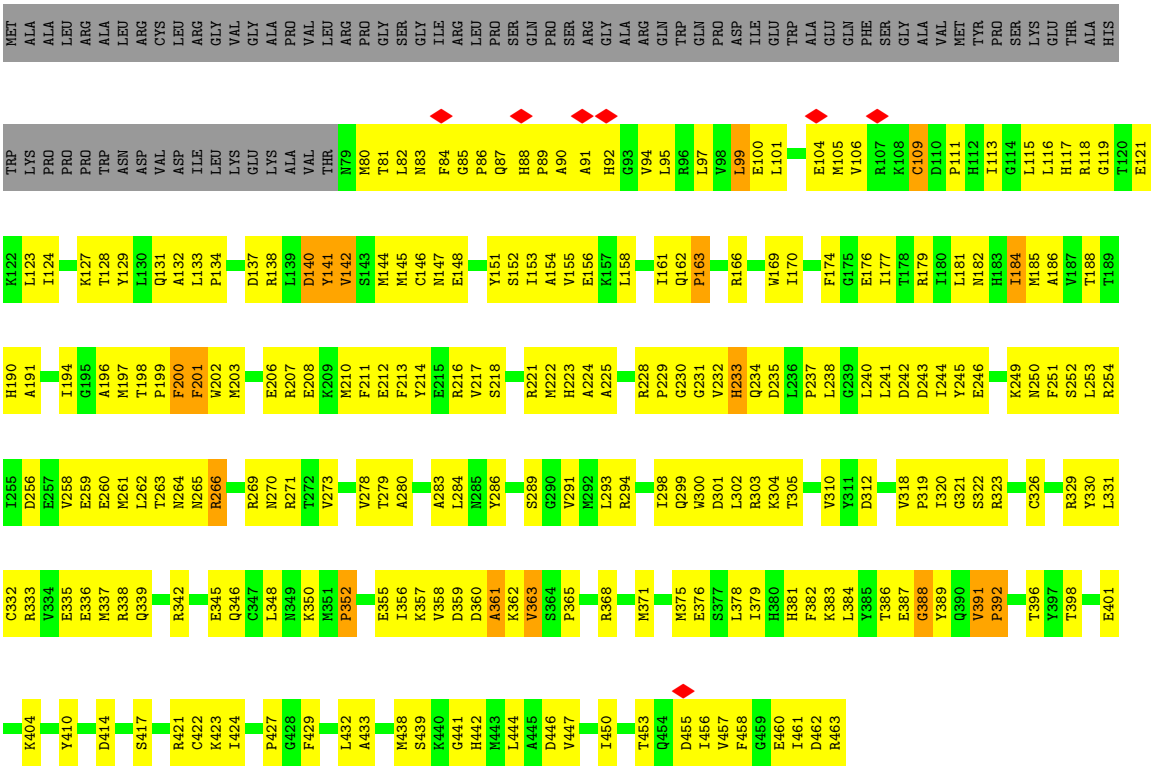




• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

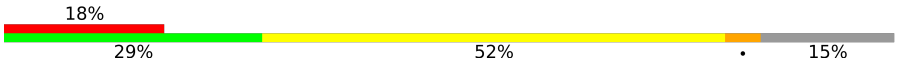
Chain D:

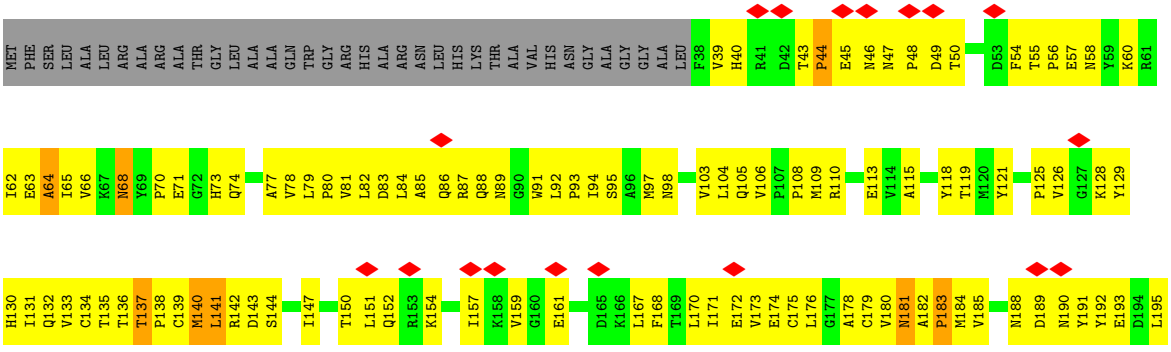




• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

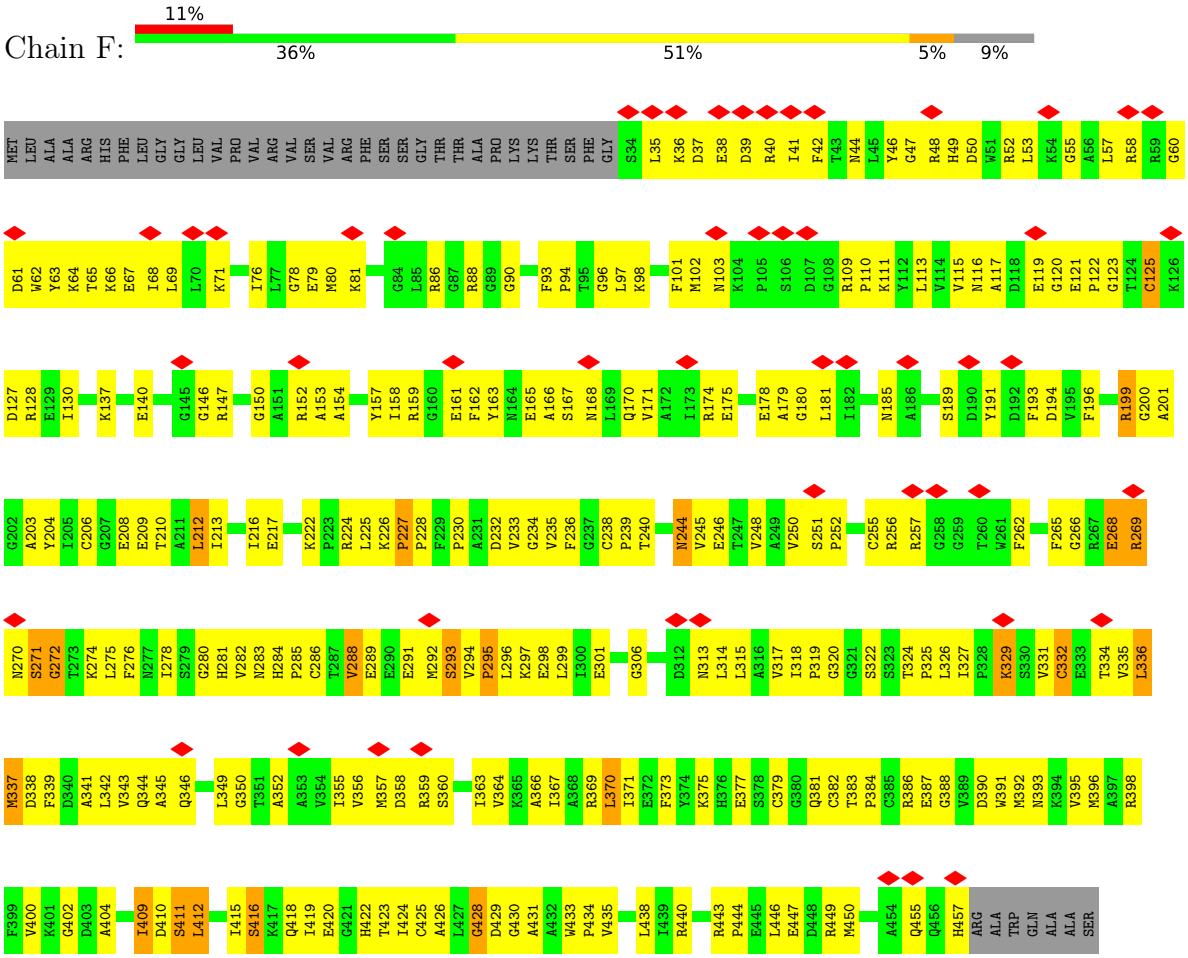
Chain E:



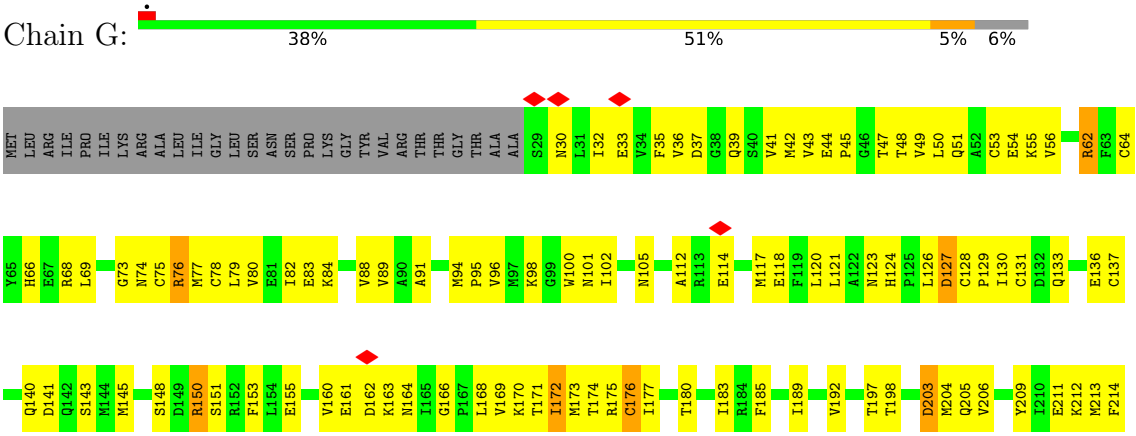


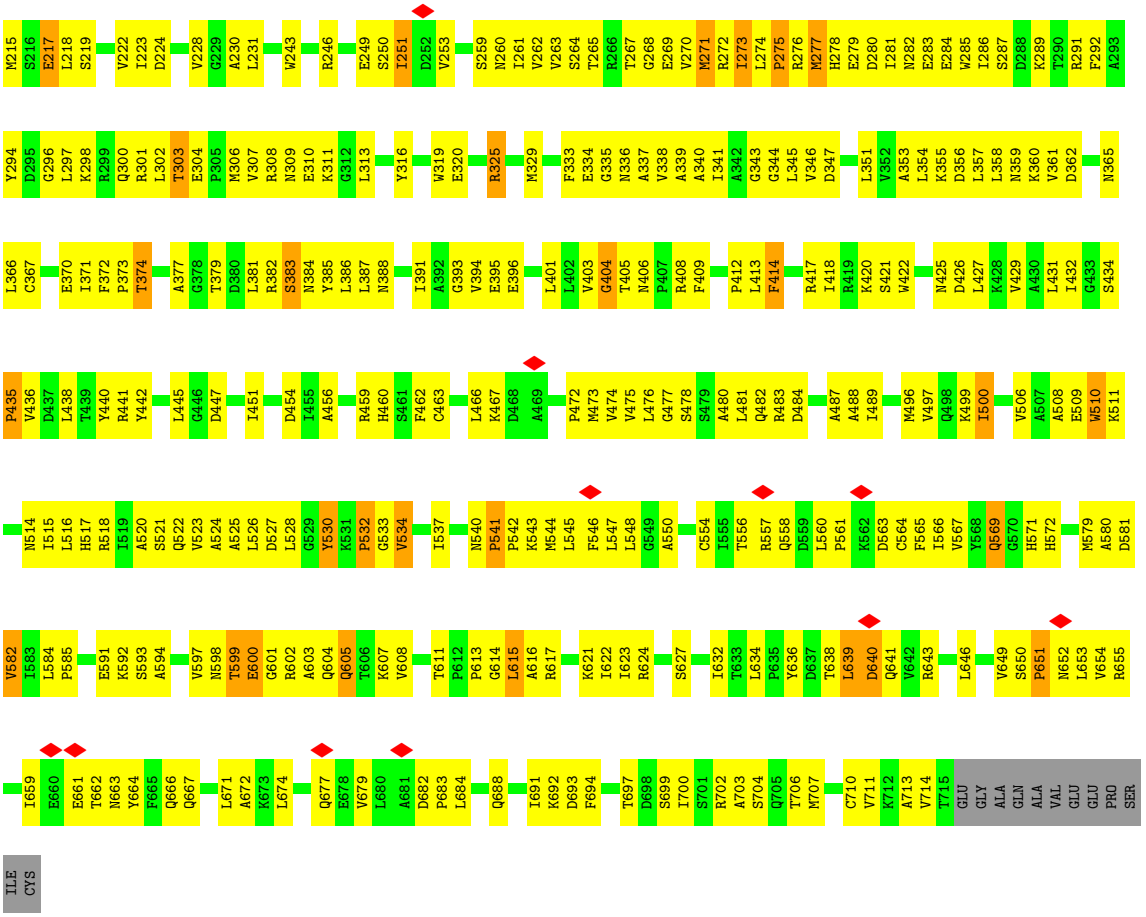


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

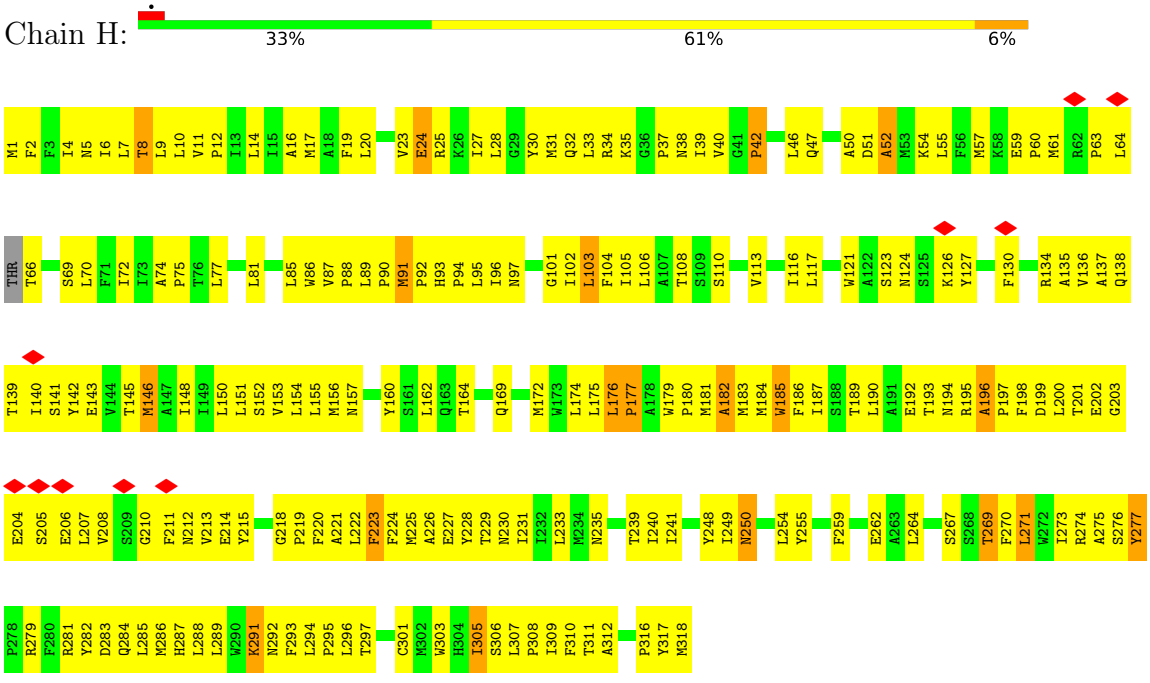


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



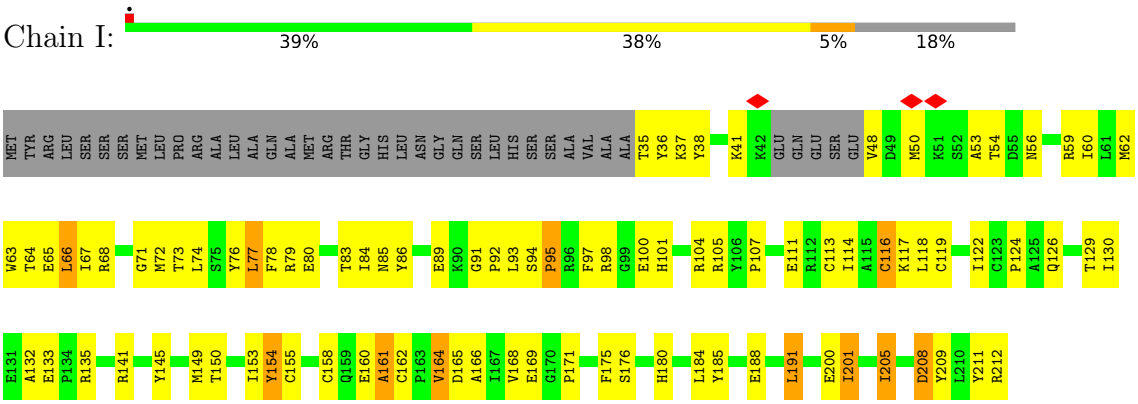


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



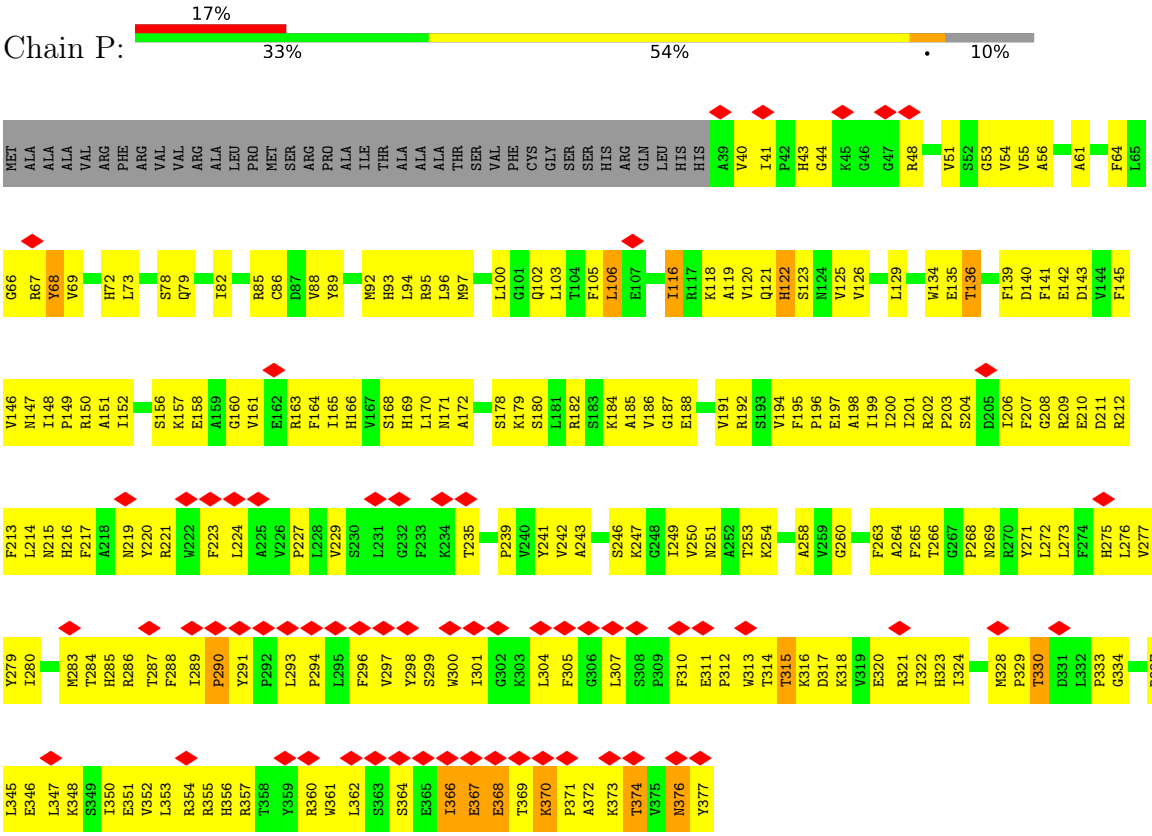
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



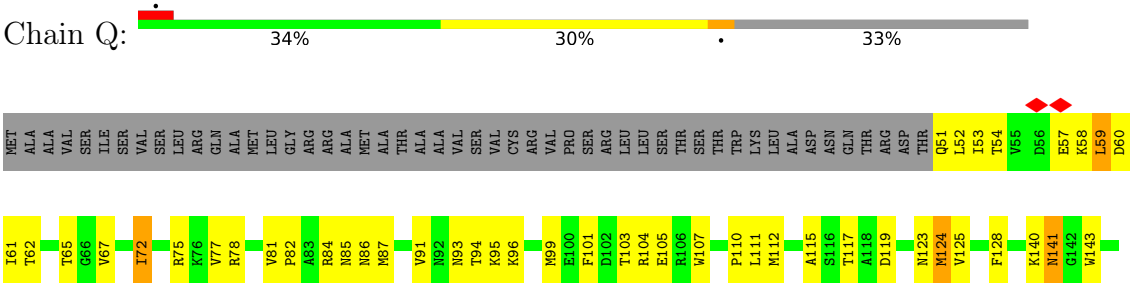
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

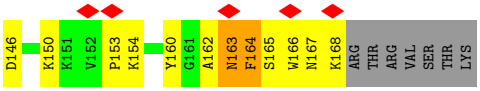
Chain P:



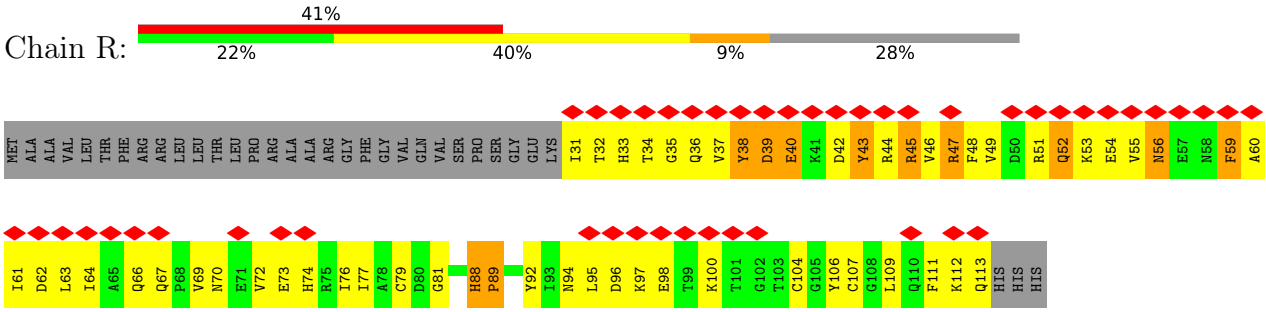
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:

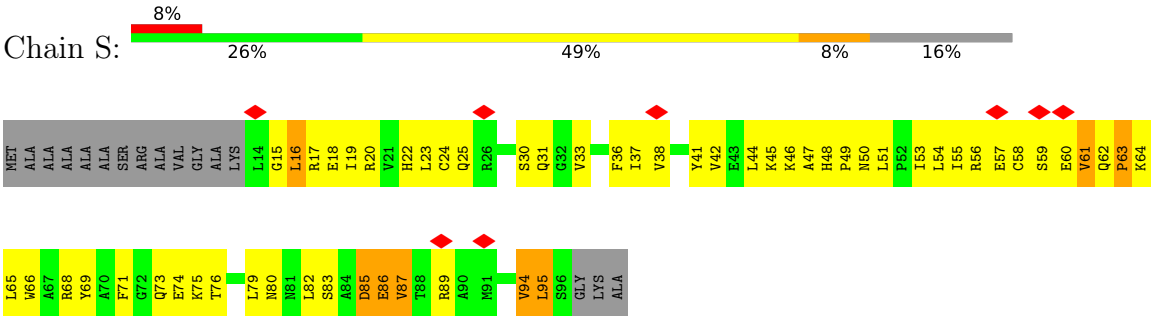




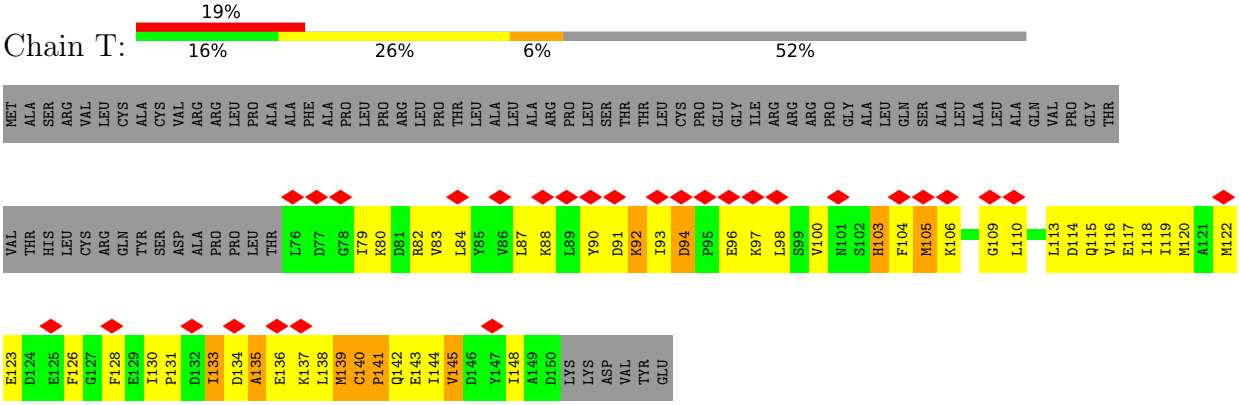
• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



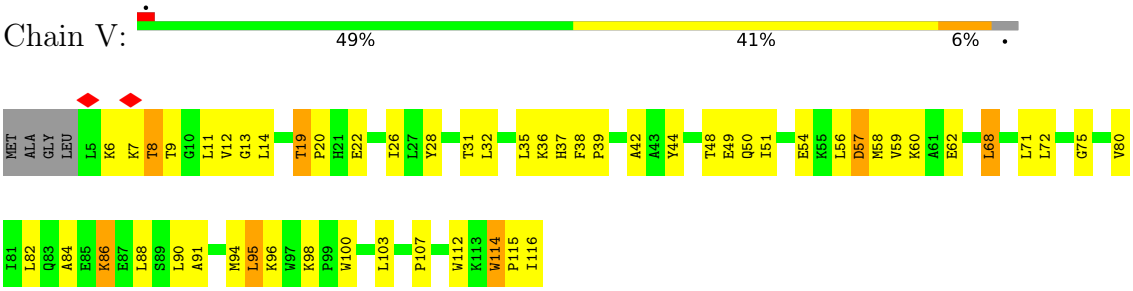
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



• Molecule 14: Acyl carrier protein, mitochondrial

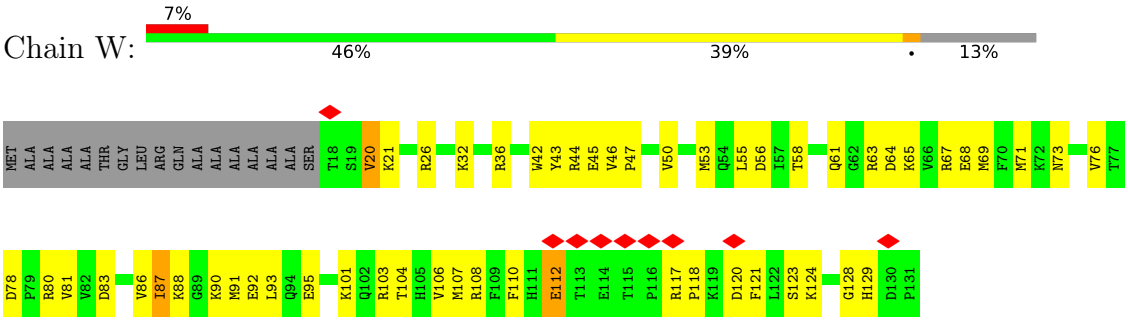


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



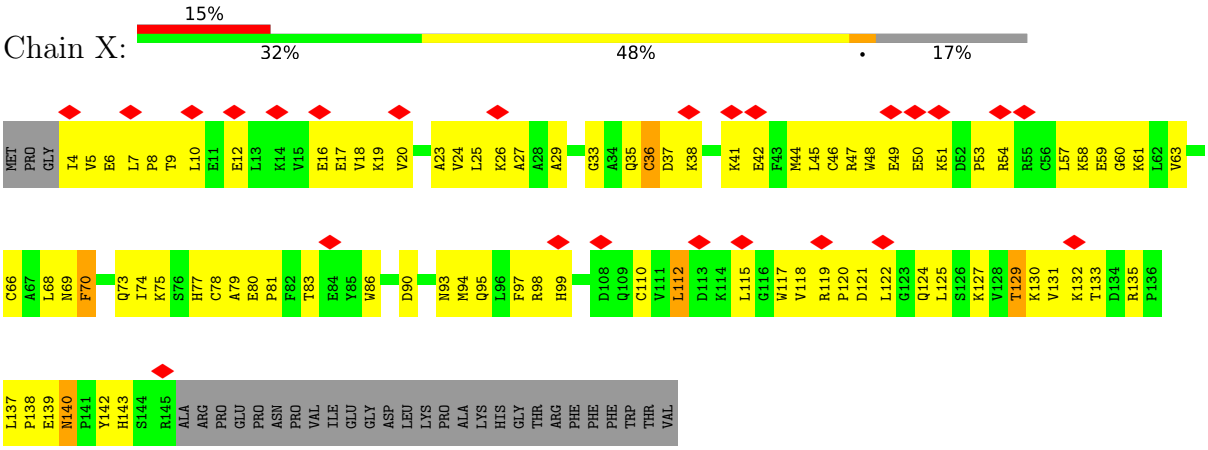
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



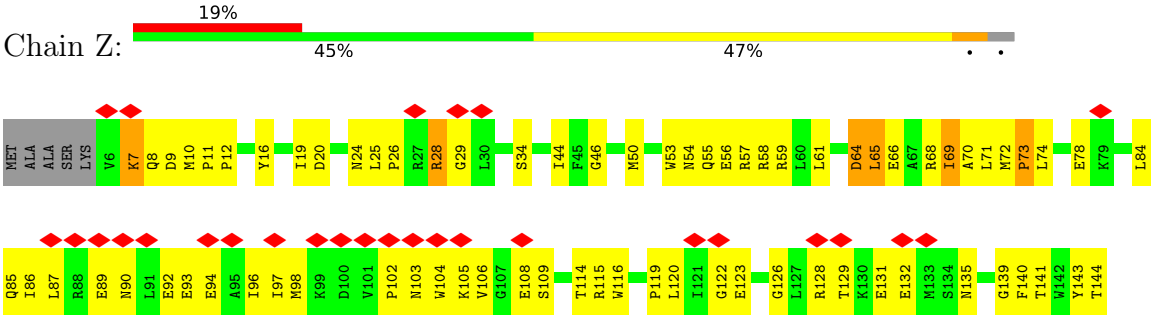
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



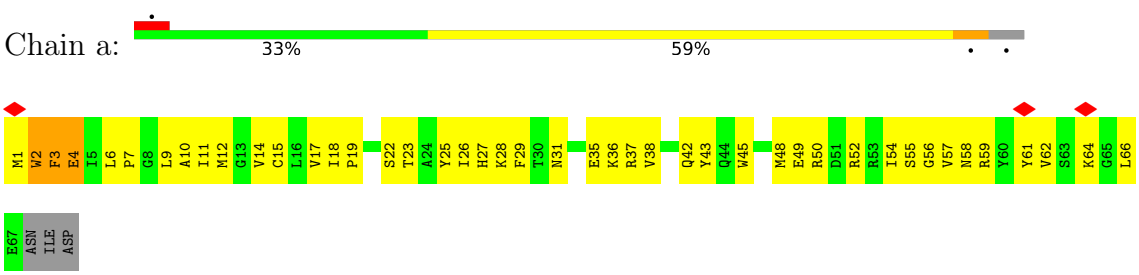
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:



• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:



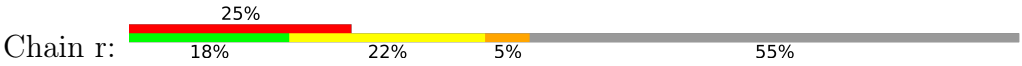


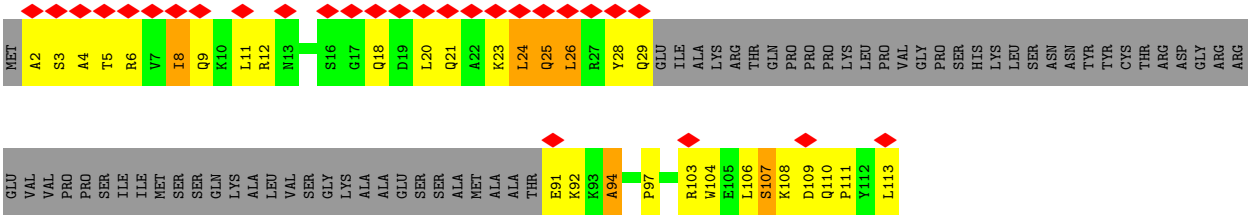
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12





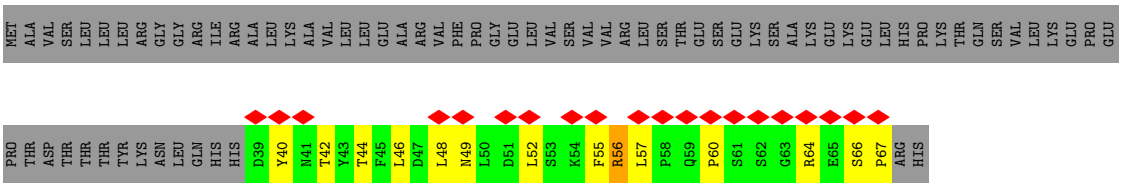
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7





• Molecule 23: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.326	Depositor
Minimum map value	-1.210	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, UQ9, 3PE, SF4, PC1, ZN, UQ1, FES, FMN, EHZ, CDL

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	0.67	0/755	0.96	3/1029 (0.3%)
2	B	0.96	4/1278 (0.3%)	1.30	11/1730 (0.6%)
3	C	0.88	2/1687 (0.1%)	1.28	13/2297 (0.6%)
4	D	0.94	5/3162 (0.2%)	1.39	30/4276 (0.7%)
5	E	0.82	3/1675 (0.2%)	1.16	18/2282 (0.8%)
6	F	0.82	4/3347 (0.1%)	1.32	41/4522 (0.9%)
7	G	0.88	8/5374 (0.1%)	1.49	86/7281 (1.2%)
8	H	0.83	2/2607 (0.1%)	1.22	30/3561 (0.8%)
9	I	0.90	1/1418 (0.1%)	1.48	18/1915 (0.9%)
10	P	0.79	4/2793 (0.1%)	1.17	23/3787 (0.6%)
11	Q	0.87	1/980 (0.1%)	1.28	12/1324 (0.9%)
12	R	1.04	4/671 (0.6%)	1.38	13/903 (1.4%)
13	S	0.94	2/678 (0.3%)	1.47	11/915 (1.2%)
14	T	1.03	1/613 (0.2%)	1.56	12/826 (1.5%)
15	V	0.86	0/937	1.47	14/1270 (1.1%)
16	W	0.73	0/993	0.95	3/1335 (0.2%)
17	X	0.70	0/1191	1.22	13/1605 (0.8%)
18	Z	0.81	1/1183 (0.1%)	1.23	11/1597 (0.7%)
19	a	0.88	0/561	1.38	8/755 (1.1%)
20	b	0.70	0/643	0.94	1/884 (0.1%)
21	q	1.04	2/1054 (0.2%)	1.53	19/1431 (1.3%)
22	r	1.16	3/426 (0.7%)	1.71	12/573 (2.1%)
23	s	0.45	0/244	1.10	2/331 (0.6%)
All	All	0.87	47/34270 (0.1%)	1.33	404/46429 (0.9%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	227	ALA	C-O	15.85	1.42	1.24
12	R	89	PRO	N-CD	-15.14	1.26	1.47
21	q	139	PRO	N-CD	-13.51	1.28	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	371	PRO	N-CD	12.90	1.65	1.47
7	G	532	PRO	N-CD	-12.58	1.30	1.47
14	T	141	PRO	N-CD	11.77	1.64	1.47
6	F	295	PRO	N-CD	-11.19	1.32	1.47
8	H	42	PRO	N-CD	10.84	1.62	1.47
22	r	91	GLU	N-CA	10.01	1.65	1.46
6	F	227	PRO	N-CD	9.93	1.61	1.47
10	P	290	PRO	N-CD	9.61	1.61	1.47
5	E	44	PRO	N-CD	-9.54	1.34	1.47
7	G	275	PRO	N-CD	-9.46	1.34	1.47
6	F	319	PRO	N-CD	9.06	1.60	1.47
9	I	107	PRO	N-CD	8.54	1.59	1.47
10	P	204	SER	C-O	-8.53	1.14	1.23
4	D	163	PRO	N-CD	-8.26	1.36	1.47
18	Z	73	PRO	N-CD	8.10	1.59	1.47
13	S	63	PRO	N-CD	-7.95	1.36	1.47
12	R	39	ASP	CA-C	7.93	1.64	1.53
4	D	352	PRO	N-CD	-7.86	1.36	1.47
11	Q	53	ILE	C-O	7.85	1.33	1.24
12	R	40	GLU	N-CA	7.84	1.56	1.46
2	B	88	SER	C-N	-7.65	1.20	1.33
22	r	111	PRO	N-CD	-7.46	1.37	1.47
2	B	96	GLY	CA-C	-7.44	1.47	1.52
7	G	541	PRO	N-CD	-6.82	1.38	1.47
7	G	203	ASP	CA-C	6.64	1.62	1.52
7	G	600	GLU	CA-C	6.45	1.61	1.52
3	C	66	GLU	C-N	6.38	1.42	1.33
2	B	153	PRO	N-CD	-6.30	1.39	1.47
7	G	127	ASP	CA-C	6.26	1.62	1.52
4	D	266	ARG	C-O	-6.23	1.16	1.24
6	F	384	PRO	N-CD	-6.17	1.39	1.47
2	B	110	PRO	C-O	-6.10	1.16	1.24
7	G	76	ARG	CA-C	6.09	1.61	1.53
22	r	25	GLN	CA-C	5.92	1.60	1.52
5	E	93	PRO	N-CD	-5.87	1.39	1.47
8	H	291	LYS	C-O	-5.81	1.16	1.24
12	R	59	PHE	CA-C	-5.81	1.45	1.52
10	P	204	SER	CA-C	-5.69	1.46	1.53
13	S	95	LEU	CA-C	5.44	1.59	1.52
4	D	392	PRO	C-O	-5.42	1.20	1.24
7	G	683	PRO	N-CD	-5.39	1.40	1.47
21	q	126	PRO	N-CD	5.33	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	266	ARG	CA-C	-5.24	1.45	1.52
3	C	61	GLY	C-N	-5.01	1.27	1.33

All (404) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	142	VAL	N-CA-CB	19.30	132.46	110.65
4	D	142	VAL	N-CA-C	-19.03	92.53	110.42
7	G	174	THR	N-CA-C	-17.48	89.04	114.39
6	F	332	CYS	N-CA-C	15.59	130.04	111.02
22	r	91	GLU	N-CA-CB	14.52	135.18	110.50
21	q	139	PRO	N-CA-CB	-13.57	95.59	103.19
7	G	251	ILE	N-CA-C	13.28	126.76	108.17
9	I	164	VAL	N-CA-C	-12.77	100.19	112.83
7	G	77	MET	N-CA-C	-12.55	97.36	113.17
7	G	500	ILE	N-CA-C	-12.54	98.74	110.53
19	a	3	PHE	CB-CA-C	-12.41	89.59	110.68
10	P	106	LEU	N-CA-C	12.21	128.73	109.07
7	G	204	MET	N-CA-C	-11.63	91.45	109.25
6	F	288	VAL	N-CA-C	11.61	121.56	110.42
6	F	449	ARG	N-CA-C	-11.60	98.71	111.36
6	F	334	THR	N-CA-CB	11.47	127.25	109.82
7	G	599	THR	N-CA-C	11.34	126.21	112.38
11	Q	60	ASP	N-CA-C	-11.33	90.32	109.24
15	V	57	ASP	N-CA-C	-11.03	99.27	111.07
9	I	77	LEU	N-CA-C	-10.44	99.70	111.71
2	B	195	PRO	N-CA-C	-10.42	97.99	110.70
14	T	139	MET	N-CA-C	-10.38	97.49	113.89
5	E	68	ASN	N-CA-C	-10.37	99.98	111.07
7	G	280	ASP	N-CA-C	10.31	122.52	111.28
23	s	55	PHE	N-CA-C	10.22	125.75	112.26
10	P	366	ILE	N-CA-C	10.22	121.04	110.62
4	D	337	MET	N-CA-C	-10.21	100.15	111.07
4	D	140	ASP	CB-CA-C	-10.19	98.07	111.42
7	G	414	PHE	N-CA-C	-10.17	101.38	113.88
9	I	161	ALA	N-CA-C	10.10	122.29	111.28
14	T	135	ALA	N-CA-C	-10.07	100.30	111.28
19	a	4	GLU	N-CA-C	10.04	124.79	112.54
14	T	133	ILE	N-CA-C	9.92	119.86	110.53
9	I	166	ALA	N-CA-C	-9.87	100.79	113.12
7	G	325	ARG	N-CA-C	-9.82	100.27	110.97
5	E	64	ALA	N-CA-C	-9.75	99.41	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	654	VAL	N-CA-C	9.71	123.23	111.09
21	q	138	VAL	CA-C-N	-9.68	112.59	119.66
21	q	138	VAL	C-N-CA	-9.68	112.59	119.66
10	P	371	PRO	N-CA-CB	9.66	111.86	103.36
16	W	87	ILE	N-CA-C	-9.63	101.17	110.42
19	a	2	TRP	N-CA-C	-9.56	101.61	113.28
6	F	418	GLN	N-CA-C	-9.56	100.81	111.14
8	H	91	MET	N-CA-C	-9.52	96.49	110.20
17	X	70	PHE	N-CA-C	-9.49	99.72	111.11
8	H	52	ALA	N-CA-C	-9.46	100.94	111.07
4	D	427	PRO	N-CA-C	-9.45	95.66	110.50
12	R	38	TYR	N-CA-C	-9.43	96.37	110.24
17	X	112	LEU	N-CA-C	-9.41	100.97	111.14
7	G	694	PHE	N-CA-C	9.38	121.50	111.28
21	q	139	PRO	CA-N-CD	9.37	125.12	112.00
7	G	692	LYS	N-CA-C	-9.28	100.53	112.23
10	P	367	GLU	N-CA-C	9.28	122.59	111.82
10	P	369	THR	N-CA-CB	9.24	123.47	110.17
18	Z	69	ILE	N-CA-C	-9.20	100.70	110.36
7	G	640	ASP	N-CA-C	-9.16	101.38	111.36
5	E	85	ALA	N-CA-C	-9.15	101.38	111.36
6	F	103	ASN	N-CA-C	-9.13	101.06	113.30
19	a	57	VAL	N-CA-C	-9.03	105.14	113.71
6	F	411	SER	N-CA-C	-8.96	101.48	111.07
7	G	133	GLN	N-CA-CB	8.81	121.55	110.45
7	G	212	LYS	N-CA-C	-8.75	94.63	108.90
16	W	20	VAL	N-CA-C	8.66	120.75	108.36
9	I	154	TYR	N-CA-CB	-8.66	99.24	111.62
19	a	3	PHE	CA-CB-CG	8.55	122.36	113.80
13	S	18	GLU	N-CA-C	8.55	123.34	109.40
13	S	86	GLU	N-CA-C	-8.52	102.08	111.36
3	C	70	LYS	N-CA-C	8.50	121.62	111.33
2	B	100	CYS	N-CA-C	-8.48	102.69	113.72
10	P	373	LYS	N-CA-C	8.47	121.87	110.35
3	C	108	LYS	N-CA-C	8.40	120.06	111.07
17	X	99	HIS	N-CA-C	-8.36	102.25	111.36
7	G	532	PRO	CA-N-CD	8.35	123.69	112.00
11	Q	54	THR	N-CA-C	8.34	123.30	109.46
7	G	558	GLN	N-CA-C	-8.29	102.20	111.07
8	H	196	ALA	N-CA-C	8.25	128.04	109.81
3	C	196	PRO	N-CA-C	8.19	124.92	113.53
7	G	691	ILE	N-CA-C	8.17	123.66	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	484	ASP	N-CA-C	8.17	121.10	111.71
15	V	86	LYS	N-CA-C	-8.14	102.35	111.14
6	F	411	SER	N-CA-CB	8.12	121.78	110.01
7	G	534	VAL	N-CA-C	-8.09	104.71	111.91
7	G	62	ARG	N-CA-C	8.07	121.56	108.32
9	I	201	ILE	N-CA-C	-8.07	102.57	110.72
7	G	500	ILE	N-CA-CB	8.01	120.82	110.57
2	B	110	PRO	N-CA-C	7.99	124.44	113.65
13	S	76	THR	N-CA-C	7.99	121.93	108.90
8	H	271	LEU	N-CA-C	-7.94	102.56	111.14
21	q	67	GLU	CB-CA-C	-7.93	99.62	112.06
7	G	651	PRO	CB-CA-C	-7.92	98.49	111.56
15	V	6	LYS	N-CA-C	-7.89	100.11	110.53
1	A	9	ILE	N-CA-C	-7.88	102.58	110.62
7	G	270	VAL	N-CA-CB	-7.86	100.65	110.31
9	I	74	LEU	N-CA-C	-7.80	102.78	111.28
9	I	160	GLU	N-CA-C	7.79	124.14	111.37
4	D	141	TYR	CA-C-N	7.76	130.19	120.72
4	D	141	TYR	C-N-CA	7.76	130.19	120.72
21	q	44	TYR	N-CA-C	-7.69	98.89	110.28
21	q	89	TRP	N-CA-C	-7.69	102.83	111.14
6	F	334	THR	N-CA-C	-7.68	101.65	111.02
12	R	47	ARG	N-CA-C	7.65	120.58	111.33
5	E	68	ASN	N-CA-CB	7.63	121.07	110.01
12	R	74	HIS	N-CA-C	7.60	121.22	110.50
7	G	569	GLN	N-CA-C	7.59	121.98	108.24
14	T	141	PRO	N-CA-C	-7.56	103.02	113.53
17	X	140	ASN	CA-C-N	-7.56	112.95	120.21
17	X	140	ASN	C-N-CA	-7.56	112.95	120.21
9	I	119	CYS	N-CA-C	-7.55	103.13	111.36
18	Z	73	PRO	N-CA-C	-7.54	103.05	113.53
2	B	183	ARG	N-CA-C	-7.54	104.32	113.97
8	H	223	PHE	CB-CA-C	-7.53	99.06	110.88
9	I	158	CYS	N-CA-C	-7.52	103.08	111.28
4	D	361	ALA	N-CA-C	-7.52	103.21	112.38
6	F	295	PRO	CA-N-CD	7.48	122.47	112.00
7	G	277	MET	N-CA-C	7.45	120.54	109.59
6	F	125	CYS	N-CA-C	-7.44	103.77	112.92
6	F	430	GLY	N-CA-C	7.42	121.63	112.73
4	D	350	LYS	CB-CA-C	-7.39	100.98	111.85
15	V	57	ASP	N-CA-CB	7.39	120.72	110.01
7	G	510	TRP	N-CA-CB	7.38	120.84	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	R	39	ASP	N-CA-C	7.35	121.25	110.59
21	q	24	LEU	N-CA-C	-7.35	103.27	111.28
7	G	303	THR	N-CA-C	7.35	122.95	113.18
14	T	105	MET	N-CA-C	7.33	119.34	111.36
13	S	94	VAL	N-CA-C	7.32	117.44	110.42
3	C	195	HIS	CB-CA-C	7.29	117.38	110.17
7	G	661	GLU	N-CA-C	7.25	118.88	110.97
15	V	68	LEU	N-CA-C	-7.25	103.37	111.28
7	G	374	THR	CB-CA-C	-7.25	99.82	111.28
7	G	384	ASN	N-CA-C	-7.22	103.44	111.82
6	F	295	PRO	N-CA-CB	-7.14	96.77	103.19
8	H	50	ALA	N-CA-C	7.13	118.70	111.07
7	G	497	VAL	N-CA-C	-7.13	103.35	110.62
8	H	176	LEU	CA-C-N	-7.12	113.47	120.52
8	H	176	LEU	C-N-CA	-7.12	113.47	120.52
4	D	99	LEU	N-CA-C	7.11	121.11	109.24
6	F	269	ARG	N-CA-C	7.09	118.66	111.07
15	V	95	LEU	N-CA-C	-7.08	103.56	111.28
11	Q	162	ALA	N-CA-C	7.08	119.00	111.28
23	s	56	ARG	N-CA-C	7.03	120.65	108.76
21	q	77	VAL	N-CA-C	-7.01	99.67	109.21
7	G	217	GLU	N-CA-C	-7.01	101.79	110.41
2	B	166	ASN	N-CA-C	-7.01	103.33	110.97
6	F	246	GLU	N-CA-C	-7.01	103.64	111.28
7	G	150	ARG	N-CA-C	7.00	119.57	109.14
6	F	455	GLN	N-CA-C	6.98	118.54	111.07
6	F	418	GLN	N-CA-CB	6.95	120.14	110.07
6	F	428	GLY	N-CA-C	-6.94	103.88	112.77
7	G	582	VAL	N-CA-C	6.94	118.47	108.48
18	Z	34	SER	N-CA-C	-6.94	103.65	111.07
6	F	103	ASN	N-CA-CB	6.94	121.08	110.61
14	T	145	VAL	N-CA-C	-6.93	103.72	110.72
7	G	294	TYR	N-CA-C	-6.91	104.66	113.23
12	R	45	ARG	N-CA-C	-6.90	104.73	113.01
7	G	300	GLN	N-CA-CB	6.86	122.44	112.08
6	F	329	LYS	N-CA-C	6.84	119.60	111.33
18	Z	28	ARG	N-CA-C	6.83	119.65	108.52
12	R	56	ASN	N-CA-C	6.81	120.00	108.90
7	G	133	GLN	N-CA-C	-6.79	101.24	110.68
7	G	268	GLY	N-CA-C	6.78	124.73	115.30
7	G	434	SER	N-CA-C	-6.75	100.97	110.29
8	H	8	THR	N-CA-C	-6.75	101.18	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	244	ASN	N-CA-C	-6.74	101.00	110.50
15	V	114	TRP	N-CA-CB	6.74	120.34	110.30
5	E	140	MET	N-CA-C	-6.73	103.87	111.07
9	I	208	ASP	N-CA-C	6.70	121.61	113.17
15	V	8	THR	N-CA-C	6.70	119.03	108.79
22	r	11	LEU	N-CA-C	-6.69	104.07	111.36
10	P	371	PRO	CA-N-CD	-6.69	102.64	112.00
6	F	344	GLN	N-CA-C	-6.66	103.95	111.07
17	X	129	THR	N-CA-C	6.66	120.89	110.17
6	F	196	PHE	N-CA-C	6.63	119.95	109.81
7	G	640	ASP	N-CA-CB	6.63	119.97	110.16
3	C	69	PRO	N-CA-C	-6.63	104.32	113.53
7	G	287	SER	N-CA-C	6.62	119.27	110.53
4	D	184	ILE	N-CA-C	-6.62	103.87	110.62
15	V	86	LYS	N-CA-CB	6.62	119.67	110.07
7	G	601	GLY	N-CA-C	6.62	124.83	115.30
10	P	116	ILE	N-CA-C	-6.61	104.05	110.72
6	F	228	PRO	N-CA-C	-6.60	98.87	112.47
8	H	208	VAL	N-CA-CB	-6.60	104.14	111.66
3	C	125	PHE	N-CA-CB	-6.59	100.68	110.17
5	E	44	PRO	CA-N-CD	6.58	121.21	112.00
7	G	435	PRO	N-CA-C	-6.58	100.18	110.50
11	Q	141	ASN	N-CA-CB	6.57	120.77	110.46
6	F	336	LEU	N-CA-CB	-6.56	101.00	111.43
8	H	182	ALA	N-CA-C	-6.55	104.06	111.07
14	T	141	PRO	N-CA-CB	6.55	110.53	103.33
8	H	267	SER	N-CA-C	-6.54	104.23	111.36
4	D	388	GLY	N-CA-C	6.53	119.65	110.38
8	H	223	PHE	N-CA-C	-6.53	104.09	111.07
13	S	16	LEU	N-CA-C	-6.51	98.28	108.90
22	r	24	LEU	N-CA-C	6.51	119.68	110.50
17	X	98	ARG	N-CA-C	6.50	120.47	112.54
18	Z	65	LEU	N-CA-C	-6.49	104.29	111.36
21	q	75	TRP	N-CA-C	6.48	121.45	112.45
7	G	361	VAL	N-CA-C	-6.47	105.02	111.88
7	G	605	GLN	N-CA-C	6.47	119.06	108.52
14	T	141	PRO	CA-N-CD	-6.45	102.97	112.00
7	G	250	SER	N-CA-C	6.44	116.78	108.34
7	G	275	PRO	CB-CA-C	-6.44	102.54	110.98
3	C	125	PHE	N-CA-C	6.44	119.58	110.50
12	R	81	GLY	N-CA-C	-6.44	106.84	115.21
15	V	49	GLU	N-CA-C	-6.44	104.26	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	78	GLY	N-CA-C	-6.43	104.54	112.77
4	D	140	ASP	N-CA-C	-6.43	96.50	107.23
8	H	177	PRO	N-CA-C	-6.41	101.58	111.13
7	G	275	PRO	CA-N-CD	6.40	120.97	112.00
6	F	370	LEU	N-CA-C	-6.39	104.39	111.36
21	q	28	PHE	N-CA-C	6.39	117.91	111.07
7	G	273	ILE	N-CA-C	-6.36	98.36	107.77
9	I	205	ILE	N-CA-C	-6.35	104.31	110.72
7	G	95	PRO	N-CA-C	-6.35	101.21	110.80
11	Q	59	LEU	N-CA-C	-6.34	100.79	110.30
5	E	141	LEU	N-CA-C	-6.33	101.74	110.35
22	r	8	ILE	N-CA-C	-6.33	104.33	110.72
8	H	271	LEU	N-CA-CB	6.33	119.24	110.07
6	F	416	SER	N-CA-C	6.32	117.84	111.07
15	V	71	LEU	N-CA-C	6.31	118.16	111.28
15	V	91	ALA	N-CA-C	-6.29	104.42	111.28
10	P	315	THR	N-CA-C	6.29	118.98	109.23
6	F	415	ILE	N-CA-C	-6.29	104.37	110.72
17	X	99	HIS	N-CA-CB	6.28	119.46	110.16
19	a	26	ILE	N-CA-C	-6.27	104.54	113.07
7	G	176	CYS	N-CA-C	6.27	119.57	110.42
7	G	383	SER	N-CA-C	-6.26	106.86	114.75
6	F	409	ILE	N-CA-C	6.26	116.43	110.42
5	E	64	ALA	N-CA-CB	6.25	119.26	109.94
4	D	141	TYR	N-CA-C	6.25	120.91	113.16
8	H	101	GLY	N-CA-C	6.24	120.19	112.64
4	D	233	HIS	N-CA-C	6.23	119.00	111.40
22	r	26	LEU	N-CA-CB	-6.22	101.08	110.35
2	B	113	ASP	N-CA-CB	6.21	119.47	109.28
8	H	52	ALA	N-CA-CB	6.21	119.01	110.01
11	Q	141	ASN	N-CA-C	-6.20	105.72	113.28
21	q	69	ASN	N-CA-CB	6.19	121.32	111.66
8	H	269	THR	N-CA-C	6.18	118.02	111.28
18	Z	69	ILE	N-CA-CB	6.17	117.36	110.51
4	D	291	VAL	N-CA-C	-6.17	103.38	111.09
6	F	212	LEU	N-CA-C	-6.16	104.56	111.28
8	H	276	SER	N-CA-C	6.16	118.97	111.82
10	P	368	GLU	N-CA-CB	6.16	119.79	110.30
10	P	118	LYS	N-CA-C	6.14	118.95	111.82
7	G	418	ILE	N-CA-C	-6.14	103.45	112.04
7	G	420	LYS	N-CA-C	6.13	118.75	111.33
6	F	272	GLY	N-CA-C	6.12	122.39	111.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	325	ARG	N-CA-CB	6.11	118.83	109.91
13	S	87	VAL	N-CA-C	-6.08	104.42	110.62
13	S	61	VAL	N-CA-C	-6.08	99.73	108.42
18	Z	65	LEU	N-CA-CB	6.08	119.15	110.16
8	H	185	TRP	N-CA-C	-6.05	104.04	112.45
8	H	24	GLU	N-CA-C	-6.04	104.05	112.45
7	G	638	THR	N-CA-C	-6.04	100.12	109.24
10	P	370	LYS	N-CA-C	6.04	119.29	108.47
7	G	508	ALA	N-CA-C	6.04	117.86	111.28
9	I	66	LEU	N-CA-C	-6.02	104.29	111.69
7	G	353	ALA	N-CA-C	-6.01	104.65	112.23
7	G	532	PRO	N-CA-CB	-6.01	97.06	103.38
22	r	108	LYS	N-CA-C	5.98	117.88	111.36
2	B	196	PRO	N-CA-C	-5.98	101.82	111.03
8	H	7	LEU	N-CA-C	-5.97	104.40	111.03
5	E	66	VAL	N-CA-C	5.95	116.61	110.36
7	G	480	ALA	N-CA-C	-5.92	104.91	111.36
4	D	352	PRO	N-CA-CB	-5.91	97.35	103.08
12	R	34	THR	N-CA-C	-5.90	106.72	112.97
22	r	92	LYS	N-CA-CB	-5.89	101.69	110.17
9	I	116	CYS	N-CA-C	-5.86	105.62	112.89
21	q	5	GLU	N-CA-C	-5.86	104.98	111.36
3	C	209	LEU	N-CA-CB	-5.85	100.64	110.83
7	G	639	LEU	N-CA-C	5.85	118.61	111.82
10	P	122	HIS	N-CA-C	5.85	120.12	112.92
8	H	208	VAL	N-CA-C	5.85	116.10	107.15
14	T	94	ASP	N-CA-CB	-5.85	105.17	111.66
21	q	65	THR	N-CA-C	5.85	119.21	110.14
7	G	672	ALA	N-CA-C	-5.84	104.91	111.28
13	S	86	GLU	N-CA-CB	5.84	118.81	110.16
10	P	330	THR	CB-CA-C	-5.84	109.83	116.54
5	E	223	CYS	CB-CA-C	-5.83	109.31	117.23
10	P	367	GLU	CB-CA-C	-5.82	99.50	110.67
15	V	19	THR	N-CA-CB	5.81	120.72	110.37
11	Q	164	PHE	N-CA-CB	5.81	119.83	110.42
17	X	36	CYS	CB-CA-C	-5.80	102.53	111.74
4	D	414	ASP	N-CA-C	-5.79	101.39	110.36
18	Z	44	ILE	N-CA-C	-5.78	104.87	110.42
19	a	3	PHE	N-CA-CB	5.78	118.73	110.06
7	G	275	PRO	N-CA-CB	-5.77	97.96	103.33
6	F	393	ASN	N-CA-C	-5.76	104.90	111.07
17	X	97	PHE	N-CA-C	5.73	118.47	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	289	LYS	N-CA-C	5.71	117.51	111.28
10	P	272	LEU	N-CA-C	-5.71	101.83	110.28
12	R	35	GLY	N-CA-C	5.70	121.81	113.48
13	S	73	GLN	N-CA-C	-5.70	100.42	109.59
5	E	137	THR	CA-C-N	-5.68	113.06	118.97
5	E	137	THR	C-N-CA	-5.68	113.06	118.97
21	q	140	PRO	N-CA-C	-5.67	102.23	110.80
6	F	457	HIS	N-CA-CB	-5.67	100.86	110.50
12	R	52	GLN	N-CA-C	5.67	118.01	110.53
4	D	352	PRO	N-CA-C	5.65	117.59	110.70
13	S	63	PRO	CA-N-CD	5.64	119.90	112.00
2	B	135	GLY	N-CA-C	5.63	118.61	111.85
2	B	112	TYR	N-CA-C	5.63	122.80	110.80
2	B	201	LEU	N-CA-C	-5.63	105.14	111.28
10	P	119	ALA	N-CA-C	-5.62	105.07	111.14
7	G	599	THR	CA-C-N	-5.61	114.19	122.83
7	G	599	THR	C-N-CA	-5.61	114.19	122.83
5	E	183	PRO	N-CA-C	-5.61	102.12	111.26
11	Q	124	MET	CA-C-N	-5.61	115.02	122.98
11	Q	124	MET	C-N-CA	-5.61	115.02	122.98
9	I	191	LEU	N-CA-C	-5.60	105.25	111.36
6	F	268	GLU	CB-CA-C	-5.59	110.11	116.54
18	Z	64	ASP	N-CA-C	5.59	119.82	112.89
21	q	68	MET	N-CA-C	5.58	119.35	112.54
5	E	119	THR	N-CA-C	-5.58	105.97	112.89
7	G	530	TYR	N-CA-C	-5.58	102.02	110.28
7	G	615	LEU	N-CA-C	-5.58	106.24	113.16
19	a	25	TYR	N-CA-C	-5.54	107.77	114.75
22	r	94	ALA	N-CA-C	-5.52	101.68	109.96
7	G	127	ASP	CA-C-O	5.52	129.01	121.89
21	q	142	THR	N-CA-CB	5.51	119.77	109.68
12	R	89	PRO	N-CA-CB	-5.51	98.31	103.27
10	P	86	CYS	N-CA-C	-5.50	103.12	110.55
21	q	71	LYS	N-CA-C	5.49	119.97	113.16
4	D	132	ALA	N-CA-C	-5.48	106.59	113.72
4	D	163	PRO	N-CA-CB	-5.48	97.76	103.08
14	T	135	ALA	N-CA-CB	5.47	118.16	110.12
4	D	231	GLY	N-CA-C	-5.46	103.05	110.43
7	G	682	ASP	CA-C-N	-5.45	114.15	119.76
7	G	682	ASP	C-N-CA	-5.45	114.15	119.76
7	G	404	GLY	N-CA-C	5.44	121.42	113.48
4	D	200	PHE	CA-CB-CG	5.43	119.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r	111	PRO	N-CA-C	-5.42	106.46	113.57
7	G	420	LYS	N-CA-CB	-5.41	101.94	110.06
7	G	150	ARG	N-CA-CB	-5.41	102.86	111.62
18	Z	55	GLN	N-CA-C	-5.41	105.39	111.28
6	F	180	GLY	N-CA-C	-5.40	108.19	115.21
17	X	27	ALA	N-CA-C	-5.40	105.05	111.69
10	P	374	THR	N-CA-C	5.39	117.52	108.73
7	G	556	THR	N-CA-C	-5.39	101.57	109.81
4	D	201	PHE	N-CA-C	-5.37	105.50	111.36
6	F	199	ARG	N-CA-C	5.37	117.49	109.59
2	B	101	ALA	N-CA-C	-5.37	105.43	111.28
12	R	88	HIS	CB-CA-C	5.37	117.29	109.08
18	Z	50	MET	N-CA-C	-5.37	105.43	111.28
4	D	141	TYR	N-CA-CB	-5.36	102.24	110.44
5	E	74	GLN	N-CA-C	-5.35	107.40	114.04
11	Q	163	ASN	CB-CA-C	-5.34	99.32	109.95
7	G	510	TRP	N-CA-C	-5.34	101.95	109.96
4	D	109	CYS	N-CA-C	5.34	118.42	107.69
14	T	92	LYS	N-CA-C	-5.33	106.37	112.92
11	Q	164	PHE	N-CA-C	-5.32	106.77	113.20
15	V	84	ALA	N-CA-C	5.31	116.75	111.07
5	E	44	PRO	N-CA-CB	-5.30	97.66	103.39
5	E	143	ASP	N-CA-C	5.29	118.93	111.52
9	I	160	GLU	N-CA-CB	-5.29	100.73	109.72
8	H	305	ILE	N-CA-C	-5.28	105.98	111.58
8	H	46	LEU	N-CA-C	-5.27	106.62	113.16
4	D	363	VAL	N-CA-C	5.27	116.34	111.81
4	D	391	VAL	CA-C-N	-5.26	115.87	119.66
4	D	391	VAL	C-N-CA	-5.26	115.87	119.66
17	X	33	GLY	N-CA-C	-5.26	107.79	114.16
11	Q	72	ILE	N-CA-C	-5.25	108.38	113.53
8	H	146	MET	N-CA-C	-5.25	105.45	111.07
8	H	103	LEU	N-CA-C	-5.25	105.45	111.07
6	F	412	LEU	N-CA-C	-5.25	105.73	111.82
7	G	277	MET	N-CA-CB	-5.24	101.64	109.71
10	P	68	TYR	N-CA-C	5.24	117.07	111.36
7	G	435	PRO	CB-CA-C	-5.23	105.86	111.56
22	r	25	GLN	N-CA-C	5.22	118.91	112.54
3	C	164	TRP	N-CA-C	5.20	117.03	111.36
7	G	600	GLU	CB-CA-C	-5.20	103.00	111.06
13	S	85	ASP	N-CA-C	5.19	117.84	111.82
22	r	111	PRO	CA-N-CD	5.19	119.26	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r	107	SER	N-CA-C	-5.17	102.20	109.96
4	D	391	VAL	N-CA-C	5.17	113.83	109.02
10	P	204	SER	CA-C-O	-5.16	115.05	121.50
7	G	172	ILE	N-CA-C	-5.15	98.62	109.34
3	C	156	VAL	N-CA-C	-5.14	104.08	111.17
6	F	271	SER	N-CA-C	-5.13	99.92	108.34
7	G	569	GLN	CB-CA-C	-5.13	104.26	112.05
9	I	95	PRO	N-CA-C	5.13	121.24	113.81
7	G	713	ALA	N-CA-C	-5.12	105.59	111.07
20	b	82	LYS	N-CA-C	-5.12	103.77	110.53
8	H	196	ALA	CA-C-N	-5.12	113.48	119.32
8	H	196	ALA	C-N-CA	-5.12	113.48	119.32
6	F	337	MET	CB-CA-C	-5.11	103.10	111.68
1	A	2	ASN	CA-C-N	-5.10	113.05	120.29
1	A	2	ASN	C-N-CA	-5.10	113.05	120.29
8	H	277	TYR	N-CA-C	5.10	117.91	110.10
6	F	293	SER	CB-CA-C	-5.09	104.37	111.80
3	C	109	SER	N-CA-C	5.08	118.10	109.76
10	P	376	ASN	CB-CA-C	-5.07	102.23	110.85
17	X	112	LEU	N-CA-CB	5.07	117.42	110.07
5	E	181	ASN	N-CA-C	-5.06	99.54	108.20
21	q	13	GLN	N-CA-C	-5.06	105.65	111.07
7	G	203	ASP	CA-C-O	5.05	127.18	121.32
7	G	280	ASP	N-CA-CB	-5.05	102.70	110.12
7	G	393	GLY	N-CA-C	-5.05	107.79	115.66
9	I	160	GLU	CB-CA-C	5.04	119.20	110.84
10	P	136	THR	N-CA-CB	-5.04	102.77	110.42
12	R	43	TYR	N-CA-CB	-5.04	103.20	110.70
3	C	208	GLU	CA-C-O	-5.03	115.71	121.40
14	T	140	CYS	CB-CA-C	-5.03	104.12	109.85
16	W	112	GLU	N-CA-C	5.02	116.83	111.36
3	C	221	GLU	N-CA-C	-5.00	102.45	108.25

There are no chirality outliers.

There are no planarity outliers.

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	737	0	800	73	0
2	B	1247	0	1256	144	0
3	C	1641	0	1596	118	0
4	D	3088	0	3059	294	0
5	E	1635	0	1626	171	0
6	F	3273	0	3231	310	0
7	G	5287	0	5323	528	0
8	H	2531	0	2619	343	0
9	I	1389	0	1352	137	0
10	P	2720	0	2740	227	0
11	Q	957	0	949	84	0
12	R	660	0	639	77	0
13	S	667	0	683	91	0
14	T	604	0	596	87	0
15	V	915	0	954	78	0
16	W	970	0	991	67	0
17	X	1164	0	1154	124	0
18	Z	1152	0	1148	84	0
19	a	548	0	562	63	0
20	b	620	0	617	76	0
21	q	1020	0	976	91	0
22	r	418	0	434	50	0
23	s	238	0	225	24	0
24	B	8	0	0	3	0
24	F	8	0	0	5	0
24	G	16	0	0	2	0
24	I	16	0	0	5	0
25	B	18	0	18	3	0
26	B	35	0	44	6	0
26	I	43	0	60	8	0
27	E	4	0	0	4	0
27	G	4	0	0	5	0
28	F	31	0	19	0	0
29	H	35	0	43	28	0
30	H	97	0	151	18	0
31	P	48	0	26	5	0
32	R	1	0	0	0	0
33	W	32	0	0	4	0
34	q	57	0	58	22	0
All	All	33934	0	33949	2840	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (2840) 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)
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.27
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.20
15:V:44:TYR:CE1	15:V:48:THR:HG21	1.77	1.18
8:H:52:ALA:HB2	29:H:401:UQ9:H23	1.26	1.13
8:H:224:PHE:CE2	29:H:401:UQ9:H17A	1.84	1.12
12:R:38:TYR:HE2	21:q:127:TYR:HB2	1.04	1.12
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.22	1.12
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.47	1.12
12:R:38:TYR:CE2	21:q:127:TYR:HB2	1.85	1.11
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.09
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.09
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.88	1.09
9:I:53:ALA:HB1	20:b:14:ALA:HB2	1.27	1.09
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.08
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.11	1.07
9:I:54:THR:HG22	20:b:13:TRP:HE1	1.02	1.07
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
17:X:4:ILE:HG22	17:X:5:VAL:H	0.96	1.06
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.70	1.06
13:S:23:LEU:HD12	13:S:23:LEU:O	1.54	1.06
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.34	1.06
6:F:270:ASN:OD1	6:F:270:ASN:O	1.70	1.06
14:T:138:LEU:HD12	14:T:138:LEU:O	1.55	1.06
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.38	1.05
15:V:44:TYR:CE1	15:V:48:THR:CG2	2.39	1.05
22:r:2:ALA:N	22:r:26:LEU:HD12	1.70	1.04
2:B:149:TYR:HA	2:B:152:MET:HE2	1.35	1.04
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.04
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.57	1.03
9:I:53:ALA:CB	20:b:14:ALA:HB2	1.88	1.03
9:I:208:ASP:O	9:I:208:ASP:OD1	1.76	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.95	1.01
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.41	1.01
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.01
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.42	1.01
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.01
21:q:66:THR:HG22	21:q:74:PHE:HB2	1.39	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
5:E:203:ILE:HG23	5:E:213:PRO:HG2	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:44:TYR:CZ	15:V:48:THR:HG21	1.97	0.99
17:X:53:PRO:HD3	18:Z:116:TRP:CD1	1.96	0.99
17:X:90:ASP:OD2	19:a:62:VAL:HG11	1.59	0.99
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.99
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.99
8:H:52:ALA:CB	29:H:401:UQ9:H23	1.93	0.98
5:E:134:CYS:HG	27:E:301:FES:FE1	0.78	0.98
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.98
8:H:30:TYR:CE1	19:a:1:MET:O	2.16	0.98
16:W:55:LEU:HB3	16:W:107:MET:CE	1.94	0.98
2:B:82:ILE:HG23	8:H:57:MET:SD	2.03	0.97
17:X:135:ARG:HH12	17:X:138:PRO:HD3	1.23	0.97
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.47	0.97
17:X:4:ILE:HG22	17:X:5:VAL:N	1.77	0.97
6:F:379:CYS:SG	24:F:502:SF4:FE1	1.56	0.97
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.97
9:I:54:THR:CG2	20:b:13:TRP:HE1	1.77	0.96
6:F:382:CYS:HG	24:F:502:SF4:FE2	0.79	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.47	0.96
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.96
10:P:376:ASN:OD1	10:P:377:TYR:N	1.98	0.96
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.96
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.95
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.95
9:I:54:THR:HG22	20:b:13:TRP:NE1	1.80	0.95
6:F:63:TYR:HB3	6:F:256:ARG:HE	1.29	0.95
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.95
5:E:189:ASP:CG	6:F:163:TYR:HB3	1.92	0.94
3:C:85:ILE:CD1	3:C:140:ILE:HD11	1.98	0.94
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.94
7:G:78:CYS:SG	27:G:803:FES:FE2	1.59	0.94
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
13:S:16:LEU:HD11	13:S:51:LEU:HD11	1.46	0.94
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.48	0.94
9:I:162:CYS:SG	24:I:303:SF4:FE4	1.60	0.93
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.47	0.93
9:I:113:CYS:SG	24:I:303:SF4:FE3	1.60	0.93
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.34	0.92
7:G:176:CYS:SG	24:G:802:SF4:FE4	1.59	0.92
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:55:LEU:HB3	16:W:107:MET:HE1	1.52	0.91
17:X:4:ILE:CG2	17:X:5:VAL:H	1.82	0.91
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.91
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.91
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.06	0.91
5:E:179:CYS:SG	27:E:301:FES:FE2	1.63	0.90
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.51	0.90
9:I:80:GLU:HG3	19:a:1:MET:SD	2.11	0.90
7:G:362:ASP:HB2	13:S:71:PHE:CE1	2.06	0.90
5:E:39:VAL:HG22	7:G:205:GLN:HE22	1.34	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
4:D:280:ALA:CB	15:V:11:LEU:HG	2.00	0.90
7:G:36:VAL:HG11	7:G:56:VAL:HG11	1.52	0.90
21:q:76:ASP:OD1	21:q:76:ASP:O	1.90	0.89
9:I:67:ILE:HG23	26:I:301:PC1:H381	1.53	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
18:Z:86:ILE:HG23	18:Z:128:ARG:HE	1.38	0.89
13:S:16:LEU:HD22	13:S:19:ILE:HD11	1.53	0.89
4:D:270:ASN:HB3	8:H:284:GLN:NE2	1.87	0.89
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.89
14:T:79:ILE:HB	14:T:145:VAL:HG13	1.55	0.88
6:F:379:CYS:HG	24:F:502:SF4:FE1	0.88	0.88
1:A:55:PHE:CZ	8:H:282:TYR:HE2	1.92	0.88
6:F:41:ILE:HG21	6:F:250:VAL:HG12	1.54	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
7:G:64:CYS:HG	27:G:803:FES:FE1	0.71	0.88
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.88
16:W:32:LYS:NZ	33:W:201:EHZ:C19	2.37	0.88
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.56	0.88
3:C:102:HIS:HE1	15:V:48:THR:HG22	1.35	0.88
6:F:55:GLY:HA2	6:F:58:ARG:HD2	1.54	0.87
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.87
8:H:52:ALA:HB2	29:H:401:UQ9:C23	2.04	0.87
7:G:78:CYS:HG	27:G:803:FES:FE2	0.57	0.87
10:P:221:ARG:HD3	10:P:286:ARG:CD	2.05	0.87
12:R:51:ARG:HH21	21:q:125:VAL:HG12	1.38	0.87
2:B:121:PHE:HB2	25:B:302:UQ1:H8	1.54	0.87
22:r:2:ALA:N	22:r:26:LEU:CD1	2.37	0.87
2:B:99:CYS:HB3	4:D:141:TYR:CD2	2.10	0.87
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.87
3:C:217:ARG:HH12	16:W:112:GLU:HB2	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:122:HIS:HB2	12:R:46:VAL:HG12	1.55	0.86
12:R:32:THR:HG22	12:R:36:GLN:H	1.40	0.86
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.56	0.86
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.54	0.86
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.03	0.86
6:F:327:ILE:HD11	6:F:331:VAL:HG11	1.56	0.86
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.86
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.56	0.86
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.55	0.86
7:G:617:ARG:NH1	16:W:129:HIS:HA	1.90	0.86
3:C:217:ARG:NH1	16:W:112:GLU:HB2	1.91	0.86
6:F:425:CYS:HG	24:F:502:SF4:FE4	0.58	0.86
13:S:16:LEU:HD12	13:S:16:LEU:O	1.76	0.86
5:E:147:ILE:HG23	5:E:200:ILE:HG12	1.57	0.85
26:B:303:PC1:H322	26:B:303:PC1:H232	1.55	0.85
2:B:116:ARG:HA	8:H:37:PRO:HA	1.56	0.85
26:B:303:PC1:H142	8:H:39:ILE:HD11	1.55	0.85
15:V:56:LEU:HD12	15:V:57:ASP:N	1.92	0.85
2:B:82:ILE:HG12	8:H:57:MET:CE	2.06	0.85
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.06	0.85
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.07	0.85
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.77	0.85
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.42	0.84
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.95	0.84
17:X:49:GLU:HG3	17:X:138:PRO:HG2	1.58	0.84
4:D:137:ASP:OD1	4:D:148:GLU:CD	2.20	0.84
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.84
3:C:114:THR:HG22	4:D:421:ARG:NH1	1.93	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.59	0.84
16:W:55:LEU:HD22	16:W:107:MET:HE2	1.58	0.84
15:V:75:GLY:HA2	22:r:103:ARG:HD2	1.59	0.84
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.84
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.83
2:B:152:MET:HB3	2:B:153:PRO:HD2	1.57	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
2:B:92:PRO:HD2	2:B:121:PHE:H	1.44	0.83
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.61	0.83
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.83
20:b:67:PRO:HD3	20:b:74:LEU:HB2	1.60	0.83
7:G:176:CYS:HG	24:G:802:SF4:FE4	0.55	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:674:LEU:HD11	13:S:46:LYS:HE2	1.60	0.83
10:P:94:LEU:HA	10:P:97:MET:HE2	1.59	0.83
4:D:254:ARG:HH11	22:r:25:GLN:HB2	1.44	0.83
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.83
13:S:48:HIS:CE1	13:S:95:LEU:HD22	2.13	0.83
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.82
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
10:P:122:HIS:CB	12:R:46:VAL:HG12	2.08	0.82
21:q:85:GLU:HG2	21:q:98:PRO:HB3	1.59	0.82
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.82
22:r:4:ALA:HB1	22:r:9:GLN:HB2	1.60	0.82
6:F:278:ILE:HD11	6:F:299:LEU:HD21	1.61	0.82
5:E:174:GLU:OE2	6:F:373:PHE:CD1	2.33	0.82
7:G:64:CYS:SG	27:G:803:FES:FE1	1.72	0.82
3:C:85:ILE:HG13	3:C:140:ILE:HD11	1.60	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.62	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.42	0.82
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.10	0.81
17:X:142:TYR:HB2	18:Z:115:ARG:HH11	1.45	0.81
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.81
13:S:36:PHE:HZ	13:S:44:LEU:HD11	1.45	0.81
16:W:55:LEU:CD2	16:W:107:MET:HE2	2.09	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.60	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
10:P:141:PHE:HD2	10:P:179:LYS:HD2	1.43	0.81
21:q:71:LYS:O	21:q:72:ASN:OD1	1.99	0.81
14:T:93:ILE:HG21	14:T:110:LEU:HD22	1.63	0.81
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
7:G:432:ILE:HG23	7:G:451:ILE:HD11	1.63	0.80
8:H:97:ASN:HD22	19:a:38:VAL:HG13	1.46	0.80
9:I:162:CYS:HG	24:I:303:SF4:FE4	0.50	0.80
8:H:187:ILE:HD12	30:H:403:3PE:H242	1.62	0.80
3:C:85:ILE:CG1	3:C:140:ILE:HD11	2.12	0.80
10:P:163:ARG:HD2	10:P:253:THR:HA	1.62	0.80
2:B:99:CYS:HB3	4:D:141:TYR:CE2	2.16	0.80
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.80
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.46	0.80
9:I:113:CYS:HG	24:I:303:SF4:FE3	0.49	0.80
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:334:GLU:OE1	13:S:71:PHE:HE1	1.64	0.80
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.79
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.63	0.79
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.79
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.79
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.96	0.79
6:F:425:CYS:SG	24:F:502:SF4:FE4	1.74	0.79
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.79
17:X:132:LYS:HB2	20:b:59:ASP:HB3	1.64	0.79
8:H:17:MET:SD	8:H:229:THR:OG1	2.41	0.79
8:H:51:ASP:OD2	29:H:401:UQ9:H15B	1.80	0.78
10:P:208:GLY:H	10:P:211:ASP:HB3	1.48	0.78
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.78
17:X:50:GLU:HG2	17:X:138:PRO:HG3	1.66	0.78
2:B:82:ILE:HA	8:H:57:MET:HE1	1.64	0.78
14:T:87:LEU:HD21	14:T:104:PHE:HZ	1.47	0.78
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.64	0.78
13:S:20:ARG:HG3	13:S:54:LEU:HB2	1.64	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.61	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.65	0.78
14:T:87:LEU:HD22	14:T:104:PHE:CE1	2.19	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.65	0.78
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	1.97	0.78
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.78
7:G:272:ARG:HD2	7:G:274:LEU:HD23	1.63	0.78
4:D:254:ARG:HE	22:r:25:GLN:NE2	1.82	0.77
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.77
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.65	0.77
17:X:20:VAL:HG22	17:X:24:VAL:HG21	1.65	0.77
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.49	0.77
17:X:135:ARG:NH1	17:X:138:PRO:HD3	1.98	0.77
19:a:3:PHE:HE2	34:q:201:CDL:HA4	1.47	0.77
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:86:TRP:CZ2	19:a:64:LYS:HB3	2.18	0.77
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.49	0.77
8:H:116:ILE:HG13	8:H:117:LEU:N	1.99	0.77
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.50	0.77
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.77
14:T:83:VAL:CG2	14:T:126:PHE:HZ	1.97	0.77
7:G:664:TYR:OH	13:S:23:LEU:HD11	1.84	0.77
18:Z:144:THR:HA	19:a:45:TRP:HZ3	1.50	0.77
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.77
7:G:454:ASP:HA	7:G:459:ARG:HH21	1.48	0.76
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.76
21:q:96:ASP:OD1	21:q:97:PRO:HD2	1.85	0.76
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.76
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.65	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
7:G:655:ARG:NH1	13:S:59:SER:HB3	2.01	0.76
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.76
4:D:271:ARG:HD2	8:H:279:ARG:O	1.85	0.76
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.67	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
7:G:355:LYS:HA	7:G:366:LEU:HD11	1.65	0.76
10:P:143:ASP:HA	10:P:147:ASN:HB2	1.67	0.76
4:D:270:ASN:HB3	8:H:284:GLN:HE22	1.51	0.76
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.76
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.75
9:I:64:THR:HG22	26:I:301:PC1:H231	1.68	0.75
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.75
14:T:93:ILE:HG23	14:T:110:LEU:HD13	1.66	0.75
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.75
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.50	0.75
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.68	0.75
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.75
16:W:55:LEU:HB3	16:W:107:MET:HE2	1.66	0.75
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.75
11:Q:167:ASN:O	11:Q:168:LYS:CD	2.35	0.75
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.75
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.00	0.75
10:P:170:LEU:HA	10:P:202:ARG:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.75
2:B:112:TYR:OH	9:I:91:GLY:CA	2.31	0.74
4:D:371:MET:SD	4:D:381:HIS:CD2	2.79	0.74
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.69	0.74
8:H:224:PHE:CD2	29:H:401:UQ9:C20	2.69	0.74
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.66	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
16:W:32:LYS:HZ3	33:W:201:EHZ:C19	1.98	0.74
20:b:35:ILE:HD12	20:b:35:ILE:O	1.88	0.74
10:P:235:THR:OG1	10:P:273:LEU:HB3	1.87	0.74
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.18	0.74
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
8:H:85:LEU:HD21	8:H:108:THR:HB	1.68	0.74
14:T:88:LYS:HG3	14:T:98:LEU:HD22	1.70	0.74
16:W:32:LYS:HZ2	33:W:201:EHZ:C19	2.01	0.74
2:B:93:MET:HE1	2:B:131:MET:HE2	1.68	0.74
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.68	0.74
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.74
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.03	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.27	0.74
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.88	0.74
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.70	0.74
14:T:117:GLU:HA	14:T:120:MET:HE3	1.67	0.74
1:A:73:LEU:O	1:A:76:PRO:HD2	1.88	0.73
14:T:94:ASP:HB3	14:T:98:LEU:HB2	1.68	0.73
14:T:103:HIS:CG	14:T:106:LYS:HD2	2.23	0.73
6:F:392:MET:CE	6:F:419:ILE:HD12	2.18	0.73
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.68	0.73
4:D:383:LYS:HD3	7:G:140:GLN:NE2	2.03	0.73
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.69	0.73
6:F:213:ILE:HG23	6:F:235:VAL:HA	1.68	0.73
8:H:64:LEU:H	8:H:64:LEU:HD23	1.52	0.73
18:Z:93:GLU:O	18:Z:97:ILE:HG13	1.88	0.73
2:B:147:LYS:HE3	2:B:151:GLN:HE21	1.51	0.73
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.73
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.73
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.69	0.73
17:X:142:TYR:HB3	18:Z:115:ARG:HD3	1.70	0.73
21:q:56:PHE:HA	21:q:59:HIS:CD2	2.24	0.73
21:q:68:MET:SD	21:q:81:MET:HB3	2.28	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:PRO:HD3	2:B:119:VAL:HG13	1.71	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
11:Q:167:ASN:O	11:Q:168:LYS:HD2	1.88	0.73
1:A:21:ALA:O	1:A:25:PRO:HD3	1.88	0.73
5:E:128:LYS:HB3	5:E:167:LEU:HA	1.71	0.73
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.73
6:F:42:PHE:HA	6:F:137:LYS:NZ	2.04	0.72
6:F:127:ASP:HB3	6:F:245:VAL:HG21	1.70	0.72
17:X:29:ALA:HB2	18:Z:71:LEU:HD11	1.70	0.72
18:Z:65:LEU:O	18:Z:69:ILE:HG12	1.89	0.72
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.72
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.89	0.72
7:G:33:GLU:HB3	7:G:98:LYS:HE2	1.70	0.72
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.72
10:P:317:ASP:HB3	10:P:321:ARG:NH2	2.04	0.72
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.72
9:I:93:LEU:O	21:q:93:MET:HG2	1.89	0.72
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.72
21:q:56:PHE:HD1	21:q:59:HIS:HE2	1.35	0.72
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.72	0.72
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.72
4:D:206:GLU:OE1	22:r:25:GLN:NE2	2.21	0.72
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.72
8:H:175:LEU:HD21	26:I:301:PC1:H2C2	1.71	0.72
10:P:166:HIS:HB3	10:P:200:ILE:HD13	1.71	0.72
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.72
8:H:307:LEU:HA	8:H:310:PHE:CE2	2.25	0.72
6:F:278:ILE:HD11	6:F:299:LEU:CD2	2.19	0.71
16:W:42:TRP:CH2	16:W:93:LEU:HA	2.25	0.71
5:E:151:LEU:HD12	5:E:204:ILE:HD11	1.72	0.71
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.71
8:H:224:PHE:CD2	29:H:401:UQ9:H20	2.25	0.71
20:b:31:ILE:HA	20:b:34:MET:HE2	1.71	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	0.71
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.71	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
5:E:174:GLU:HG2	6:F:369:ARG:NH1	1.96	0.71
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.72	0.71
7:G:126:LEU:HD11	12:R:89:PRO:CB	2.20	0.71
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.71
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.71
3:C:70:LYS:O	15:V:103:LEU:HD12	1.90	0.71
5:E:179:CYS:HG	27:E:301:FES:FE2	0.48	0.71
6:F:37:ASP:HA	6:F:40:ARG:HD2	1.72	0.71
6:F:327:ILE:HG23	6:F:332:CYS:SG	2.29	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
8:H:61:MET:HE3	8:H:63:PRO:HA	1.72	0.71
17:X:8:PRO:HD3	17:X:54:ARG:HD3	1.71	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.71
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.56	0.71
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	1.88	0.71
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.56	0.70
4:D:137:ASP:OD1	4:D:148:GLU:CG	2.39	0.70
4:D:261:MET:O	4:D:265:ASN:HB2	1.91	0.70
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.26	0.70
8:H:33:LEU:CD2	22:r:25:GLN:HG2	2.21	0.70
2:B:123:ALA:HB1	4:D:89:PRO:HG3	1.73	0.70
7:G:117:MET:HE3	7:G:143:SER:HA	1.73	0.70
8:H:104:PHE:CE2	30:H:402:3PE:H362	2.26	0.70
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.70
4:D:254:ARG:NH1	22:r:25:GLN:HB2	2.06	0.70
10:P:172:ALA:O	10:P:185:ALA:HB2	1.91	0.70
15:V:56:LEU:HD12	15:V:56:LEU:C	2.16	0.70
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.55	0.70
4:D:141:TYR:O	4:D:144:MET:SD	2.49	0.70
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.71	0.70
7:G:463:CYS:O	7:G:467:LYS:HG2	1.92	0.70
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.72	0.70
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.70
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.70
17:X:124:GLN:O	20:b:70:PRO:HB2	1.91	0.70
8:H:274:ARG:HH22	29:H:401:UQ9:H1MB	1.57	0.70
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.70
17:X:18:VAL:HG21	18:Z:74:LEU:HD11	1.74	0.70
7:G:362:ASP:HB2	13:S:71:PHE:CD1	2.27	0.70
9:I:62:MET:HE2	9:I:62:MET:HA	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:ILE:HD11	6:F:262:PHE:HE1	1.56	0.70
10:P:55:VAL:HG12	10:P:123:SER:HA	1.74	0.69
8:H:93:HIS:HB3	19:a:27:HIS:ND1	2.07	0.69
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.41	0.69
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.69
8:H:30:TYR:CZ	19:a:1:MET:O	2.45	0.69
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.74	0.69
17:X:50:GLU:CG	17:X:138:PRO:HG3	2.23	0.69
2:B:131:MET:HE3	2:B:152:MET:CE	2.23	0.69
6:F:63:TYR:HB3	6:F:256:ARG:NE	2.04	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.69
5:E:222:PHE:H	5:E:225:GLU:HG2	1.55	0.69
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.69
8:H:92:PRO:HD3	8:H:255:TYR:CD2	2.27	0.69
8:H:274:ARG:NH2	29:H:401:UQ9:H1MB	2.06	0.69
12:R:67:GLN:HG2	12:R:109:LEU:CD2	2.21	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.74	0.69
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.22	0.69
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.28	0.69
8:H:116:ILE:HA	8:H:211:PHE:CE1	2.27	0.69
10:P:320:GLU:O	10:P:324:ILE:HG12	1.93	0.69
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.69
14:T:138:LEU:HD13	14:T:144:ILE:CG1	2.22	0.69
2:B:92:PRO:HG3	2:B:119:VAL:HG13	1.73	0.69
2:B:99:CYS:HB2	4:D:141:TYR:CG	2.28	0.69
4:D:279:THR:HG23	15:V:13:GLY:CA	2.19	0.69
5:E:151:LEU:HD23	5:E:170:LEU:HD13	1.73	0.69
6:F:81:LYS:HE2	6:F:97:LEU:HD23	1.75	0.69
7:G:43:VAL:HG12	7:G:55:LYS:HD3	1.75	0.69
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.69
8:H:23:VAL:HG11	19:a:9:LEU:HD21	1.72	0.69
2:B:92:PRO:HG2	2:B:121:PHE:HA	1.75	0.69
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.69
4:D:254:ARG:HH11	22:r:25:GLN:CB	2.06	0.69
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.69
7:G:335:GLY:HA2	7:G:362:ASP:O	1.93	0.69
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.28	0.69
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.69
13:S:51:LEU:HD13	13:S:95:LEU:HD12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ILE:CD1	3:C:140:ILE:CD1	2.70	0.68
8:H:90:PRO:HD3	8:H:162:LEU:HD23	1.75	0.68
8:H:224:PHE:HB3	29:H:401:UQ9:C20	2.22	0.68
6:F:41:ILE:HD11	6:F:262:PHE:CE1	2.28	0.68
7:G:341:ILE:HG13	7:G:545:LEU:HD11	1.74	0.68
9:I:78:PHE:HB3	22:r:8:ILE:HG22	1.76	0.68
3:C:141:ARG:NH1	4:D:410:TYR:HE1	1.90	0.68
8:H:34:ARG:HH22	29:H:401:UQ9:H4M	1.58	0.68
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.74	0.68
14:T:87:LEU:HD22	14:T:104:PHE:HE1	1.58	0.68
14:T:100:VAL:HB	14:T:142:GLN:HB2	1.74	0.68
17:X:142:TYR:O	17:X:143:HIS:C	2.36	0.68
4:D:259:GLU:O	4:D:263:THR:HG22	1.93	0.68
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.75	0.68
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.58	0.68
5:E:39:VAL:HG22	7:G:205:GLN:NE2	2.09	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
7:G:651:PRO:HG3	13:S:57:GLU:H	1.58	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
4:D:279:THR:HA	15:V:12:VAL:CG1	2.24	0.68
4:D:279:THR:HA	15:V:12:VAL:HG13	1.75	0.68
17:X:142:TYR:CB	18:Z:115:ARG:HD3	2.23	0.68
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.08	0.68
22:r:20:LEU:C	22:r:20:LEU:HD12	2.18	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
2:B:110:PRO:HB3	8:H:33:LEU:O	1.93	0.68
6:F:39:ASP:HB3	6:F:265:PHE:CZ	2.29	0.68
8:H:224:PHE:CG	29:H:401:UQ9:H20	2.29	0.68
10:P:317:ASP:HB3	10:P:321:ARG:HH22	1.58	0.68
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
5:E:206:GLU:HB2	5:E:213:PRO:HG3	1.76	0.67
6:F:296:LEU:HD23	6:F:332:CYS:HB3	1.75	0.67
8:H:51:ASP:OD2	29:H:401:UQ9:H16A	1.94	0.67
8:H:54:LYS:HG3	8:H:55:LEU:N	2.08	0.67
10:P:185:ALA:O	10:P:188:GLU:HG2	1.94	0.67
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.76	0.67
17:X:44:MET:O	17:X:48:TRP:HE3	1.77	0.67
8:H:224:PHE:CD2	29:H:401:UQ9:H17A	2.28	0.67
13:S:16:LEU:HB3	13:S:69:TYR:HD1	1.58	0.67
16:W:121:PHE:HA	16:W:124:LYS:HE2	1.75	0.67
17:X:41:LYS:HD2	20:b:56:PRO:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ILE:HD11	3:C:140:ILE:HD11	1.76	0.67
4:D:375:MET:HE1	7:G:126:LEU:HA	1.75	0.67
6:F:225:LEU:H	11:Q:160:TYR:HE2	1.43	0.67
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.58	0.67
8:H:33:LEU:HD21	22:r:25:GLN:HG2	1.74	0.67
12:R:48:PHE:CD2	21:q:125:VAL:HG21	2.29	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.27	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
14:T:87:LEU:CD2	14:T:104:PHE:CZ	2.78	0.67
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.76	0.67
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.58	0.67
7:G:304:GLU:OE2	10:P:41:ILE:HG12	1.94	0.67
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.25	0.67
15:V:116:ILE:HG23	15:V:116:ILE:O	1.92	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.67
7:G:382:ARG:HD2	13:S:56:ARG:CD	2.25	0.67
9:I:92:PRO:HA	21:q:91:HIS:O	1.95	0.67
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.56	0.67
6:F:42:PHE:HA	6:F:137:LYS:HZ2	1.58	0.67
21:q:13:GLN:HE22	34:q:201:CDL:HA31	1.60	0.67
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.73	0.66
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.66
2:B:92:PRO:CD	2:B:119:VAL:HG13	2.26	0.66
7:G:617:ARG:HH12	16:W:129:HIS:N	1.93	0.66
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.78	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
9:I:68:ARG:HH22	18:Z:26:PRO:HD2	1.60	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
8:H:92:PRO:HD3	8:H:255:TYR:HD2	1.58	0.66
17:X:44:MET:CE	18:Z:73:PRO:HA	2.25	0.66
2:B:98:ALA:HB2	2:B:136:THR:H	1.61	0.66
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.77	0.66
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.28	0.66
7:G:655:ARG:NH1	13:S:59:SER:CB	2.58	0.66
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.66
14:T:83:VAL:HG22	14:T:126:PHE:CZ	2.31	0.66
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.66
1:A:3:LEU:HD23	30:H:402:3PE:H251	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.66
13:S:24:CYS:SG	13:S:61:VAL:O	2.53	0.66
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.66
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.31	0.66
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.66
5:E:43:THR:OG1	5:E:44:PRO:HD2	1.96	0.66
7:G:388:ASN:H	7:G:514:ASN:HB3	1.61	0.66
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.66
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.78	0.66
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.31	0.66
5:E:138:PRO:HD2	27:E:301:FES:S2	2.36	0.66
10:P:288:PHE:CZ	10:P:290:PRO:HB3	2.30	0.66
9:I:200:GLU:OE2	21:q:93:MET:SD	2.53	0.65
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.65
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.65
8:H:90:PRO:HG2	8:H:240:ILE:HG21	1.77	0.65
14:T:118:ILE:HG23	14:T:122:MET:HE3	1.78	0.65
16:W:65:LYS:HE2	16:W:110:PHE:HA	1.78	0.65
3:C:102:HIS:CE1	15:V:48:THR:HG22	2.27	0.65
10:P:263:PHE:HD1	10:P:333:PRO:HB2	1.60	0.65
12:R:42:ASP:HB3	12:R:44:ARG:HH11	1.61	0.65
13:S:16:LEU:HB3	13:S:69:TYR:CD1	2.32	0.65
15:V:44:TYR:CE1	15:V:48:THR:HG23	2.30	0.65
10:P:135:GLU:HB2	10:P:140:ASP:HA	1.78	0.65
12:R:32:THR:HG22	12:R:36:GLN:N	2.09	0.65
13:S:58:CYS:HB2	13:S:61:VAL:HG12	1.78	0.65
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.32	0.65
3:C:73:GLN:NE2	15:V:112:TRP:HE1	1.95	0.65
4:D:101:LEU:HD11	4:D:106:VAL:HG22	1.78	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
8:H:221:ALA:HA	29:H:401:UQ9:H20A	1.79	0.65
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.77	0.65
5:E:147:ILE:HD11	5:E:183:PRO:HB3	1.77	0.65
7:G:126:LEU:CD1	12:R:89:PRO:HB3	2.25	0.65
8:H:138:GLN:HG3	8:H:139:THR:N	2.11	0.65
13:S:48:HIS:CE1	13:S:95:LEU:CD2	2.80	0.65
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
10:P:141:PHE:CD2	10:P:179:LYS:HD2	2.28	0.65
14:T:130:ILE:HG23	14:T:131:PRO:HD2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ALA:CB	2:B:136:THR:H	2.10	0.65
6:F:110:PRO:HB3	6:F:152:ARG:HH12	1.62	0.65
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.65
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.32	0.65
5:E:79:LEU:HB2	5:E:80:PRO:HD3	1.78	0.64
5:E:136:THR:HG22	5:E:137:THR:H	1.62	0.64
6:F:152:ARG:NH2	23:s:60:PRO:HG3	2.13	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.13	0.64
8:H:90:PRO:HD3	8:H:162:LEU:CD2	2.27	0.64
10:P:166:HIS:HB3	10:P:200:ILE:CD1	2.27	0.64
11:Q:163:ASN:OD1	11:Q:164:PHE:N	2.31	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.64
12:R:52:GLN:HE21	21:q:122:GLU:C	2.04	0.64
14:T:120:MET:HG2	16:W:44:ARG:HH11	1.61	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	0.64
4:D:137:ASP:OD1	4:D:148:GLU:OE2	2.14	0.64
7:G:386:LEU:HD21	7:G:523:VAL:CG1	2.28	0.64
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.64
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.64
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.59	0.64
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.27	0.64
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.64
2:B:70:ARG:HG3	2:B:73:TYR:H	1.63	0.64
2:B:99:CYS:CB	4:D:141:TYR:CG	2.80	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
10:P:88:VAL:HG12	10:P:92:MET:HE2	1.80	0.64
10:P:169:HIS:H	10:P:184:LYS:HE3	1.63	0.64
13:S:15:GLY:HA3	13:S:17:ARG:HH22	1.63	0.64
13:S:16:LEU:HD12	13:S:16:LEU:C	2.22	0.64
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.80	0.64
6:F:388:GLY:HA3	6:F:419:ILE:HD11	1.80	0.64
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.80	0.64
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.64
14:T:83:VAL:HG23	14:T:126:PHE:HZ	1.63	0.64
14:T:87:LEU:HD21	14:T:104:PHE:CZ	2.32	0.64
18:Z:65:LEU:O	18:Z:68:ARG:HG2	1.98	0.64
20:b:48:ALA:O	20:b:49:THR:C	2.40	0.64
1:A:52:SER:HB3	1:A:55:PHE:HB2	1.80	0.64
6:F:278:ILE:HG22	6:F:282:VAL:HG21	1.80	0.64
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.64
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:206:TYR:C	3:C:223:VAL:HG23	2.23	0.63
4:D:97:LEU:O	4:D:99:LEU:HG	1.98	0.63
8:H:145:THR:HG22	8:H:289:LEU:HD11	1.79	0.63
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.63
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.63
34:q:201:CDL:H1	22:r:3:SER:HB2	1.80	0.63
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.79	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.28	0.63
14:T:93:ILE:CG2	14:T:110:LEU:HD13	2.28	0.63
10:P:284:THR:HG23	10:P:356:HIS:HB2	1.79	0.63
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.80	0.63
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.63
10:P:163:ARG:CD	10:P:253:THR:HA	2.27	0.63
18:Z:70:ALA:O	18:Z:73:PRO:HD2	1.99	0.63
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.63
10:P:166:HIS:HE1	10:P:168:SER:HB2	1.63	0.63
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.63
2:B:99:CYS:CB	4:D:141:TYR:CD2	2.82	0.63
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.64	0.63
5:E:176:LEU:HB2	5:E:184:MET:CE	2.29	0.63
7:G:117:MET:HE3	7:G:143:SER:CA	2.28	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
2:B:92:PRO:HD2	2:B:121:PHE:N	2.13	0.63
4:D:142:VAL:HG13	4:D:207:ARG:NH1	2.14	0.63
4:D:348:LEU:O	18:Z:11:PRO:HB3	1.98	0.63
5:E:245:GLN:HB2	6:F:257:ARG:C	2.23	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.63
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.63
10:P:165:ILE:HA	10:P:199:ILE:O	1.98	0.63
4:D:253:LEU:HD22	22:r:23:LYS:HB2	1.81	0.63
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.63
13:S:16:LEU:HA	13:S:69:TYR:HA	1.79	0.63
20:b:66:VAL:HG22	20:b:75:GLY:HA3	1.81	0.63
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.62
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.34	0.62
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.80	0.62
14:T:138:LEU:HD12	14:T:138:LEU:C	2.24	0.62
14:T:138:LEU:O	14:T:138:LEU:CD1	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:25:LEU:HD11	19:a:50:ARG:NH2	2.13	0.62
22:r:109:ASP:O	22:r:110:GLN:HG2	1.99	0.62
5:E:48:PRO:HA	5:E:95:SER:HB2	1.81	0.62
7:G:127:ASP:HA	12:R:106:TYR:OH	1.99	0.62
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.63	0.62
10:P:172:ALA:H	10:P:202:ARG:HH21	1.45	0.62
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.63	0.62
16:W:55:LEU:CB	16:W:107:MET:HE2	2.30	0.62
17:X:130:LYS:HZ2	20:b:63:MET:HB2	1.64	0.62
5:E:140:MET:HE1	6:F:366:ALA:HA	1.81	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
8:H:51:ASP:HA	8:H:54:LYS:HG2	1.80	0.62
8:H:248:TYR:HB3	8:H:250:ASN:OD1	2.00	0.62
6:F:35:LEU:HD11	6:F:39:ASP:O	1.99	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
12:R:51:ARG:NH2	21:q:125:VAL:HG12	2.14	0.62
16:W:55:LEU:CB	16:W:107:MET:CE	2.75	0.62
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.62
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
26:I:301:PC1:H361	26:I:301:PC1:H322	1.79	0.62
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.34	0.62
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.62
8:H:289:LEU:HD23	8:H:289:LEU:C	2.25	0.62
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.34	0.62
2:B:99:CYS:HB2	4:D:141:TYR:CD1	2.35	0.62
2:B:154:GLU:HB3	2:B:155:PRO:HD3	1.81	0.62
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.77	0.62
7:G:339:ALA:C	7:G:545:LEU:HD12	2.25	0.62
7:G:445:LEU:HD21	7:G:462:PHE:HB2	1.81	0.62
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.82	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.62
8:H:289:LEU:HD23	8:H:289:LEU:O	1.99	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.64	0.62
17:X:69:ASN:O	17:X:73:GLN:HG3	2.00	0.62
17:X:130:LYS:NZ	20:b:63:MET:HB2	2.14	0.62
22:r:20:LEU:HD12	22:r:21:GLN:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.63	0.62
6:F:71:LYS:HE2	6:F:71:LYS:HA	1.82	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.62
20:b:67:PRO:HD2	20:b:72:ASP:HB2	1.82	0.62
1:A:73:LEU:N	1:A:74:PRO:HD2	2.15	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
5:E:131:ILE:HD11	5:E:168:PHE:HD2	1.65	0.62
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.62
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.82	0.62
7:G:311:LYS:HE3	7:G:313:LEU:HD13	1.82	0.62
18:Z:28:ARG:HG3	18:Z:28:ARG:O	1.99	0.62
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.58	0.61
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.82	0.61
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61
12:R:98:GLU:CD	12:R:98:GLU:H	2.07	0.61
4:D:109:CYS:O	4:D:111:PRO:HD3	1.99	0.61
5:E:222:PHE:N	5:E:225:GLU:HG2	2.15	0.61
17:X:129:THR:HG23	20:b:68:SER:HA	1.81	0.61
7:G:334:GLU:OE1	13:S:71:PHE:CE1	2.51	0.61
8:H:81:LEU:HD22	8:H:108:THR:HG23	1.82	0.61
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
14:T:103:HIS:ND1	14:T:140:CYS:SG	2.73	0.61
2:B:142:ALA:HB3	2:B:143:PRO:HD3	1.82	0.61
4:D:94:VAL:O	4:D:94:VAL:HG23	1.99	0.61
6:F:266:GLY:HA3	6:F:271:SER:HA	1.82	0.61
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.81	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
21:q:10:GLY:HA2	34:q:201:CDL:OA6	2.00	0.61
21:q:34:ARG:NE	21:q:58:ARG:NH2	2.48	0.61
3:C:73:GLN:HE21	15:V:112:TRP:HE1	1.47	0.61
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.28	0.61
5:E:222:PHE:CE1	6:F:48:ARG:HG3	2.36	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
8:H:87:VAL:HG13	8:H:95:LEU:HD23	1.83	0.61
8:H:224:PHE:HB3	29:H:401:UQ9:H20B	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:48:HIS:HE1	13:S:95:LEU:HD22	1.63	0.61
21:q:71:LYS:O	21:q:72:ASN:CG	2.43	0.61
2:B:98:ALA:O	24:B:301:SF4:S3	2.59	0.61
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.61
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.61
8:H:116:ILE:HD12	8:H:135:ALA:CB	2.30	0.61
8:H:301:CYS:O	8:H:305:ILE:HG13	2.01	0.61
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.61
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.61
5:E:193:GLU:HB2	5:E:217:PRO:HG3	1.81	0.61
5:E:204:ILE:HG22	5:E:208:LYS:HG3	1.82	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.61
11:Q:167:ASN:O	11:Q:168:LYS:CG	2.48	0.61
8:H:127:TYR:CD2	8:H:207:LEU:HG	2.36	0.61
5:E:182:ALA:O	5:E:183:PRO:C	2.43	0.60
12:R:32:THR:HA	12:R:55:VAL:HG23	1.83	0.60
20:b:11:ASN:O	20:b:15:LYS:N	2.31	0.60
21:q:74:PHE:CD2	21:q:75:TRP:CD1	2.88	0.60
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.83	0.60
7:G:35:PHE:O	7:G:101:ASN:HA	2.01	0.60
7:G:64:CYS:HG	7:G:75:CYS:HG	1.47	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
13:S:23:LEU:O	13:S:23:LEU:CD1	2.41	0.60
14:T:79:ILE:CB	14:T:145:VAL:HG13	2.28	0.60
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.60
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.37	0.60
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.60
18:Z:143:TYR:O	18:Z:144:THR:C	2.45	0.60
4:D:80:MET:O	4:D:100:GLU:HA	2.02	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
4:D:304:LYS:HE2	9:I:35:THR:N	2.16	0.60
5:E:175:CYS:SG	6:F:122:PRO:HA	2.42	0.60
10:P:55:VAL:CG1	10:P:123:SER:HA	2.30	0.60
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.02	0.60
7:G:306:MET:HG2	7:G:316:TYR:HA	1.84	0.60
8:H:195:ARG:O	8:H:199:ASP:HB2	2.02	0.60
9:I:64:THR:HG21	26:I:301:PC1:H121	1.83	0.60
17:X:127:LYS:HD3	20:b:66:VAL:HG21	1.83	0.60
22:r:12:ARG:HB3	22:r:20:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:TYR:CB	9:I:153:ILE:HG21	2.31	0.60
7:G:126:LEU:HD11	12:R:89:PRO:HB3	1.82	0.60
7:G:391:ILE:HG22	7:G:417:ARG:HE	1.66	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.84	0.60
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.60
6:F:158:ILE:CD1	6:F:166:ALA:HB2	2.32	0.60
7:G:343:GLY:HA3	7:G:550:ALA:HA	1.82	0.60
6:F:191:TYR:HE2	6:F:193:PHE:HD2	1.50	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
10:P:136:THR:CG2	10:P:139:PHE:HB2	2.31	0.60
13:S:16:LEU:CB	13:S:69:TYR:HD1	2.15	0.60
2:B:141:MET:HE2	4:D:115:LEU:HD23	1.84	0.60
3:C:84:GLU:OE2	3:C:141:ARG:NH1	2.35	0.60
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.83	0.60
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.66	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.60
10:P:146:VAL:HG23	10:P:187:GLY:HA2	1.83	0.60
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.32	0.60
17:X:20:VAL:HG12	17:X:25:LEU:HD21	1.84	0.60
6:F:44:ASN:OD1	6:F:49:HIS:HB2	2.02	0.60
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.60
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.59
4:D:253:LEU:HB2	22:r:23:LYS:CD	2.31	0.59
5:E:225:GLU:HG3	5:E:226:PRO:O	2.01	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.17	0.59
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.59
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.32	0.59
8:H:104:PHE:HE2	30:H:402:3PE:H362	1.66	0.59
10:P:229:VAL:HB	10:P:323:HIS:CD2	2.37	0.59
1:A:7:ILE:HD12	30:H:402:3PE:H392	1.84	0.59
2:B:115:ASP:HA	2:B:119:VAL:O	2.02	0.59
6:F:90:GLY:O	6:F:350:GLY:HA2	2.01	0.59
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.59
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.59
16:W:64:ASP:O	16:W:68:GLU:HG3	2.02	0.59
19:a:3:PHE:CE2	34:q:201:CDL:HA4	2.35	0.59
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.59
7:G:388:ASN:H	7:G:514:ASN:CB	2.15	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:164:PHE:HB3	10:P:198:ALA:HB1	1.83	0.59
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.59
8:H:116:ILE:HD12	8:H:135:ALA:HB1	1.85	0.59
10:P:180:SER:O	10:P:184:LYS:HG3	2.03	0.59
11:Q:167:ASN:HB3	23:s:64:ARG:HE	1.67	0.59
12:R:40:GLU:HA	12:R:45:ARG:CZ	2.33	0.59
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.59
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.02	0.59
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.59
8:H:183:MET:HE2	26:I:301:PC1:H291	1.85	0.59
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.85	0.59
14:T:83:VAL:CG2	14:T:126:PHE:CZ	2.83	0.59
16:W:104:THR:O	16:W:108:ARG:HG3	2.02	0.59
21:q:51:ASP:O	21:q:59:HIS:HB2	2.02	0.59
21:q:96:ASP:OD1	21:q:97:PRO:CD	2.50	0.59
21:q:98:PRO:O	21:q:99:THR:C	2.45	0.59
21:q:137:TRP:CZ2	21:q:140:PRO:HD3	2.38	0.59
2:B:92:PRO:CG	2:B:119:VAL:HG13	2.31	0.59
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.33	0.59
8:H:224:PHE:CD2	29:H:401:UQ9:H20B	2.37	0.59
10:P:328:MET:HG3	10:P:330:THR:H	1.67	0.59
10:P:357:ARG:HD3	10:P:361:TRP:O	2.03	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
2:B:98:ALA:HB3	2:B:135:GLY:HA2	1.85	0.59
3:C:102:HIS:HE1	15:V:48:THR:CG2	2.12	0.59
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.59
12:R:42:ASP:HB3	12:R:44:ARG:NH1	2.17	0.59
18:Z:98:MET:HB2	18:Z:104:TRP:NE1	2.18	0.59
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.68	0.59
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.59
7:G:337:ALA:O	7:G:543:LYS:N	2.36	0.59
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.59
18:Z:105:LYS:O	18:Z:106:VAL:C	2.46	0.59
20:b:8:PHE:HA	20:b:11:ASN:ND2	2.18	0.59
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.61	0.59
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.59
17:X:44:MET:HE1	18:Z:73:PRO:HA	1.84	0.59
20:b:6:SER:O	20:b:9:LEU:HB3	2.03	0.59
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.36	0.58
14:T:90:TYR:CE2	14:T:92:LYS:HB3	2.38	0.58
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:q:201:CDL:H722	34:q:201:CDL:H512	1.84	0.58
3:C:186:ILE:HG13	3:C:187:LEU:N	2.18	0.58
6:F:410:ASP:OD1	6:F:411:SER:N	2.36	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
14:T:103:HIS:HB2	14:T:106:LYS:HB2	1.83	0.58
17:X:53:PRO:HD3	18:Z:116:TRP:CG	2.38	0.58
18:Z:144:THR:HA	19:a:45:TRP:CZ3	2.35	0.58
17:X:78:CYS:SG	17:X:110:CYS:HB3	2.42	0.58
17:X:127:LYS:HD3	20:b:66:VAL:CG2	2.34	0.58
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.19	0.58
4:D:388:GLY:HA3	4:D:417:SER:OG	2.03	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
10:P:318:LYS:O	10:P:322:ILE:HG13	2.02	0.58
11:Q:166:TRP:CE3	23:s:67:PRO:HG3	2.38	0.58
13:S:47:ALA:O	13:S:49:PRO:HD3	2.03	0.58
18:Z:122:GLY:O	18:Z:126:GLY:N	2.34	0.58
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.58
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.58
13:S:16:LEU:HD11	13:S:51:LEU:CD1	2.29	0.58
1:A:55:PHE:O	1:A:56:PHE:C	2.46	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.86	0.58
4:D:375:MET:HE1	7:G:126:LEU:CA	2.34	0.58
7:G:49:VAL:HB	7:G:91:ALA:HA	1.86	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
8:H:288:LEU:HA	8:H:292:ASN:HB2	1.86	0.58
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.58
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.04	0.58
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.04	0.58
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.69	0.58
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
5:E:126:VAL:HG21	5:E:130:HIS:ND1	2.19	0.58
5:E:150:THR:O	5:E:154:LYS:HG2	2.02	0.58
6:F:116:ASN:OD1	6:F:244:ASN:HA	2.03	0.58
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.86	0.58
2:B:112:TYR:CZ	9:I:84:ILE:HD11	2.37	0.58
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.85	0.58
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.58
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.58
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.58
7:G:387:LEU:HD21	7:G:516:LEU:HB3	1.85	0.58
11:Q:166:TRP:HE3	23:s:67:PRO:HG3	1.67	0.58
14:T:90:TYR:CE2	14:T:92:LYS:CB	2.87	0.58
17:X:20:VAL:C	19:a:54:ILE:HD13	2.29	0.58
5:E:135:THR:OG1	5:E:172:GLU:CG	2.52	0.57
6:F:109:ARG:NH2	6:F:232:ASP:O	2.36	0.57
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.17	0.57
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.57
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.85	0.57
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.57
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.57
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.57
18:Z:129:THR:HB	18:Z:132:GLU:HG3	1.86	0.57
1:A:25:PRO:HG3	8:H:60:PRO:HD3	1.85	0.57
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.22	0.57
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.57
7:G:372:PHE:H	7:G:532:PRO:HB2	1.69	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.57
18:Z:86:ILE:HG23	18:Z:128:ARG:NE	2.15	0.57
10:P:56:ALA:HA	10:P:125:VAL:O	2.03	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.04	0.57
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.34	0.57
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.57
18:Z:120:LEU:HB2	18:Z:123:GLU:HG3	1.87	0.57
3:C:104:ASN:O	22:r:97:PRO:HD3	2.04	0.57
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.87	0.57
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.57
7:G:73:GLY:HA2	27:G:803:FES:S1	2.45	0.57
8:H:64:LEU:HD12	10:P:362:LEU:HD11	1.86	0.57
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.86	0.57
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.86	0.57
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.87	0.57
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.19	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
4:D:137:ASP:OD1	4:D:148:GLU:HG3	2.04	0.57
6:F:76:ILE:HG23	6:F:255:CYS:SG	2.45	0.57
8:H:90:PRO:HA	8:H:94:PRO:HB3	1.86	0.57
8:H:210:GLY:HA2	8:H:213:VAL:HG23	1.87	0.57
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.57
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.57
11:Q:167:ASN:O	11:Q:168:LYS:HG2	2.04	0.57
17:X:58:LYS:HA	17:X:61:LYS:HE2	1.87	0.57
4:D:84:PHE:CE2	4:D:91:ALA:HB2	2.40	0.57
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.85	0.57
8:H:86:TRP:NE1	8:H:233:LEU:HB2	2.20	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
14:T:130:ILE:HD11	14:T:148:ILE:HD11	1.86	0.57
4:D:148:GLU:OE2	4:D:225:ALA:HA	2.04	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.57
7:G:171:THR:HB	7:G:173:MET:HG3	1.87	0.57
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.57
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.57
21:q:65:THR:HG22	21:q:66:THR:N	2.20	0.57
7:G:41:VAL:HG21	7:G:56:VAL:HB	1.86	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
10:P:211:ASP:OD1	10:P:214:LEU:HB3	2.04	0.56
21:q:14:VAL:HG13	21:q:23:LEU:CD2	2.35	0.56
7:G:102:ILE:H	7:G:102:ILE:HD12	1.70	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
8:H:113:VAL:O	8:H:116:ILE:HG12	2.05	0.56
18:Z:7:LYS:HB2	18:Z:7:LYS:NZ	2.20	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.87	0.56
26:B:303:PC1:H143	21:q:29:ARG:O	2.05	0.56
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.15	0.56
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.56
5:E:151:LEU:CD2	5:E:170:LEU:HD13	2.35	0.56
6:F:171:VAL:HA	6:F:174:ARG:HH12	1.70	0.56
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.56
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.56
8:H:19:PHE:CE1	19:a:11:ILE:HD12	2.40	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.40	0.56
10:P:168:SER:HA	10:P:184:LYS:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:38:TYR:HE2	21:q:127:TYR:CB	1.97	0.56
12:R:62:ASP:O	12:R:66:GLN:HG3	2.05	0.56
14:T:134:ASP:OD1	14:T:134:ASP:O	2.23	0.56
17:X:137:LEU:HD13	20:b:58:ARG:HE	1.70	0.56
21:q:129:THR:O	21:q:129:THR:HG22	2.03	0.56
2:B:98:ALA:H	2:B:135:GLY:HA3	1.69	0.56
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.37	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.40	0.56
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.86	0.56
12:R:37:VAL:O	12:R:38:TYR:C	2.44	0.56
12:R:59:PHE:O	12:R:63:LEU:HG	2.06	0.56
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.56
4:D:359:ASP:O	7:G:150:ARG:NH2	2.38	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
8:H:90:PRO:CG	8:H:162:LEU:HB3	2.31	0.56
11:Q:110:PRO:HB3	12:R:43:TYR:OH	2.06	0.56
2:B:69:SER:O	2:B:70:ARG:C	2.48	0.56
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.56
5:E:84:LEU:HD12	23:s:46:LEU:HD13	1.88	0.56
5:E:200:ILE:O	5:E:204:ILE:HG13	2.06	0.56
8:H:19:PHE:HB3	19:a:12:MET:HG3	1.87	0.56
8:H:142:TYR:HE1	8:H:285:LEU:HD23	1.71	0.56
10:P:145:PHE:O	10:P:149:PRO:HG2	2.05	0.56
17:X:44:MET:SD	17:X:48:TRP:HZ3	2.29	0.56
17:X:142:TYR:HB2	18:Z:115:ARG:NH1	2.17	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.56
6:F:39:ASP:HB3	6:F:265:PHE:HZ	1.69	0.56
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.56
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
8:H:4:ILE:H	8:H:4:ILE:HD12	1.71	0.56
8:H:142:TYR:HE1	8:H:285:LEU:CD2	2.19	0.56
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.88	0.56
9:I:35:THR:CG2	22:r:107:SER:HA	2.36	0.56
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.56
9:I:80:GLU:HB3	22:r:26:LEU:HD11	1.88	0.56
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.56
5:E:180:VAL:HG21	6:F:286:CYS:HA	1.88	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:318:MET:HE3	18:Z:57:ARG:HH21	1.71	0.56
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.56
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.56
14:T:90:TYR:HE2	14:T:92:LYS:CB	2.19	0.56
17:X:124:GLN:C	17:X:125:LEU:HD12	2.31	0.56
18:Z:85:GLN:O	18:Z:89:GLU:HG3	2.06	0.56
18:Z:92:GLU:O	18:Z:96:ILE:HG13	2.05	0.56
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.41	0.55
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.21	0.55
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.55
10:P:251:ASN:OD1	10:P:254:LYS:HE3	2.06	0.55
11:Q:166:TRP:CE3	23:s:67:PRO:CG	2.88	0.55
14:T:87:LEU:HD22	14:T:104:PHE:CZ	2.41	0.55
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.88	0.55
1:A:96:THR:O	1:A:100:LEU:HG	2.06	0.55
4:D:199:PRO:HD3	4:D:261:MET:HE1	1.87	0.55
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.55
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.41	0.55
10:P:188:GLU:HA	10:P:191:VAL:HG12	1.89	0.55
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.49	0.55
20:b:8:PHE:CG	20:b:9:LEU:N	2.74	0.55
6:F:213:ILE:CG2	6:F:235:VAL:HA	2.36	0.55
7:G:264:SER:HB2	7:G:272:ARG:HG2	1.88	0.55
7:G:666:GLN:NE2	13:S:38:VAL:HG13	2.21	0.55
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.42	0.55
10:P:265:PHE:CZ	10:P:338:LEU:HD12	2.41	0.55
12:R:36:GLN:HG2	21:q:127:TYR:CD2	2.40	0.55
1:A:22:PHE:O	1:A:25:PRO:HD2	2.05	0.55
1:A:54:LYS:HE3	1:A:111:LEU:O	2.06	0.55
3:C:217:ARG:HH12	16:W:112:GLU:CB	2.13	0.55
4:D:145:MET:O	4:D:148:GLU:N	2.39	0.55
4:D:254:ARG:HH11	22:r:25:GLN:CA	2.19	0.55
7:G:94:MET:CE	7:G:100:TRP:HH2	2.20	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.86	0.55
3:C:85:ILE:HD11	3:C:140:ILE:CD1	2.34	0.55
4:D:128:THR:H	4:D:131:GLN:NE2	2.00	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
7:G:126:LEU:CD1	12:R:89:PRO:HB2	2.37	0.55
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:ARG:HH11	29:H:401:UQ9:H15	1.72	0.55
10:P:206:ILE:HG13	31:P:401:NDP:H42N	1.88	0.55
10:P:235:THR:OG1	10:P:273:LEU:CB	2.54	0.55
21:q:68:MET:HE1	21:q:81:MET:O	2.06	0.55
2:B:95:PHE:HE2	2:B:97:LEU:HD11	1.71	0.55
2:B:210:ARG:HD3	21:q:76:ASP:HB2	1.88	0.55
5:E:170:LEU:HD12	5:E:171:ILE:N	2.20	0.55
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.37	0.55
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.55
10:P:64:PHE:HE1	10:P:209:ARG:O	1.90	0.55
10:P:208:GLY:O	10:P:209:ARG:C	2.48	0.55
10:P:258:ALA:HA	10:P:263:PHE:HZ	1.71	0.55
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.89	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
7:G:356:ASP:O	7:G:360:LYS:HG3	2.06	0.55
10:P:219:ASN:ND2	10:P:313:TRP:HE1	2.04	0.55
11:Q:165:SER:HB3	11:Q:168:LYS:O	2.06	0.55
14:T:128:PHE:CE2	14:T:130:ILE:HG13	2.42	0.55
21:q:64:TYR:CE2	21:q:82:VAL:HG13	2.42	0.55
4:D:262:LEU:O	4:D:263:THR:C	2.49	0.55
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
10:P:196:PRO:O	10:P:197:GLU:HB2	2.07	0.55
18:Z:56:GLU:HA	18:Z:59:ARG:HH11	1.72	0.55
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.55
1:A:103:ALA:O	1:A:107:THR:HG23	2.06	0.55
4:D:97:LEU:HG	4:D:99:LEU:HD21	1.89	0.55
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.55
8:H:51:ASP:CA	8:H:54:LYS:HG2	2.37	0.55
9:I:53:ALA:CA	20:b:14:ALA:HB2	2.36	0.55
19:a:1:MET:HG3	34:q:201:CDL:HB21	1.87	0.55
1:A:105:GLU:CG	1:A:111:LEU:HB3	2.37	0.55
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.55
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.55
10:P:195:PHE:HD1	10:P:198:ALA:HB2	1.72	0.55
10:P:208:GLY:H	10:P:211:ASP:CB	2.18	0.55
13:S:30:SER:O	13:S:31:GLN:C	2.49	0.55
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.72	0.54
1:A:49:LEU:HD12	1:A:50:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.37	0.54
6:F:270:ASN:OD1	6:F:270:ASN:C	2.48	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.07	0.54
7:G:617:ARG:HH12	16:W:128:GLY:C	2.14	0.54
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.88	0.54
8:H:212:ASN:HB3	8:H:215:TYR:HB2	1.89	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
10:P:199:ILE:HD13	10:P:258:ALA:HB1	1.89	0.54
15:V:50:GLN:HE22	22:r:94:ALA:H	1.54	0.54
4:D:81:THR:HG22	4:D:100:GLU:HG2	1.88	0.54
4:D:202:TRP:CH2	9:I:72:MET:HG2	2.42	0.54
4:D:232:VAL:HG23	4:D:356:ILE:HD13	1.88	0.54
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.54
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.54
7:G:456:ALA:O	7:G:499:LYS:HE2	2.06	0.54
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.89	0.54
10:P:213:PHE:CE2	10:P:239:PRO:HB3	2.42	0.54
10:P:300:TRP:O	10:P:304:LEU:HG	2.08	0.54
10:P:315:THR:O	10:P:316:LYS:C	2.49	0.54
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.54
14:T:97:LYS:HG3	14:T:97:LYS:O	2.08	0.54
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.54
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.06	0.54
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.54
6:F:275:LEU:HA	6:F:289:GLU:HA	1.90	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.54
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.22	0.54
19:a:58:ASN:HB2	19:a:61:TYR:CD2	2.43	0.54
20:b:8:PHE:O	20:b:9:LEU:C	2.50	0.54
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.43	0.54
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.89	0.54
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.54
5:E:40:HIS:HB2	7:G:209:TYR:CZ	2.41	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
10:P:376:ASN:OD1	10:P:376:ASN:C	2.50	0.54
17:X:8:PRO:HG2	17:X:57:LEU:HD11	1.90	0.54
2:B:141:MET:CE	4:D:115:LEU:HD23	2.37	0.54
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:152:ARG:CZ	23:s:60:PRO:HG3	2.38	0.54
6:F:152:ARG:HD3	23:s:57:LEU:HD11	1.87	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
7:G:360:LYS:HB2	7:G:632:ILE:CD1	2.28	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
16:W:53:MET:HB2	16:W:55:LEU:HG	1.89	0.54
3:C:73:GLN:NE2	15:V:107:PRO:HB3	2.22	0.54
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.89	0.54
10:P:209:ARG:N	10:P:352:VAL:HG22	2.23	0.54
10:P:315:THR:HG22	10:P:316:LYS:N	2.21	0.54
11:Q:160:TYR:CZ	11:Q:164:PHE:HZ	2.26	0.54
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.54
6:F:109:ARG:HE	6:F:239:PRO:HD3	1.73	0.54
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
7:G:50:LEU:O	7:G:54:GLU:HG2	2.07	0.54
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.54
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.90	0.54
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.43	0.54
16:W:67:ARG:HD2	16:W:71:MET:HE2	1.89	0.54
16:W:88:LYS:O	16:W:92:GLU:HG2	2.08	0.54
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.23	0.54
19:a:31:ASN:HD21	19:a:36:LYS:HB2	1.71	0.54
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.23	0.54
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.54
6:F:67:GLU:O	6:F:71:LYS:HG2	2.07	0.54
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.54
6:F:171:VAL:HA	6:F:174:ARG:NH1	2.23	0.54
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.54
7:G:355:LYS:HG3	7:G:366:LEU:CD1	2.38	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:617:ARG:NH1	16:W:128:GLY:C	2.66	0.54
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.54
10:P:258:ALA:HA	10:P:263:PHE:CZ	2.43	0.54
14:T:83:VAL:HG22	14:T:126:PHE:HZ	1.66	0.54
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.54
6:F:127:ASP:HB3	6:F:245:VAL:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:94:MET:HE2	7:G:100:TRP:HH2	1.73	0.54
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.54
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.54
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.54
10:P:142:GLU:HA	10:P:146:VAL:HG12	1.90	0.54
11:Q:52:LEU:HG	16:W:21:LYS:HG2	1.90	0.54
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.54
2:B:92:PRO:HG3	2:B:119:VAL:CG1	2.36	0.53
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.53
6:F:297:LYS:O	6:F:301:GLU:HG2	2.08	0.53
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.53
8:H:303:TRP:CZ3	20:b:28:LEU:HG	2.43	0.53
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.53
10:P:311:GLU:O	10:P:312:PRO:C	2.49	0.53
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.53
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.53
21:q:95:ASP:OD1	21:q:96:ASP:N	2.41	0.53
1:A:68:GLU:CD	1:A:98:LEU:HG	2.33	0.53
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.43	0.53
3:C:224:GLU:OE1	10:P:48:ARG:O	2.26	0.53
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.53
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.53
8:H:69:SER:O	8:H:72:ILE:HG13	2.08	0.53
10:P:211:ASP:OD2	10:P:352:VAL:HG11	2.08	0.53
10:P:355:ARG:HH11	10:P:356:HIS:CE1	2.25	0.53
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.53
21:q:125:VAL:HG23	21:q:125:VAL:O	2.08	0.53
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.53
8:H:172:MET:HE1	18:Z:46:GLY:HA3	1.91	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
14:T:118:ILE:HG23	14:T:122:MET:CE	2.37	0.53
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.53
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.91	0.53
2:B:114:MET:SD	2:B:119:VAL:HG12	2.48	0.53
2:B:135:GLY:O	2:B:165:ALA:HB2	2.08	0.53
6:F:276:PHE:HD1	6:F:352:ALA:HB1	1.72	0.53
7:G:382:ARG:HD2	13:S:56:ARG:HD3	1.90	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53
10:P:164:PHE:HB3	10:P:198:ALA:CB	2.38	0.53
21:q:56:PHE:HD1	21:q:59:HIS:NE2	2.06	0.53
1:A:58:VAL:HG11	8:H:286:MET:HE1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:235:VAL:HG12	6:F:240:THR:OG1	2.09	0.53
6:F:270:ASN:ND2	6:F:338:ASP:HB2	2.23	0.53
6:F:388:GLY:CA	6:F:419:ILE:HD11	2.37	0.53
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.09	0.53
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.53
9:I:78:PHE:CG	22:r:8:ILE:HG23	2.44	0.53
17:X:25:LEU:HD11	19:a:50:ARG:CZ	2.39	0.53
17:X:120:PRO:HG3	20:b:71:GLN:HE21	1.73	0.53
21:q:132:LYS:HD3	21:q:135:HIS:ND1	2.23	0.53
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.44	0.53
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	2.97	0.53
5:E:77:ALA:C	5:E:80:PRO:HD2	2.33	0.53
5:E:135:THR:OG1	5:E:135:THR:O	2.21	0.53
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.53
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.91	0.53
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.90	0.53
10:P:122:HIS:CB	12:R:46:VAL:CG1	2.85	0.53
10:P:370:LYS:HG3	10:P:370:LYS:O	2.08	0.53
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.53
5:E:129:TYR:CZ	5:E:207:LEU:HB3	2.43	0.53
7:G:163:LYS:HE2	12:R:97:LYS:NZ	2.24	0.53
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.53
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.53
18:Z:116:TRP:CZ2	18:Z:119:PRO:HD3	2.44	0.53
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.43	0.53
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.51	0.53
9:I:153:ILE:HD12	9:I:153:ILE:O	2.09	0.53
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.53
14:T:103:HIS:HD1	14:T:140:CYS:HG	1.51	0.53
17:X:80:GLU:HB3	17:X:81:PRO:HD3	1.91	0.53
21:q:68:MET:SD	21:q:81:MET:CB	2.95	0.53
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.53
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.53
5:E:39:VAL:CG2	7:G:205:GLN:HE22	2.16	0.53
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
7:G:347:ASP:N	7:G:347:ASP:OD1	2.41	0.53
10:P:94:LEU:O	10:P:97:MET:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:VAL:HG12	8:H:25:ARG:NH2	2.22	0.53
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.43	0.53
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.91	0.53
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.22	0.53
5:E:47:ASN:OD1	5:E:50:THR:HG23	2.09	0.53
5:E:131:ILE:HD13	5:E:151:LEU:HD11	1.90	0.53
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.53
12:R:69:VAL:HG12	12:R:112:LYS:N	2.24	0.53
13:S:16:LEU:O	13:S:16:LEU:CD1	2.51	0.53
13:S:16:LEU:HD13	13:S:19:ILE:CD1	2.38	0.53
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.53
19:a:3:PHE:HE2	34:q:201:CDL:H112	1.74	0.53
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.89	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
7:G:634:LEU:HD13	7:G:636:TYR:CZ	2.43	0.52
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.52
8:H:102:ILE:CD1	8:H:154:LEU:HD21	2.39	0.52
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.52
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.52
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.52
2:B:141:MET:HE1	4:D:86:PRO:HB2	1.90	0.52
7:G:140:GLN:HG3	7:G:141:ASP:OD1	2.09	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.52
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.74	0.52
12:R:98:GLU:HA	12:R:113:GLN:CD	2.33	0.52
4:D:80:MET:SD	8:H:126:LYS:HD3	2.49	0.52
7:G:30:ASN:O	7:G:45:PRO:HD3	2.09	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.91	0.52
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.91	0.52
10:P:239:PRO:HG2	10:P:345:LEU:CD1	2.40	0.52
10:P:283:MET:HE2	10:P:366:ILE:HG22	1.92	0.52
10:P:353:LEU:HA	10:P:356:HIS:HD2	1.74	0.52
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.52
14:T:114:ASP:OD1	16:W:67:ARG:NH1	2.42	0.52
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.35	0.52
21:q:3:LEU:HD13	34:q:201:CDL:OB6	2.09	0.52
2:B:125:PRO:HG3	2:B:148:VAL:HG13	1.90	0.52
5:E:178:ALA:HA	6:F:125:CYS:SG	2.49	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.52
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.52
8:H:317:TYR:O	8:H:318:MET:C	2.52	0.52
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52
21:q:6:VAL:HG11	34:q:201:CDL:HB4	1.91	0.52
2:B:103:GLU:O	2:B:106:HIS:HB2	2.10	0.52
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.91	0.52
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.45	0.52
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.52
7:G:36:VAL:CG1	7:G:56:VAL:HG11	2.34	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.52
1:A:87:MET:HE1	8:H:309:ILE:HD11	1.91	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
14:T:87:LEU:HD23	14:T:122:MET:HE1	1.91	0.52
14:T:130:ILE:CG2	14:T:131:PRO:HD2	2.40	0.52
17:X:37:ASP:OD1	17:X:38:LYS:N	2.43	0.52
17:X:49:GLU:HG2	17:X:138:PRO:HD2	1.91	0.52
21:q:13:GLN:HE22	34:q:201:CDL:CA3	2.21	0.52
21:q:29:ARG:HD3	21:q:74:PHE:CD1	2.44	0.52
2:B:173:TYR:O	3:C:203:LEU:HD22	2.09	0.52
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.52
4:D:368:ARG:HA	4:D:371:MET:HG2	1.90	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.52
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.52
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.42	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.09	0.52
5:E:188:ASN:O	5:E:189:ASP:HB3	2.10	0.52
5:E:240:PRO:HG3	6:F:60:GLY:HA2	1.91	0.52
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.52
16:W:42:TRP:CH2	33:W:201:EHZ:O1	2.63	0.52
17:X:77:HIS:HD2	17:X:115:LEU:HD21	1.75	0.52
1:A:104:TYR:O	1:A:105:GLU:C	2.51	0.52
3:C:114:THR:CG2	4:D:421:ARG:HH12	2.17	0.52
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
7:G:30:ASN:O	7:G:44:GLU:HA	2.09	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.52
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.52
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.52
1:A:19:LEU:O	1:A:20:VAL:C	2.50	0.52
5:E:192:TYR:CE2	5:E:213:PRO:HB2	2.45	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.45	0.52
7:G:671:LEU:CD1	13:S:42:VAL:HG12	2.40	0.52
10:P:195:PHE:CD1	10:P:198:ALA:HB2	2.45	0.52
14:T:79:ILE:CG2	14:T:145:VAL:HG13	2.40	0.52
16:W:73:ASN:O	16:W:76:VAL:HG12	2.10	0.52
17:X:129:THR:CG2	20:b:68:SER:HA	2.39	0.52
20:b:68:SER:O	20:b:69:HIS:C	2.51	0.52
21:q:29:ARG:HD3	21:q:74:PHE:CE1	2.44	0.52
21:q:89:TRP:HB2	21:q:98:PRO:HD3	1.92	0.52
3:C:124:ARG:HD2	11:Q:140:LYS:HZ2	1.75	0.51
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.74	0.51
6:F:63:TYR:H	6:F:256:ARG:HH21	1.57	0.51
7:G:47:THR:O	7:G:96:VAL:HG12	2.10	0.51
7:G:275:PRO:HB2	11:Q:86:ASN:ND2	2.25	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.51
7:G:614:GLY:O	16:W:129:HIS:NE2	2.41	0.51
8:H:51:ASP:OD2	29:H:401:UQ9:C16	2.58	0.51
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.45	0.51
22:r:28:TYR:O	22:r:29:GLN:C	2.53	0.51
2:B:92:PRO:CD	2:B:121:PHE:H	2.18	0.51
2:B:170:TYR:HB2	9:I:153:ILE:CG2	2.33	0.51
4:D:106:VAL:HG21	4:D:447:VAL:CG2	2.41	0.51
6:F:217:GLU:CD	11:Q:166:TRP:HE1	2.18	0.51
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.51
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.51
14:T:130:ILE:HG23	14:T:131:PRO:CD	2.40	0.51
18:Z:61:LEU:O	18:Z:64:ASP:OD1	2.28	0.51
18:Z:65:LEU:HB2	20:b:50:PRO:HG2	1.91	0.51
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.33	0.51
5:E:129:TYR:CE2	5:E:207:LEU:HB3	2.46	0.51
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:75:CYS:SG	7:G:76:ARG:N	2.84	0.51
7:G:367:CYS:HB3	7:G:533:GLY:O	2.10	0.51
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.44	0.51
8:H:51:ASP:O	8:H:54:LYS:HG2	2.10	0.51
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.51
2:B:126:ARG:HG3	8:H:214:GLU:HA	1.91	0.51
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.51
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.51
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.45	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.51
9:I:38:TYR:HB3	9:I:41:LYS:HB2	1.93	0.51
9:I:209:TYR:HA	9:I:212:ARG:CG	2.39	0.51
21:q:65:THR:CG2	21:q:66:THR:N	2.72	0.51
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.51
7:G:41:VAL:HG21	7:G:56:VAL:CB	2.41	0.51
7:G:253:VAL:O	7:G:253:VAL:HG12	2.11	0.51
7:G:304:GLU:HB2	7:G:316:TYR:HD2	1.75	0.51
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.41	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:386:LEU:HD21	7:G:523:VAL:HG13	1.91	0.51
10:P:207:PHE:O	10:P:241:TYR:HA	2.10	0.51
19:a:1:MET:HG3	34:q:201:CDL:CB2	2.41	0.51
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.10	0.51
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.51
6:F:42:PHE:CE1	6:F:130:ILE:HD12	2.46	0.51
7:G:355:LYS:HA	7:G:366:LEU:CD1	2.37	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:33:LEU:HD23	22:r:25:GLN:HG2	1.92	0.51
8:H:51:ASP:OD2	29:H:401:UQ9:C15	2.56	0.51
8:H:142:TYR:CE1	8:H:285:LEU:HD21	2.46	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
20:b:36:SER:HB3	20:b:39:THR:OG1	2.10	0.51
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
8:H:23:VAL:HG11	19:a:9:LEU:CD2	2.39	0.51
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.98	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
10:P:305:PHE:CG	10:P:314:THR:HG22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:42:GLN:O	19:a:43:TYR:C	2.51	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.91	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
4:D:299:GLN:OE1	22:r:104:TRP:HB2	2.10	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.11	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.51
7:G:358:LEU:HD12	7:G:366:LEU:CD2	2.40	0.51
7:G:401:LEU:HD21	7:G:462:PHE:CE2	2.46	0.51
7:G:401:LEU:HD21	7:G:466:LEU:HD21	1.92	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:42:PRO:HB3	21:q:27:PHE:HE2	1.76	0.51
8:H:90:PRO:CG	8:H:240:ILE:HG21	2.39	0.51
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.51
14:T:140:CYS:HB2	14:T:143:GLU:CG	2.40	0.51
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.51
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.51
2:B:116:ARG:O	8:H:39:ILE:HG22	2.09	0.51
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.51
5:E:180:VAL:HG22	5:E:221:ARG:HH12	1.75	0.51
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.51
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.93	0.51
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.91	0.51
10:P:367:GLU:HG2	10:P:368:GLU:N	2.26	0.51
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.51
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.51
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.51
4:D:166:ARG:CZ	18:Z:8:GLN:HG2	2.41	0.51
8:H:142:TYR:CE1	8:H:285:LEU:CD2	2.94	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.51
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.51
14:T:105:MET:HB2	14:T:139:MET:SD	2.51	0.51
20:b:11:ASN:OD1	20:b:12:ALA:N	2.44	0.51
1:A:59:ALA:O	1:A:62:PHE:HB3	2.11	0.50
4:D:84:PHE:HB2	4:D:97:LEU:HB3	1.93	0.50
4:D:253:LEU:HB2	22:r:23:LYS:HD3	1.92	0.50
4:D:280:ALA:CB	15:V:11:LEU:CG	2.81	0.50
6:F:122:PRO:HG3	6:F:373:PHE:CZ	2.46	0.50
7:G:382:ARG:O	7:G:386:LEU:HD12	2.10	0.50
9:I:71:GLY:HA2	26:I:301:PC1:H351	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.50
11:Q:167:ASN:C	11:Q:168:LYS:HG2	2.36	0.50
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.92	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.76	0.50
17:X:25:LEU:O	17:X:29:ALA:N	2.44	0.50
2:B:174:SER:HA	3:C:203:LEU:CD2	2.41	0.50
4:D:444:LEU:HD21	8:H:206:GLU:O	2.12	0.50
5:E:128:LYS:CB	5:E:167:LEU:HA	2.42	0.50
7:G:617:ARG:NH1	16:W:129:HIS:N	2.57	0.50
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.50
8:H:74:ALA:HB3	8:H:75:PRO:HD3	1.93	0.50
14:T:87:LEU:HD23	14:T:122:MET:CE	2.41	0.50
19:a:3:PHE:CE2	34:q:201:CDL:H112	2.47	0.50
21:q:6:VAL:HG12	34:q:201:CDL:OA9	2.11	0.50
4:D:145:MET:O	4:D:146:CYS:C	2.54	0.50
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.50
5:E:227:ALA:HB3	6:F:284:HIS:ND1	2.26	0.50
10:P:68:TYR:CD1	10:P:242:VAL:HG21	2.46	0.50
10:P:172:ALA:H	10:P:202:ARG:NH2	2.08	0.50
11:Q:167:ASN:HA	23:s:64:ARG:HD3	1.94	0.50
1:A:57:LEU:O	1:A:61:THR:HG23	2.12	0.50
5:E:43:THR:HG23	5:E:46:ASN:H	1.75	0.50
6:F:238:CYS:O	6:F:239:PRO:C	2.54	0.50
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.92	0.50
12:R:55:VAL:HG22	12:R:56:ASN:H	1.77	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.50
4:D:266:ARG:HD3	30:H:403:3PE:O12	2.11	0.50
5:E:136:THR:HG22	5:E:137:THR:N	2.27	0.50
6:F:113:LEU:HB3	6:F:154:ALA:HB2	1.92	0.50
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.94	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.50
10:P:374:THR:HG23	10:P:374:THR:O	2.10	0.50
2:B:125:PRO:O	2:B:152:MET:HA	2.10	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50
10:P:150:ARG:O	10:P:151:ALA:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.11	0.50
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.50
19:a:4:GLU:O	19:a:7:PRO:HD2	2.11	0.50
22:r:6:ARG:HG2	22:r:6:ARG:O	2.11	0.50
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.50
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.93	0.50
8:H:103:LEU:HG	8:H:160:TYR:CD1	2.46	0.50
8:H:172:MET:SD	18:Z:46:GLY:HA2	2.52	0.50
15:V:44:TYR:CD1	15:V:48:THR:HG23	2.46	0.50
16:W:95:GLU:HB3	16:W:101:LYS:HG3	1.94	0.50
20:b:35:ILE:O	20:b:35:ILE:CD1	2.59	0.50
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.50
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.47	0.50
4:D:289:SER:N	4:D:293:LEU:HG	2.26	0.50
6:F:295:PRO:HD2	6:F:298:GLU:OE2	2.11	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.50
10:P:157:LYS:O	10:P:158:GLU:C	2.53	0.50
13:S:36:PHE:CZ	13:S:44:LEU:HD11	2.37	0.50
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.50
17:X:8:PRO:HD3	17:X:54:ARG:CD	2.40	0.50
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.51	0.50
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.42	0.50
4:D:460:GLU:O	4:D:463:ARG:HG2	2.12	0.50
6:F:174:ARG:O	6:F:178:GLU:HG3	2.11	0.50
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.50
8:H:224:PHE:CG	29:H:401:UQ9:C20	2.93	0.50
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.50
12:R:32:THR:CG2	12:R:36:GLN:H	2.18	0.50
17:X:36:CYS:SG	17:X:36:CYS:O	2.69	0.50
4:D:105:MET:SD	4:D:441:GLY:HA2	2.52	0.49
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.49
5:E:130:HIS:O	5:E:132:GLN:HG3	2.12	0.49
5:E:152:GLN:HE21	5:E:159:VAL:HB	1.76	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
8:H:85:LEU:CD2	8:H:108:THR:HB	2.37	0.49
10:P:246:SER:O	10:P:247:LYS:C	2.55	0.49
15:V:56:LEU:C	15:V:56:LEU:CD1	2.85	0.49
15:V:56:LEU:HA	15:V:59:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:7:LEU:CD1	18:Z:87:LEU:HB3	2.41	0.49
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.49
18:Z:140:PHE:O	18:Z:141:THR:C	2.55	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.95	0.49
5:E:233:LEU:HD13	6:F:48:ARG:HH22	1.76	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.47	0.49
7:G:304:GLU:HB2	7:G:316:TYR:CD2	2.46	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
8:H:12:PRO:O	19:a:15:CYS:HB3	2.13	0.49
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.46	0.49
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.94	0.49
18:Z:129:THR:HG22	18:Z:131:GLU:H	1.77	0.49
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.49
20:b:66:VAL:HG22	20:b:75:GLY:CA	2.40	0.49
2:B:170:TYR:OH	4:D:131:GLN:O	2.30	0.49
3:C:100:ARG:HH12	15:V:86:LYS:NZ	2.10	0.49
3:C:216:LYS:HG3	10:P:209:ARG:HH11	1.76	0.49
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.49
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.49
5:E:135:THR:O	6:F:369:ARG:NE	2.41	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.13	0.49
7:G:298:LYS:O	21:q:134:ILE:HA	2.12	0.49
8:H:202:GLU:OE2	8:H:211:PHE:HB3	2.12	0.49
21:q:97:PRO:C	21:q:99:THR:N	2.70	0.49
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.77	0.49
26:B:303:PC1:H232	26:B:303:PC1:C32	2.37	0.49
5:E:91:TRP:CE3	5:E:125:PRO:HB3	2.48	0.49
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.13	0.49
17:X:7:LEU:HD13	18:Z:87:LEU:HB3	1.93	0.49
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.30	0.49
5:E:244:VAL:HG23	6:F:256:ARG:CG	2.42	0.49
8:H:17:MET:CE	8:H:225:MET:HB3	2.41	0.49
8:H:63:PRO:O	8:H:66:THR:HG22	2.12	0.49
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.49
10:P:178:SER:O	10:P:179:LYS:C	2.55	0.49
10:P:208:GLY:N	10:P:211:ASP:HB3	2.20	0.49
17:X:59:GLU:O	17:X:63:VAL:HG23	2.12	0.49
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.38	0.49
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.12	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:171:VAL:O	6:F:175:GLU:HG2	2.12	0.49
6:F:225:LEU:HB2	11:Q:160:TYR:CD2	2.45	0.49
7:G:43:VAL:CG1	7:G:55:LYS:HD3	2.41	0.49
8:H:93:HIS:O	19:a:23:THR:HG22	2.13	0.49
8:H:222:LEU:O	8:H:223:PHE:C	2.51	0.49
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.49
10:P:168:SER:O	10:P:202:ARG:HA	2.13	0.49
13:S:42:VAL:O	13:S:46:LYS:HG3	2.12	0.49
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.49
2:B:91:TRP:N	2:B:91:TRP:CD1	2.80	0.49
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.38	0.49
7:G:117:MET:HE3	7:G:143:SER:N	2.27	0.49
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
8:H:66:THR:HA	8:H:124:ASN:OD1	2.12	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.95	0.49
8:H:224:PHE:CB	29:H:401:UQ9:C20	2.89	0.49
10:P:211:ASP:O	10:P:215:ASN:HB2	2.12	0.49
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.49
17:X:73:GLN:OE1	17:X:117:TRP:HZ2	1.96	0.49
17:X:115:LEU:HD13	17:X:117:TRP:CZ3	2.48	0.49
18:Z:66:GLU:HA	18:Z:69:ILE:HG12	1.93	0.49
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.95	0.49
1:A:105:GLU:HG3	1:A:111:LEU:HD22	1.95	0.49
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49
4:D:339:GLN:HE21	9:I:37:LYS:NZ	2.11	0.49
5:E:235:GLU:HB2	6:F:37:ASP:CB	2.43	0.49
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.93	0.49
6:F:146:GLY:O	6:F:150:GLY:N	2.46	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49
6:F:224:ARG:HD2	11:Q:164:PHE:CE1	2.48	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.49
8:H:274:ARG:HH22	29:H:401:UQ9:C1M	2.23	0.49
10:P:166:HIS:CE1	10:P:168:SER:HB2	2.45	0.49
12:R:67:GLN:HG2	12:R:109:LEU:HD21	1.94	0.49
13:S:24:CYS:N	13:S:58:CYS:SG	2.85	0.49
14:T:138:LEU:HD13	14:T:144:ILE:CD1	2.42	0.49
14:T:140:CYS:O	14:T:144:ILE:HG13	2.12	0.49
1:A:89:ILE:O	1:A:93:ILE:HG12	2.13	0.49
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.49
6:F:35:LEU:HB2	6:F:291:GLU:HB2	1.94	0.49
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.49
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.49
7:G:344:GLY:O	7:G:345:LEU:HB2	2.12	0.49
7:G:386:LEU:HD21	7:G:523:VAL:HG11	1.95	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
8:H:70:LEU:HD22	8:H:121:TRP:CZ3	2.48	0.49
14:T:88:LYS:NZ	14:T:96:GLU:H	2.11	0.49
14:T:104:PHE:CZ	14:T:118:ILE:HG21	2.48	0.49
17:X:112:LEU:HD13	17:X:118:VAL:HG22	1.94	0.49
1:A:97:ILE:HG13	1:A:98:LEU:HD22	1.93	0.49
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.48	0.49
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.49
6:F:36:LYS:HB3	6:F:38:GLU:HG2	1.93	0.49
6:F:66:LYS:HG2	6:F:189:SER:HB3	1.95	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
8:H:116:ILE:HA	8:H:211:PHE:HE1	1.75	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.49
10:P:354:ARG:NH2	16:W:56:ASP:OD1	2.45	0.49
14:T:90:TYR:HE2	14:T:92:LYS:HB3	1.78	0.49
1:A:24:LEU:N	1:A:25:PRO:CD	2.76	0.48
2:B:194:CYS:HB2	9:I:153:ILE:O	2.12	0.48
5:E:134:CYS:SG	5:E:139:CYS:SG	3.11	0.48
5:E:227:ALA:H	6:F:284:HIS:HB3	1.76	0.48
7:G:357:LEU:HD13	7:G:627:SER:OG	2.12	0.48
8:H:311:THR:O	8:H:312:ALA:C	2.56	0.48
17:X:69:ASN:O	17:X:70:PHE:C	2.56	0.48
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.48
19:a:37:ARG:CB	19:a:48:MET:HE2	2.43	0.48
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.48
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.48
8:H:179:TRP:CZ3	9:I:62:MET:HE1	2.48	0.48
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.48
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.48
16:W:46:VAL:N	16:W:47:PRO:HD2	2.28	0.48
17:X:44:MET:HE2	18:Z:73:PRO:HA	1.95	0.48
17:X:139:GLU:O	17:X:140:ASN:C	2.55	0.48
22:r:12:ARG:HE	22:r:20:LEU:HD21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.48
5:E:201:GLU:HA	5:E:204:ILE:HD12	1.96	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
10:P:122:HIS:HB3	12:R:46:VAL:CG1	2.43	0.48
10:P:265:PHE:HZ	10:P:338:LEU:HD12	1.78	0.48
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.48
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.48
16:W:103:ARG:O	16:W:104:THR:C	2.55	0.48
1:A:18:ILE:O	1:A:21:ALA:HB3	2.13	0.48
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.48
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.94	0.48
6:F:288:VAL:O	6:F:289:GLU:HB3	2.13	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
8:H:30:TYR:HE1	19:a:1:MET:O	1.87	0.48
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48
2:B:115:ASP:O	2:B:116:ARG:C	2.54	0.48
6:F:116:ASN:O	6:F:245:VAL:HG13	2.13	0.48
6:F:289:GLU:O	6:F:289:GLU:CD	2.56	0.48
7:G:662:THR:HB	13:S:25:GLN:NE2	2.28	0.48
8:H:91:MET:O	8:H:92:PRO:C	2.54	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.95	0.48
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.48
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.78	0.48
23:s:64:ARG:HD2	23:s:64:ARG:N	2.29	0.48
2:B:97:LEU:CD2	4:D:94:VAL:HG11	2.44	0.48
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.77	0.48
3:C:134:LEU:H	3:C:134:LEU:HD12	1.79	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
7:G:32:ILE:N	7:G:43:VAL:O	2.46	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
8:H:85:LEU:HB3	8:H:233:LEU:CD2	2.42	0.48
10:P:66:GLY:O	10:P:67:ARG:C	2.54	0.48
10:P:79:GLN:NE2	10:P:102:GLN:O	2.47	0.48
10:P:197:GLU:HA	10:P:260:GLY:HA2	1.96	0.48
14:T:133:ILE:O	14:T:136:GLU:N	2.46	0.48
16:W:120:ASP:OD1	16:W:121:PHE:N	2.46	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
1:A:84:THR:HG23	20:b:46:ASN:HD21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.44	0.48
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.67	0.48
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.48
6:F:227:PRO:HG3	7:G:94:MET:SD	2.54	0.48
7:G:53:CYS:O	7:G:56:VAL:HG12	2.13	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
7:G:432:ILE:CG2	7:G:451:ILE:HD11	2.39	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
9:I:80:GLU:CB	22:r:26:LEU:HD11	2.43	0.48
10:P:328:MET:O	10:P:330:THR:HG23	2.13	0.48
17:X:17:GLU:HB3	17:X:19:LYS:HG3	1.96	0.48
1:A:4:TYR:CE1	30:H:402:3PE:H282	2.48	0.48
26:B:303:PC1:H132	21:q:29:ARG:HA	1.96	0.48
7:G:66:HIS:HB3	7:G:69:LEU:HB2	1.96	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.48
8:H:64:LEU:H	8:H:64:LEU:CD2	2.24	0.48
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.48	0.48
8:H:130:PHE:O	8:H:134:ARG:HG3	2.14	0.48
30:H:403:3PE:H3E1	30:H:403:3PE:H3I2	1.95	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.48	0.48
10:P:235:THR:HB	10:P:273:LEU:HB2	1.95	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.48
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.48
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.96	0.48
5:E:221:ARG:HH22	6:F:285:PRO:HB2	1.78	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.40	0.48
10:P:360:ARG:HD3	10:P:360:ARG:O	2.14	0.48
16:W:46:VAL:O	16:W:50:VAL:HG23	2.14	0.48
17:X:80:GLU:O	17:X:81:PRO:C	2.56	0.48
21:q:23:LEU:HD11	21:q:33:ILE:HG12	1.96	0.48
2:B:131:MET:HE3	2:B:152:MET:HE2	1.95	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.48
5:E:43:THR:OG1	5:E:44:PRO:CD	2.61	0.48
6:F:146:GLY:HA3	6:F:193:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.49	0.48
8:H:96:ILE:HG12	18:Z:143:TYR:OH	2.14	0.48
8:H:116:ILE:HG13	8:H:117:LEU:H	1.75	0.48
10:P:294:PRO:HB3	10:P:296:PHE:HD1	1.79	0.48
14:T:117:GLU:HG2	16:W:43:TYR:CZ	2.49	0.48
2:B:126:ARG:HB2	2:B:127:GLN:NE2	2.29	0.47
2:B:141:MET:HE1	4:D:86:PRO:CB	2.44	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
10:P:44:GLY:HA2	11:Q:107:TRP:CE3	2.49	0.47
12:R:36:GLN:HG2	21:q:127:TYR:HD2	1.78	0.47
12:R:79:CYS:O	12:R:88:HIS:CE1	2.67	0.47
13:S:50:ASN:O	13:S:51:LEU:C	2.57	0.47
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.96	0.47
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.49	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.47
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.15	0.47
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.47
10:P:97:MET:O	10:P:103:LEU:HD11	2.15	0.47
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.95	0.47
21:q:68:MET:SD	21:q:81:MET:HG2	2.55	0.47
1:A:73:LEU:N	1:A:74:PRO:CD	2.77	0.47
1:A:106:TRP:CZ2	8:H:291:LYS:HA	2.49	0.47
4:D:142:VAL:HG13	4:D:207:ARG:HH12	1.78	0.47
6:F:57:LEU:HD23	6:F:61:ASP:OD1	2.13	0.47
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.48	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
8:H:127:TYR:HD2	8:H:207:LEU:HG	1.78	0.47
10:P:221:ARG:HD2	10:P:286:ARG:HD3	1.91	0.47
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.14	0.47
14:T:117:GLU:HA	14:T:120:MET:CE	2.41	0.47
17:X:133:THR:OG1	17:X:135:ARG:HG2	2.14	0.47
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
6:F:209:GLU:OE2	6:F:230:PRO:HG2	2.15	0.47
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
8:H:20:LEU:HA	19:a:12:MET:SD	2.53	0.47
8:H:210:GLY:HA2	8:H:213:VAL:CG2	2.44	0.47
10:P:157:LYS:HD3	10:P:194:VAL:O	2.14	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.47
2:B:210:ARG:CD	21:q:76:ASP:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:ARG:NH1	4:D:410:TYR:CE1	2.76	0.47
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.78	0.47
4:D:235:ASP:OD2	18:Z:8:GLN:NE2	2.42	0.47
6:F:230:PRO:HA	6:F:233:VAL:O	2.15	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.97	0.47
10:P:304:LEU:O	10:P:307:LEU:HB3	2.14	0.47
10:P:340:VAL:HG13	10:P:340:VAL:O	2.14	0.47
17:X:20:VAL:CG2	17:X:24:VAL:HG21	2.40	0.47
4:D:254:ARG:NH1	22:r:25:GLN:N	2.62	0.47
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.43	0.47
7:G:651:PRO:CD	13:S:56:ARG:HB3	2.45	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.47
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.48	0.47
13:S:58:CYS:HB2	13:S:61:VAL:CG1	2.43	0.47
14:T:119:ILE:HG13	14:T:135:ALA:HB1	1.95	0.47
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.37	0.47
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
5:E:45:GLU:HB3	5:E:91:TRP:HH2	1.78	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
8:H:200:LEU:CD2	8:H:285:LEU:HD13	2.44	0.47
10:P:85:ARG:HE	31:P:401:NDP:C2A	2.27	0.47
10:P:210:GLU:HG3	10:P:210:GLU:O	2.15	0.47
13:S:19:ILE:HD12	13:S:94:VAL:CG1	2.44	0.47
17:X:120:PRO:CB	17:X:125:LEU:CD1	2.91	0.47
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.50	0.47
22:r:12:ARG:HB3	22:r:20:LEU:CD2	2.44	0.47
23:s:49:ASN:HA	23:s:52:LEU:HD12	1.97	0.47
2:B:95:PHE:CE2	2:B:97:LEU:HD11	2.50	0.47
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.47
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.47
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.47
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.47
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.30	0.47
6:F:382:CYS:HA	7:G:74:ASN:O	2.15	0.47
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.47
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.30	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.47
4:D:259:GLU:O	4:D:260:GLU:C	2.55	0.47
5:E:47:ASN:H	5:E:50:THR:HG23	1.79	0.47
5:E:226:PRO:HD2	5:E:230:LEU:HB3	1.97	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
8:H:1:MET:HE3	19:a:29:PHE:CE1	2.50	0.47
15:V:56:LEU:HD12	15:V:57:ASP:CA	2.44	0.47
16:W:32:LYS:O	16:W:36:ARG:HG3	2.15	0.47
17:X:129:THR:HG23	20:b:68:SER:CA	2.44	0.47
19:a:22:SER:O	19:a:23:THR:C	2.57	0.47
20:b:55:VAL:HG13	20:b:56:PRO:HD2	1.97	0.47
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.96	0.47
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.47
2:B:138:THR:HG21	4:D:116:LEU:HA	1.97	0.47
3:C:149:LEU:CD1	16:W:80:ARG:HH21	2.23	0.47
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.47
5:E:135:THR:OG1	5:E:172:GLU:OE2	2.31	0.47
6:F:46:TYR:O	6:F:48:ARG:HG3	2.15	0.47
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.47
7:G:382:ARG:NH1	7:G:386:LEU:HD11	2.30	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.95	0.47
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.47
10:P:209:ARG:O	10:P:210:GLU:HB3	2.15	0.47
11:Q:166:TRP:CZ3	23:s:67:PRO:HG2	2.50	0.47
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.47
15:V:22:GLU:O	15:V:26:ILE:HG12	2.15	0.47
17:X:41:LYS:HB2	17:X:131:VAL:HG11	1.96	0.47
2:B:121:PHE:CB	25:B:302:UQ1:H8	2.35	0.46
4:D:83:ASN:O	4:D:84:PHE:C	2.55	0.46
4:D:198:THR:HG23	8:H:275:ALA:O	2.15	0.46
5:E:141:LEU:HD22	6:F:281:HIS:NE2	2.30	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
8:H:306:SER:OG	20:b:33:PRO:HG3	2.15	0.46
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.96	0.46
14:T:87:LEU:CD2	14:T:104:PHE:CE1	2.94	0.46
17:X:4:ILE:CG2	17:X:5:VAL:N	2.50	0.46
17:X:51:LYS:CE	17:X:142:TYR:HD1	2.28	0.46
17:X:115:LEU:HD13	17:X:117:TRP:CZ2	2.51	0.46
1:A:75:LEU:O	1:A:79:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.46
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.46
7:G:401:LEU:HD12	7:G:474:VAL:HG22	1.96	0.46
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.46
15:V:116:ILE:O	15:V:116:ILE:CG2	2.61	0.46
17:X:35:GLN:HG3	17:X:70:PHE:HE1	1.80	0.46
17:X:53:PRO:HD2	17:X:54:ARG:H	1.80	0.46
18:Z:72:MET:N	18:Z:73:PRO:CD	2.78	0.46
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.46
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.46
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.46
9:I:105:ARG:NH2	12:R:56:ASN:ND2	2.63	0.46
12:R:38:TYR:CD1	12:R:44:ARG:HB2	2.50	0.46
15:V:56:LEU:HD13	15:V:60:LYS:HE2	1.98	0.46
16:W:50:VAL:HA	16:W:55:LEU:HD12	1.97	0.46
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.40	0.46
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.43	0.46
20:b:41:TYR:HD1	20:b:80:TRP:CZ3	2.33	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
4:D:142:VAL:HG21	4:D:185:MET:HG2	1.98	0.46
5:E:45:GLU:CD	5:E:45:GLU:H	2.23	0.46
5:E:154:LYS:HE3	5:E:201:GLU:HB2	1.97	0.46
6:F:168:ASN:ND2	23:s:40:TYR:HE2	2.13	0.46
6:F:278:ILE:CG2	6:F:282:VAL:HG21	2.46	0.46
7:G:140:GLN:HG3	7:G:141:ASP:N	2.30	0.46
7:G:360:LYS:CE	7:G:632:ILE:HB	2.41	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.46
8:H:249:ILE:HG13	19:a:35:GLU:OE2	2.15	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.59	0.46
20:b:28:LEU:O	20:b:32:MET:HG2	2.15	0.46
21:q:76:ASP:OD1	21:q:76:ASP:C	2.57	0.46
22:r:109:ASP:O	22:r:110:GLN:OE1	2.32	0.46
1:A:60:ILE:O	1:A:64:LEU:HG	2.16	0.46
2:B:164:CYS:SG	24:B:301:SF4:S4	3.14	0.46
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.46
4:D:260:GLU:HG2	18:Z:25:LEU:HD22	1.97	0.46
10:P:163:ARG:HH11	10:P:199:ILE:HD11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:328:MET:HB2	10:P:329:PRO:HD2	1.98	0.46
12:R:39:ASP:CG	12:R:40:GLU:N	2.74	0.46
17:X:36:CYS:CB	17:X:66:CYS:HG	2.21	0.46
17:X:135:ARG:HH12	17:X:138:PRO:CD	2.11	0.46
2:B:77:LYS:HD3	2:B:77:LYS:HA	1.64	0.46
2:B:154:GLU:O	10:P:89:TYR:OH	2.33	0.46
4:D:238:LEU:HA	18:Z:9:ASP:HB2	1.97	0.46
6:F:270:ASN:C	6:F:292:MET:HE3	2.40	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.46
9:I:48:VAL:O	20:b:10:LYS:NZ	2.48	0.46
9:I:89:GLU:HG3	21:q:61:TRP:HB3	1.97	0.46
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.46
17:X:49:GLU:HB3	17:X:135:ARG:HH22	1.81	0.46
34:q:201:CDL:OB7	22:r:8:ILE:HD11	2.16	0.46
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.46
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.46
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.46
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.80	0.46
12:R:33:HIS:HE1	12:R:56:ASN:HD22	1.64	0.46
17:X:143:HIS:CG	18:Z:114:THR:HG1	2.33	0.46
1:A:63:LEU:O	1:A:67:LEU:HG	2.15	0.46
1:A:109:LYS:HG2	1:A:112:GLU:HB2	1.98	0.46
2:B:104:MET:HE3	2:B:132:ILE:HD12	1.97	0.46
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.46
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.46
4:D:381:HIS:HE1	9:I:161:ALA:O	1.99	0.46
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.44	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.98	0.46
7:G:401:LEU:HD11	7:G:466:LEU:HD21	1.98	0.46
10:P:157:LYS:O	10:P:160:GLY:N	2.49	0.46
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.46
16:W:45:GLU:O	16:W:46:VAL:C	2.58	0.46
17:X:122:LEU:HD21	20:b:81:LEU:HD23	1.98	0.46
20:b:38:TYR:O	20:b:39:THR:C	2.58	0.46
21:q:86:TRP:HA	21:q:98:PRO:HG2	1.98	0.46
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.46
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.16	0.46
2:B:123:ALA:HB3	8:H:204:GLU:OE2	2.16	0.46
4:D:198:THR:HA	8:H:32:GLN:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
5:E:141:LEU:O	5:E:142:ARG:HB2	2.15	0.46
5:E:204:ILE:O	5:E:208:LYS:HG3	2.16	0.46
5:E:238:LYS:HE2	5:E:242:PHE:CZ	2.51	0.46
6:F:102:MET:HE3	6:F:102:MET:HB2	1.73	0.46
6:F:111:LYS:HG2	6:F:239:PRO:HB2	1.97	0.46
6:F:146:GLY:HA3	6:F:193:PHE:HE2	1.81	0.46
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.46
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.46
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.46
9:I:80:GLU:N	19:a:1:MET:HE1	2.31	0.46
10:P:276:LEU:O	10:P:280:ILE:HG13	2.14	0.46
10:P:285:HIS:CE1	10:P:364:SER:HB3	2.51	0.46
10:P:287:THR:HG23	10:P:289:ILE:HD11	1.97	0.46
14:T:87:LEU:CD2	14:T:122:MET:HE1	2.46	0.46
19:a:58:ASN:HB2	19:a:61:TYR:CE2	2.50	0.46
1:A:52:SER:HB3	1:A:55:PHE:CD2	2.50	0.46
4:D:83:ASN:C	4:D:85:GLY:N	2.69	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.97	0.46
6:F:41:ILE:CD1	6:F:262:PHE:HE1	2.25	0.46
6:F:41:ILE:O	6:F:137:LYS:NZ	2.47	0.46
6:F:81:LYS:HE3	6:F:96:GLY:C	2.41	0.46
7:G:83:GLU:HB2	7:G:101:ASN:HB3	1.98	0.46
7:G:308:ARG:HH11	7:G:580:ALA:H	1.64	0.46
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.46
10:P:169:HIS:ND1	31:P:401:NDP:H5N	2.31	0.46
10:P:334:GLY:O	10:P:337:ASP:HB3	2.15	0.46
23:s:48:LEU:O	23:s:52:LEU:HG	2.15	0.46
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.98	0.45
6:F:86:ARG:HB2	6:F:88:ARG:HH12	1.81	0.45
6:F:213:ILE:HG23	6:F:235:VAL:CA	2.41	0.45
6:F:292:MET:HG2	6:F:293:SER:H	1.80	0.45
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.99	0.45
8:H:274:ARG:HH22	29:H:401:UQ9:C1	2.29	0.45
10:P:95:ARG:HG2	10:P:105:PHE:CE2	2.51	0.45
10:P:170:LEU:HD13	10:P:264:ALA:HB1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:264:ALA:O	10:P:266:THR:HG23	2.17	0.45
12:R:32:THR:HA	12:R:55:VAL:CG2	2.45	0.45
19:a:49:GLU:CD	19:a:52:ARG:HH11	2.22	0.45
21:q:10:GLY:HA2	34:q:201:CDL:CA5	2.46	0.45
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.45
6:F:168:ASN:HD21	23:s:40:TYR:HE2	1.64	0.45
7:G:36:VAL:O	7:G:39:GLN:HG2	2.16	0.45
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.45
8:H:34:ARG:NH2	29:H:401:UQ9:H4M	2.28	0.45
8:H:248:TYR:CD1	8:H:254:LEU:HD23	2.51	0.45
8:H:293:PHE:CE1	30:H:403:3PE:H32	2.52	0.45
10:P:206:ILE:HB	31:P:401:NDP:N7N	2.30	0.45
12:R:39:ASP:H	12:R:42:ASP:CG	2.21	0.45
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.45
21:q:6:VAL:HG13	34:q:201:CDL:CA2	2.47	0.45
21:q:14:VAL:HA	21:q:23:LEU:HD22	1.98	0.45
5:E:134:CYS:SG	5:E:175:CYS:HA	2.55	0.45
6:F:179:ALA:HB3	6:F:181:LEU:HG	1.98	0.45
10:P:207:PHE:CZ	10:P:345:LEU:HA	2.51	0.45
14:T:133:ILE:HG23	14:T:134:ASP:N	2.32	0.45
3:C:243:ALA:C	7:G:105:ASN:ND2	2.75	0.45
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.45
5:E:87:ARG:HD2	23:s:42:THR:HB	1.98	0.45
5:E:184:MET:HG3	5:E:192:TYR:O	2.16	0.45
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.43	0.45
8:H:200:LEU:HD22	8:H:282:TYR:HD1	1.82	0.45
10:P:55:VAL:HA	10:P:79:GLN:O	2.17	0.45
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.45
17:X:53:PRO:CD	17:X:54:ARG:H	2.29	0.45
34:q:201:CDL:OB7	34:q:201:CDL:HB62	2.16	0.45
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.98	0.45
1:A:75:LEU:HB2	8:H:155:LEU:HD21	1.99	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.45
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.45
6:F:69:LEU:HD22	6:F:147:ARG:HB2	1.98	0.45
6:F:154:ALA:HB2	6:F:193:PHE:HZ	1.82	0.45
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.45
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.30	0.45
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:H:403:3PE:H272	30:H:403:3PE:H241	1.56	0.45
10:P:192:ARG:HH11	10:P:197:GLU:HA	1.81	0.45
10:P:208:GLY:N	10:P:211:ASP:OD2	2.49	0.45
2:B:71:ALA:O	2:B:75:VAL:N	2.47	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
6:F:110:PRO:CB	6:F:152:ARG:HH22	2.30	0.45
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.99	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
8:H:250:ASN:OD1	8:H:250:ASN:N	2.49	0.45
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.45
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.45
15:V:56:LEU:HD11	15:V:57:ASP:OD1	2.17	0.45
1:A:4:TYR:CE2	30:H:402:3PE:H231	2.52	0.45
2:B:129:ASP:CG	8:H:54:LYS:HZ1	2.24	0.45
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.26	0.45
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.45
5:E:137:THR:HA	5:E:140:MET:HE2	1.98	0.45
5:E:180:VAL:CG2	6:F:286:CYS:HA	2.46	0.45
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD21	1.99	0.45
7:G:454:ASP:OD1	7:G:459:ARG:NH2	2.50	0.45
8:H:140:ILE:HG13	8:H:141:SER:N	2.32	0.45
8:H:240:ILE:HD11	8:H:259:PHE:CD1	2.51	0.45
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.45
14:T:83:VAL:HG21	14:T:145:VAL:HG22	1.99	0.45
16:W:83:ASP:O	16:W:87:ILE:HG12	2.17	0.45
18:Z:66:GLU:HA	18:Z:69:ILE:CG1	2.46	0.45
4:D:198:THR:OG1	4:D:261:MET:HE1	2.17	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.45
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.45
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.99	0.45
8:H:212:ASN:O	8:H:213:VAL:C	2.60	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
10:P:68:TYR:CZ	10:P:242:VAL:HG11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:227:PRO:HA	10:P:291:TYR:O	2.16	0.45
11:Q:166:TRP:CE3	23:s:67:PRO:HG2	2.51	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.45
14:T:82:ARG:NH2	14:T:126:PHE:HD1	2.15	0.45
19:a:48:MET:HE3	19:a:48:MET:HB2	1.77	0.45
21:q:71:LYS:HB2	21:q:73:THR:HG23	1.98	0.45
2:B:123:ALA:HB2	25:B:302:UQ1:O1	2.17	0.45
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.45
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.45
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.45
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.52	0.45
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.99	0.45
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.31	0.45
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
7:G:381:LEU:HD23	13:S:55:ILE:HG13	1.98	0.45
7:G:401:LEU:HD11	7:G:466:LEU:CD2	2.47	0.45
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
8:H:135:ALA:HB2	8:H:201:THR:HG22	1.98	0.45
9:I:56:ASN:O	9:I:60:ILE:HG13	2.16	0.45
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.45
10:P:315:THR:CG2	10:P:316:LYS:N	2.80	0.45
14:T:90:TYR:O	14:T:91:ASP:HB2	2.17	0.45
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.35	0.45
5:E:180:VAL:HG11	5:E:224:CYS:CB	2.47	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
6:F:268:GLU:CG	6:F:269:ARG:H	2.30	0.45
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.99	0.45
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.45
7:G:432:ILE:HG12	7:G:451:ILE:HD11	1.99	0.45
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.45
10:P:169:HIS:N	10:P:184:LYS:HE3	2.29	0.45
10:P:182:ARG:O	10:P:186:VAL:HG23	2.17	0.45
11:Q:51:GLN:HB3	16:W:26:ARG:HH22	1.82	0.45
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.45
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.44
5:E:128:LYS:HD3	5:E:167:LEU:HG	2.00	0.44
6:F:209:GLU:CD	6:F:230:PRO:HG2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
30:H:403:3PE:H331	9:I:63:TRP:CZ2	2.51	0.44
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.98	0.44
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.52	0.44
4:D:202:TRP:HZ2	9:I:73:THR:HG22	1.82	0.44
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.44
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.44
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.44
5:E:147:ILE:CG2	5:E:200:ILE:HG12	2.37	0.44
6:F:158:ILE:HD13	6:F:166:ALA:HB2	1.98	0.44
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.98	0.44
7:G:163:LYS:HE2	12:R:97:LYS:HZ3	1.82	0.44
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.44
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.44
8:H:305:ILE:O	8:H:308:PRO:HD2	2.17	0.44
10:P:178:SER:O	10:P:182:ARG:HG3	2.17	0.44
17:X:45:LEU:HD23	17:X:135:ARG:HH21	1.82	0.44
17:X:54:ARG:HA	17:X:57:LEU:HG	1.99	0.44
18:Z:68:ARG:O	18:Z:69:ILE:C	2.60	0.44
18:Z:98:MET:HB2	18:Z:104:TRP:CE2	2.52	0.44
19:a:2:TRP:HZ2	34:q:201:CDL:OB7	2.00	0.44
1:A:62:PHE:O	1:A:63:LEU:C	2.60	0.44
1:A:109:LYS:HG2	1:A:109:LYS:O	2.17	0.44
2:B:98:ALA:N	2:B:135:GLY:HA3	2.33	0.44
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.44
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.81	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.18	0.44
5:E:246:ALA:O	5:E:247:GLY:C	2.60	0.44
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.99	0.44
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.44
8:H:288:LEU:O	8:H:293:PHE:N	2.50	0.44
10:P:323:HIS:O	10:P:323:HIS:CG	2.71	0.44
12:R:44:ARG:C	12:R:46:VAL:N	2.73	0.44
13:S:42:VAL:HB	13:S:46:LYS:HE3	1.98	0.44
14:T:119:ILE:CD1	14:T:138:LEU:HD11	2.43	0.44
18:Z:66:GLU:HG3	20:b:50:PRO:HG3	1.98	0.44
22:r:113:LEU:HD12	22:r:113:LEU:HA	1.77	0.44
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.47	0.44
4:D:201:PHE:HB2	8:H:32:GLN:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.53	0.44
6:F:98:LYS:HA	6:F:101:PHE:CE2	2.52	0.44
6:F:234:GLY:HA3	6:F:240:THR:HB	1.98	0.44
7:G:43:VAL:HG12	7:G:55:LYS:CD	2.46	0.44
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.99	0.44
8:H:200:LEU:HD21	8:H:285:LEU:HD13	1.99	0.44
9:I:59:ARG:HA	9:I:64:THR:HG23	1.99	0.44
14:T:92:LYS:O	14:T:92:LYS:HG2	2.16	0.44
17:X:46:CYS:HA	17:X:135:ARG:CZ	2.48	0.44
17:X:57:LEU:HD21	18:Z:84:LEU:HD11	1.98	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.44
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.44
5:E:131:ILE:HD11	5:E:168:PHE:CD2	2.49	0.44
6:F:50:ASP:OD2	6:F:52:ARG:HB2	2.17	0.44
6:F:168:ASN:ND2	23:s:40:TYR:CE2	2.85	0.44
6:F:226:LYS:O	6:F:227:PRO:C	2.60	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.44
7:G:607:LYS:HG2	11:Q:78:ARG:HH11	1.82	0.44
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.44
8:H:264:LEU:HD23	8:H:264:LEU:HA	1.81	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
13:S:20:ARG:HG3	13:S:54:LEU:CB	2.43	0.44
14:T:79:ILE:O	14:T:83:VAL:HG23	2.17	0.44
14:T:109:GLY:O	14:T:110:LEU:C	2.61	0.44
22:r:5:THR:HG22	22:r:5:THR:O	2.18	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.83	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:94:ILE:O	5:E:98:ASN:ND2	2.50	0.44
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.44
6:F:283:ASN:ND2	6:F:306:GLY:H	2.16	0.44
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.44
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.44
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.44
8:H:289:LEU:O	8:H:294:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:32:THR:HG21	21:q:129:THR:HG23	2.00	0.44
14:T:113:LEU:O	14:T:116:VAL:HB	2.17	0.44
16:W:86:VAL:O	16:W:90:LYS:HG3	2.18	0.44
4:D:88:HIS:HE1	8:H:205:SER:O	2.01	0.44
5:E:49:ASP:O	5:E:50:THR:C	2.60	0.44
5:E:81:VAL:O	5:E:82:LEU:C	2.59	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
6:F:47:GLY:C	6:F:49:HIS:H	2.24	0.44
6:F:93:PHE:O	6:F:94:PRO:C	2.59	0.44
7:G:114:GLU:HG3	7:G:148:SER:HB3	2.00	0.44
7:G:346:VAL:O	7:G:521:SER:HB3	2.17	0.44
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.44
30:H:402:3PE:H2I2	30:H:402:3PE:H2E1	2.00	0.44
10:P:96:LEU:C	10:P:96:LEU:HD12	2.43	0.44
10:P:165:ILE:HG12	10:P:199:ILE:HB	1.99	0.44
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.44
13:S:48:HIS:HE1	13:S:95:LEU:CD2	2.25	0.44
1:A:75:LEU:CB	8:H:155:LEU:HD21	2.48	0.44
4:D:201:PHE:CB	8:H:32:GLN:HB3	2.48	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44
5:E:196:THR:O	5:E:197:PRO:C	2.61	0.44
6:F:109:ARG:NE	6:F:239:PRO:HD3	2.33	0.44
6:F:274:LYS:HZ2	6:F:352:ALA:HB3	1.82	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:666:GLN:HE22	13:S:38:VAL:HG13	1.82	0.44
10:P:55:VAL:HG11	10:P:122:HIS:O	2.18	0.44
10:P:163:ARG:NE	10:P:253:THR:HA	2.33	0.44
10:P:246:SER:O	10:P:249:ILE:N	2.51	0.44
10:P:321:ARG:CZ	10:P:321:ARG:HB2	2.48	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.44
16:W:87:ILE:O	16:W:91:MET:HG3	2.18	0.44
19:a:37:ARG:HB2	19:a:48:MET:HE2	2.00	0.44
1:A:81:THR:O	20:b:46:ASN:ND2	2.51	0.44
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.44
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.44
6:F:147:ARG:HD2	6:F:191:TYR:CD1	2.53	0.44
7:G:279:GLU:HG3	11:Q:154:LYS:HG3	2.00	0.44
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.44
7:G:462:PHE:CD2	7:G:466:LEU:HG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
8:H:16:ALA:HB2	19:a:15:CYS:HB2	1.99	0.44
8:H:39:ILE:HG13	21:q:31:ASN:ND2	2.33	0.44
8:H:116:ILE:CG1	8:H:117:LEU:N	2.74	0.44
13:S:51:LEU:CD1	13:S:95:LEU:HD12	2.46	0.44
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.48	0.43
1:A:24:LEU:HD23	1:A:24:LEU:C	2.43	0.43
1:A:49:LEU:HD12	1:A:50:PRO:CD	2.47	0.43
2:B:95:PHE:CE2	2:B:97:LEU:HD21	2.53	0.43
2:B:114:MET:SD	2:B:119:VAL:CG1	3.06	0.43
5:E:235:GLU:HB2	6:F:37:ASP:HB2	2.00	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:306:MET:HA	7:G:316:TYR:HA	1.99	0.43
7:G:355:LYS:HG2	7:G:359:ASN:ND2	2.33	0.43
7:G:651:PRO:HB3	13:S:57:GLU:O	2.18	0.43
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.43
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.99	0.43
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.43
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.43
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.43
18:Z:87:LEU:HD21	18:Z:119:PRO:HG3	2.00	0.43
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.43
4:D:378:LEU:HD23	7:G:126:LEU:HB2	2.00	0.43
6:F:62:TRP:CH2	6:F:140:GLU:HA	2.53	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
8:H:17:MET:HE1	8:H:225:MET:HE3	2.00	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.18	0.43
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.43
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.43
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.43
13:S:23:LEU:HB3	13:S:33:VAL:HG12	2.01	0.43
21:q:74:PHE:HD2	21:q:75:TRP:CD1	2.33	0.43
1:A:105:GLU:HG2	1:A:111:LEU:HB3	1.99	0.43
5:E:63:GLU:O	5:E:64:ALA:C	2.61	0.43
5:E:87:ARG:NH2	6:F:163:TYR:CD1	2.87	0.43
5:E:179:CYS:SG	6:F:123:GLY:HA2	2.58	0.43
7:G:306:MET:HG2	7:G:316:TYR:CA	2.46	0.43
7:G:336:ASN:HB3	7:G:540:ASN:ND2	2.33	0.43
7:G:338:VAL:HA	7:G:544:MET:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:116:ILE:HD12	8:H:135:ALA:HB3	1.99	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
10:P:211:ASP:CG	10:P:214:LEU:HB3	2.43	0.43
13:S:24:CYS:SG	13:S:61:VAL:HG12	2.58	0.43
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.43
15:V:56:LEU:CD1	15:V:57:ASP:OD1	2.67	0.43
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.52	0.43
20:b:82:LYS:HB3	20:b:82:LYS:HE2	1.81	0.43
2:B:70:ARG:HG3	2:B:70:ARG:O	2.18	0.43
2:B:81:LEU:HD23	26:B:303:PC1:H251	2.00	0.43
3:C:85:ILE:HD12	3:C:140:ILE:CD1	2.48	0.43
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.43
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.43
4:D:299:GLN:HB3	22:r:104:TRP:CE3	2.53	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43
7:G:355:LYS:HG3	7:G:366:LEU:HD12	2.00	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
10:P:156:SER:HB2	10:P:161:VAL:CG2	2.47	0.43
10:P:172:ALA:N	10:P:202:ARG:HH21	2.13	0.43
13:S:85:ASP:O	13:S:89:ARG:N	2.41	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.82	0.43
16:W:20:VAL:HG21	16:W:80:ARG:CZ	2.48	0.43
18:Z:28:ARG:O	18:Z:28:ARG:CG	2.64	0.43
1:A:23:TRP:O	1:A:26:GLN:HG3	2.19	0.43
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.88	0.43
2:B:163:SER:HB2	9:I:150:THR:O	2.18	0.43
2:B:192:PRO:HD3	9:I:176:SER:HA	1.99	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
5:E:81:VAL:HB	5:E:104:LEU:HD11	2.00	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.43
6:F:412:LEU:CD2	6:F:435:VAL:HG13	2.48	0.43
7:G:169:VAL:HG11	7:G:231:LEU:HD13	2.00	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.43
7:G:662:THR:HB	13:S:25:GLN:HE21	1.84	0.43
8:H:186:PHE:CE2	30:H:403:3PE:H2B1	2.54	0.43
10:P:310:PHE:O	10:P:311:GLU:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:376:ASN:O	10:P:377:TYR:C	2.61	0.43
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.43
18:Z:10:MET:HE2	18:Z:10:MET:HB3	1.72	0.43
1:A:78:ALA:HA	1:A:81:THR:HG23	2.01	0.43
1:A:105:GLU:O	1:A:110:GLY:N	2.52	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.43
4:D:197:MET:HG3	8:H:32:GLN:NE2	2.33	0.43
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.43
5:E:157:ILE:HG13	5:E:161:GLU:HB3	2.01	0.43
5:E:170:LEU:HD12	5:E:171:ILE:H	1.83	0.43
6:F:88:ARG:HH21	6:F:262:PHE:HZ	1.66	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
7:G:126:LEU:HD13	12:R:89:PRO:HB3	2.01	0.43
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.43
8:H:89:LEU:HG	8:H:90:PRO:HD2	1.99	0.43
12:R:47:ARG:HG3	12:R:48:PHE:N	2.32	0.43
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.43
21:q:129:THR:O	21:q:129:THR:CG2	2.67	0.43
1:A:81:THR:O	1:A:82:ILE:C	2.62	0.43
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.19	0.43
4:D:263:THR:HG23	4:D:264:ASN:OD1	2.18	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
5:E:126:VAL:HG21	5:E:130:HIS:CG	2.53	0.43
5:E:233:LEU:CD2	6:F:40:ARG:HD3	2.48	0.43
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.43
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.43
7:G:347:ASP:O	7:G:351:LEU:HG	2.18	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
10:P:203:PRO:HG2	31:P:401:NDP:C5N	2.48	0.43
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.01	0.43
13:S:30:SER:O	13:S:33:VAL:N	2.51	0.43
16:W:120:ASP:HB3	16:W:123:SER:OG	2.18	0.43
17:X:49:GLU:CG	17:X:138:PRO:HG2	2.39	0.43
19:a:2:TRP:NE1	34:q:201:CDL:OB4	2.51	0.43
22:r:109:ASP:O	22:r:110:GLN:CG	2.64	0.43
2:B:126:ARG:HG3	8:H:213:VAL:O	2.18	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
4:D:339:GLN:HE22	9:I:37:LYS:HZ1	1.64	0.43
5:E:183:PRO:HB2	5:E:195:LEU:N	2.34	0.43
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
8:H:77:LEU:O	8:H:81:LEU:HG	2.19	0.43
8:H:140:ILE:O	8:H:143:GLU:HB3	2.19	0.43
10:P:169:HIS:H	10:P:184:LYS:CE	2.30	0.43
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.43
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.43
17:X:36:CYS:SG	17:X:66:CYS:CB	3.05	0.43
18:Z:129:THR:HG22	18:Z:131:GLU:N	2.33	0.43
3:C:240:ALA:O	3:C:241:PHE:C	2.62	0.43
4:D:92:HIS:HD2	4:D:456:ILE:O	2.02	0.43
4:D:232:VAL:CG2	4:D:356:ILE:HB	2.48	0.43
6:F:64:LYS:O	6:F:68:ILE:HG13	2.19	0.43
6:F:226:LYS:N	6:F:227:PRO:CD	2.82	0.43
7:G:381:LEU:HD23	13:S:55:ILE:CG1	2.49	0.43
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
8:H:54:LYS:CG	8:H:55:LEU:N	2.78	0.43
8:H:157:ASN:ND2	8:H:164:THR:OG1	2.49	0.43
8:H:224:PHE:HD2	29:H:401:UQ9:H20B	1.79	0.43
10:P:73:LEU:HD23	10:P:73:LEU:HA	1.89	0.43
10:P:235:THR:O	10:P:273:LEU:N	2.52	0.43
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.83	0.43
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.43
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.43
18:Z:108:GLU:O	18:Z:109:SER:C	2.61	0.43
20:b:15:LYS:O	20:b:15:LYS:HG3	2.18	0.43
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.43
1:A:61:THR:O	1:A:62:PHE:C	2.62	0.43
2:B:111:ARG:CZ	4:D:208:GLU:HG2	2.49	0.43
2:B:131:MET:HE1	2:B:149:TYR:HB2	2.00	0.43
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.43
4:D:104:GLU:CG	8:H:130:PHE:HZ	2.32	0.43
5:E:180:VAL:HG22	5:E:221:ARG:NH1	2.33	0.43
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.43
7:G:388:ASN:O	7:G:511:LYS:HE2	2.19	0.43
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.43
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.43
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.43
13:S:30:SER:HB3	13:S:63:PRO:HG3	2.00	0.43
14:T:87:LEU:HD11	14:T:141:PRO:HB3	2.01	0.43
4:D:318:VAL:HG21	22:r:104:TRP:CZ3	2.54	0.42
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.42
6:F:128:ARG:HD2	6:F:162:PHE:CE1	2.54	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
10:P:134:TRP:CD1	10:P:134:TRP:O	2.72	0.42
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.42
14:T:130:ILE:CG2	14:T:131:PRO:CD	2.95	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.62	0.42
17:X:10:LEU:H	17:X:10:LEU:HD12	1.84	0.42
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.42
20:b:67:PRO:O	20:b:68:SER:C	2.61	0.42
1:A:68:GLU:O	1:A:71:LEU:N	2.50	0.42
4:D:162:GLN:HB2	4:D:163:PRO:HD2	2.01	0.42
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.42
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.42
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.42
6:F:272:GLY:O	6:F:292:MET:HB2	2.19	0.42
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
9:I:153:ILE:CD1	9:I:155:CYS:HB3	2.38	0.42
9:I:188:GLU:OE2	12:R:56:ASN:HB2	2.19	0.42
10:P:313:TRP:CE3	10:P:314:THR:HB	2.54	0.42
10:P:354:ARG:HG3	10:P:362:LEU:CD2	2.48	0.42
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.42
13:S:16:LEU:HD13	13:S:19:ILE:HD11	2.02	0.42
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.42
16:W:65:LYS:O	16:W:69:MET:HG2	2.19	0.42
17:X:8:PRO:CG	17:X:54:ARG:HG2	2.49	0.42
17:X:47:ARG:NH1	17:X:51:LYS:O	2.52	0.42
18:Z:74:LEU:O	18:Z:78:GLU:HG3	2.20	0.42
19:a:28:LYS:HE3	19:a:35:GLU:HG2	2.01	0.42
21:q:85:GLU:CG	21:q:98:PRO:HB3	2.39	0.42
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.33	0.42
3:C:236:SER:OG	7:G:145:MET:HE1	2.19	0.42
5:E:109:MET:HE1	7:G:198:THR:CG2	2.50	0.42
6:F:120:GLY:O	6:F:121:GLU:C	2.61	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
8:H:200:LEU:CD2	8:H:282:TYR:HA	2.49	0.42
8:H:293:PHE:O	8:H:296:LEU:N	2.52	0.42
10:P:241:TYR:HD2	10:P:243:ALA:HB3	1.84	0.42
12:R:31:ILE:HG22	12:R:55:VAL:HG21	2.02	0.42
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:87:LEU:CD2	14:T:104:PHE:HZ	2.12	0.42
17:X:75:LYS:O	17:X:79:ALA:HB2	2.19	0.42
19:a:55:SER:O	19:a:56:GLY:C	2.61	0.42
1:A:106:TRP:N	1:A:106:TRP:CD1	2.85	0.42
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.43	0.42
2:B:154:GLU:CB	8:H:59:GLU:HB2	2.49	0.42
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.83	0.42
4:D:379:ILE:HG23	7:G:140:GLN:HB2	2.01	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.20	0.42
6:F:65:THR:HA	6:F:68:ILE:HD12	2.01	0.42
6:F:410:ASP:OD1	6:F:410:ASP:C	2.62	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
9:I:50:MET:O	9:I:54:THR:HG23	2.19	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
10:P:223:PHE:O	10:P:224:LEU:C	2.62	0.42
10:P:300:TRP:NE1	10:P:304:LEU:HD21	2.35	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.54	0.42
16:W:61:GLN:O	16:W:64:ASP:HB2	2.19	0.42
4:D:90:ALA:O	4:D:91:ALA:C	2.61	0.42
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.42
5:E:84:LEU:HD12	23:s:46:LEU:CD1	2.49	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
5:E:233:LEU:HB2	6:F:48:ARG:HH12	1.84	0.42
6:F:226:LYS:HA	6:F:226:LYS:HD3	1.86	0.42
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.19	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
9:I:93:LEU:O	21:q:93:MET:CG	2.65	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.42
10:P:247:LYS:NZ	10:P:340:VAL:HG23	2.35	0.42
12:R:45:ARG:HA	12:R:48:PHE:HE1	1.83	0.42
14:T:80:LYS:O	14:T:84:LEU:HG	2.20	0.42
17:X:20:VAL:O	19:a:54:ILE:CD1	2.67	0.42
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.42
4:D:258:VAL:O	4:D:259:GLU:C	2.61	0.42
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.42
5:E:180:VAL:HG11	5:E:224:CYS:HB2	2.02	0.42
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.54	0.42
6:F:295:PRO:O	6:F:296:LEU:C	2.60	0.42
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
13:S:19:ILE:O	13:S:53:ILE:HD12	2.20	0.42
16:W:58:THR:O	16:W:61:GLN:HB3	2.20	0.42
17:X:50:GLU:OE2	17:X:135:ARG:NH1	2.53	0.42
19:a:49:GLU:OE2	19:a:49:GLU:HA	2.20	0.42
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.42
4:D:339:GLN:HE21	9:I:37:LYS:HZ2	1.67	0.42
5:E:62:ILE:HD12	5:E:81:VAL:HG13	2.00	0.42
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.42
5:E:128:LYS:HB3	5:E:167:LEU:CA	2.45	0.42
6:F:81:LYS:HE2	6:F:97:LEU:CD2	2.47	0.42
6:F:110:PRO:O	6:F:238:CYS:HB3	2.20	0.42
6:F:153:ALA:HB1	6:F:194:ASP:O	2.19	0.42
6:F:166:ALA:O	6:F:167:SER:C	2.63	0.42
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.42
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.42
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.53	0.42
8:H:196:ALA:C	8:H:198:PHE:N	2.77	0.42
8:H:287:HIS:O	8:H:291:LYS:N	2.51	0.42
10:P:216:HIS:CD2	10:P:318:LYS:HE3	2.54	0.42
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.42
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	2.01	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
14:T:90:TYR:CD2	14:T:92:LYS:HB3	2.54	0.42
16:W:120:ASP:OD1	16:W:120:ASP:C	2.61	0.42
1:A:55:PHE:CZ	8:H:282:TYR:CE2	2.85	0.42
1:A:98:LEU:HD13	1:A:98:LEU:HA	1.90	0.42
1:A:104:TYR:HA	1:A:107:THR:OG1	2.20	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.20	0.42
4:D:144:MET:HG2	4:D:223:HIS:H	1.85	0.42
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.42
5:E:179:CYS:SG	6:F:123:GLY:CA	3.08	0.42
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.42
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.81	0.42
10:P:207:PHE:HB3	10:P:213:PHE:HD2	1.85	0.42
12:R:54:GLU:HB2	21:q:124:TYR:HD1	1.84	0.42
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.42
2:B:124:SER:HB2	2:B:127:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.42
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.42
6:F:53:LEU:O	6:F:57:LEU:HG	2.20	0.42
6:F:113:LEU:HB3	6:F:154:ALA:CB	2.49	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.20	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
8:H:19:PHE:CB	19:a:12:MET:HG3	2.49	0.42
8:H:25:ARG:NH1	29:H:401:UQ9:H15	2.34	0.42
8:H:203:GLY:O	8:H:205:SER:N	2.49	0.42
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.42
9:I:80:GLU:CG	19:a:1:MET:SD	2.98	0.42
11:Q:167:ASN:C	11:Q:168:LYS:CG	2.93	0.42
13:S:16:LEU:CB	13:S:69:TYR:CD1	2.97	0.42
16:W:117:ARG:HA	16:W:118:PRO:HD3	1.95	0.42
17:X:26:LYS:HD3	17:X:95:GLN:OE1	2.19	0.42
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.42
20:b:41:TYR:CD1	20:b:80:TRP:CZ3	3.08	0.42
22:r:18:GLN:OE1	22:r:18:GLN:N	2.53	0.42
3:C:121:ARG:NH2	15:V:114:TRP:HA	2.35	0.42
5:E:230:LEU:HD13	5:E:232:SER:O	2.19	0.42
6:F:38:GLU:HG3	6:F:39:ASP:OD1	2.20	0.42
6:F:315:LEU:HD23	6:F:315:LEU:O	2.20	0.42
7:G:365:ASN:HB3	7:G:537:ILE:HD11	2.02	0.42
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.42
8:H:8:THR:O	8:H:9:LEU:CB	2.67	0.42
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.42
14:T:87:LEU:CD2	14:T:122:MET:CE	2.98	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42
1:A:49:LEU:HA	1:A:50:PRO:HD3	1.92	0.41
1:A:94:LEU:O	1:A:97:ILE:HG12	2.19	0.41
2:B:84:TRP:HA	2:B:87:ARG:HG2	2.02	0.41
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.48	0.41
3:C:75:VAL:HG13	3:C:83:LEU:HD11	2.02	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.41
4:D:345:GLU:HB2	18:Z:19:ILE:HD12	2.02	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.34	0.41
5:E:47:ASN:CG	5:E:49:ASP:HB3	2.45	0.41
6:F:115:VAL:HG22	6:F:248:VAL:HG21	2.02	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.54	0.41
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.41
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.41
12:R:60:ALA:O	12:R:61:ILE:C	2.63	0.41
14:T:93:ILE:HD11	14:T:118:ILE:HD11	2.00	0.41
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.35	0.41
16:W:101:LYS:HB3	16:W:101:LYS:NZ	2.34	0.41
20:b:31:ILE:O	20:b:32:MET:C	2.63	0.41
21:q:74:PHE:HE2	21:q:75:TRP:HE1	1.68	0.41
2:B:194:CYS:O	24:B:301:SF4:S2	2.78	0.41
5:E:213:PRO:O	5:E:215:PRO:HD3	2.20	0.41
6:F:170:GLN:HG2	23:s:52:LEU:HD11	2.02	0.41
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.41
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.41
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.41
8:H:110:SER:O	8:H:113:VAL:HG12	2.19	0.41
9:I:54:THR:HA	20:b:13:TRP:NE1	2.35	0.41
10:P:208:GLY:O	10:P:211:ASP:N	2.53	0.41
12:R:55:VAL:HG22	12:R:56:ASN:N	2.35	0.41
14:T:115:GLN:O	14:T:116:VAL:C	2.63	0.41
16:W:53:MET:SD	16:W:106:VAL:HG21	2.60	0.41
18:Z:102:PRO:O	18:Z:103:ASN:C	2.62	0.41
19:a:17:VAL:O	19:a:18:ILE:C	2.62	0.41
20:b:35:ILE:O	20:b:35:ILE:CG1	2.67	0.41
2:B:93:MET:HG2	4:D:87:GLN:NE2	2.35	0.41
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.41
6:F:76:ILE:O	6:F:79:GLU:HB2	2.20	0.41
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:253:VAL:O	7:G:253:VAL:CG1	2.68	0.41
8:H:96:ILE:HG23	18:Z:143:TYR:CE1	2.54	0.41
8:H:123:SER:O	8:H:124:ASN:HB2	2.21	0.41
17:X:44:MET:HG3	20:b:53:TYR:OH	2.20	0.41
17:X:70:PHE:CE1	17:X:117:TRP:CZ3	3.08	0.41
20:b:11:ASN:O	20:b:15:LYS:HG2	2.20	0.41
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.03	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
6:F:62:TRP:CE2	6:F:181:LEU:HD13	2.56	0.41
6:F:208:GLU:OE1	6:F:210:THR:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:270:ASN:CG	6:F:338:ASP:HB2	2.46	0.41
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.41
7:G:41:VAL:HG21	7:G:56:VAL:CA	2.51	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
8:H:14:LEU:HD23	8:H:14:LEU:HA	1.86	0.41
8:H:25:ARG:HH11	29:H:401:UQ9:C15	2.34	0.41
8:H:42:PRO:HG3	21:q:28:PHE:HE1	1.85	0.41
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.41
17:X:37:ASP:OD1	17:X:37:ASP:C	2.62	0.41
17:X:137:LEU:HD13	20:b:58:ARG:NE	2.34	0.41
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.41
20:b:15:LYS:O	20:b:16:GLU:HB2	2.20	0.41
21:q:50:GLU:HA	21:q:59:HIS:O	2.20	0.41
22:r:12:ARG:HH21	22:r:20:LEU:CD1	2.33	0.41
1:A:111:LEU:HD23	1:A:112:GLU:H	1.86	0.41
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.01	0.41
3:C:70:LYS:O	15:V:103:LEU:HA	2.21	0.41
3:C:243:ALA:C	7:G:105:ASN:HD21	2.28	0.41
4:D:140:ASP:O	4:D:147:ASN:ND2	2.53	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
5:E:62:ILE:HG21	5:E:103:VAL:HG11	2.01	0.41
7:G:102:ILE:HD12	7:G:102:ILE:N	2.34	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.41
8:H:87:VAL:O	8:H:95:LEU:HB3	2.21	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
9:I:78:PHE:HD1	19:a:2:TRP:CD1	2.37	0.41
10:P:355:ARG:HH11	10:P:356:HIS:HE1	1.66	0.41
17:X:38:LYS:HD2	17:X:38:LYS:HA	1.75	0.41
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.55	0.41
2:B:114:MET:SD	2:B:121:PHE:HD2	2.42	0.41
3:C:72:VAL:O	3:C:72:VAL:HG23	2.20	0.41
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.19	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.03	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
8:H:306:SER:O	8:H:307:LEU:C	2.63	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41
13:S:20:ARG:HD2	13:S:22:HIS:NE2	2.35	0.41
17:X:70:PHE:O	17:X:74:ILE:HG13	2.21	0.41
20:b:16:GLU:N	20:b:17:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:O	1:A:21:ALA:C	2.62	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
4:D:301:ASP:N	22:r:104:TRP:HH2	2.18	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
6:F:274:LYS:HB3	6:F:276:PHE:CZ	2.56	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.41
7:G:309:ASN:CG	7:G:310:GLU:H	2.29	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.51	0.41
8:H:283:ASP:OD1	8:H:284:GLN:N	2.54	0.41
8:H:288:LEU:HD23	8:H:288:LEU:C	2.45	0.41
10:P:212:ARG:O	10:P:213:PHE:C	2.61	0.41
10:P:263:PHE:CD1	10:P:333:PRO:HB2	2.49	0.41
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.85	0.41
15:V:98:LYS:HG2	15:V:100:TRP:CZ2	2.55	0.41
16:W:78:ASP:HB3	16:W:81:VAL:HG23	2.03	0.41
20:b:53:TYR:CE2	20:b:55:VAL:HA	2.56	0.41
21:q:132:LYS:HE2	21:q:135:HIS:HA	2.01	0.41
5:E:71:GLU:HB3	23:s:60:PRO:O	2.21	0.41
6:F:225:LEU:HD13	11:Q:160:TYR:CZ	2.56	0.41
6:F:265:PHE:HB3	6:F:291:GLU:CG	2.51	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
7:G:277:MET:HE1	11:Q:153:PRO:HD3	2.03	0.41
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.41
7:G:649:VAL:HA	13:S:20:ARG:NH1	2.36	0.41
7:G:651:PRO:HG3	13:S:57:GLU:N	2.29	0.41
10:P:170:LEU:O	10:P:171:ASN:C	2.62	0.41
10:P:293:LEU:HD12	10:P:294:PRO:HD2	2.01	0.41
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.41
17:X:23:ALA:HB2	17:X:95:GLN:HE22	1.82	0.41
20:b:11:ASN:CG	20:b:15:LYS:HE3	2.46	0.41
34:q:201:CDL:H112	34:q:201:CDL:H312	2.02	0.41
1:A:16:THR:O	1:A:20:VAL:HG23	2.21	0.41
2:B:224:ARG:HG3	10:P:85:ARG:HH22	1.85	0.41
4:D:104:GLU:HG3	8:H:130:PHE:CZ	2.56	0.41
4:D:119:GLY:O	4:D:123:LEU:HD23	2.21	0.41
4:D:198:THR:N	4:D:199:PRO:CD	2.84	0.41
6:F:47:GLY:O	6:F:48:ARG:HB2	2.21	0.41
6:F:102:MET:O	6:F:102:MET:HG3	2.21	0.41
6:F:210:THR:HG23	6:F:226:LYS:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:280:GLY:O	6:F:281:HIS:C	2.63	0.41
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.35	0.41
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.41
7:G:48:THR:O	7:G:49:VAL:C	2.63	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:388:ASN:N	7:G:514:ASN:CB	2.83	0.41
7:G:404:GLY:HA3	7:G:684:LEU:CD1	2.34	0.41
7:G:404:GLY:HA2	7:G:684:LEU:HD11	2.00	0.41
8:H:95:LEU:HG	8:H:96:ILE:HG13	2.03	0.41
8:H:136:VAL:HG13	8:H:137:ALA:N	2.35	0.41
30:H:403:3PE:H122	9:I:60:ILE:HG21	2.03	0.41
9:I:36:TYR:CZ	22:r:106:LEU:HD23	2.56	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.55	0.41
9:I:162:CYS:SG	24:I:303:SF4:S3	3.18	0.41
10:P:61:ALA:HA	10:P:66:GLY:HA3	2.02	0.41
10:P:93:HIS:O	10:P:96:LEU:HG	2.21	0.41
10:P:146:VAL:HG13	10:P:147:ASN:OD1	2.21	0.41
10:P:201:ILE:HD13	10:P:265:PHE:CZ	2.55	0.41
11:Q:85:ASN:C	11:Q:87:MET:N	2.76	0.41
11:Q:166:TRP:O	11:Q:167:ASN:C	2.64	0.41
14:T:100:VAL:O	14:T:141:PRO:HD2	2.20	0.41
14:T:123:GLU:HG2	14:T:130:ILE:HD12	2.02	0.41
14:T:140:CYS:HB2	14:T:143:GLU:HB2	2.02	0.41
18:Z:19:ILE:HG22	18:Z:20:ASP:N	2.36	0.41
21:q:5:GLU:HG2	21:q:9:ARG:HE	1.85	0.41
1:A:1:MET:O	1:A:2:ASN:C	2.64	0.41
1:A:65:PHE:O	1:A:69:ILE:HG13	2.20	0.41
4:D:90:ALA:HB2	8:H:205:SER:O	2.21	0.41
4:D:235:ASP:OD2	18:Z:8:GLN:HG3	2.21	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
5:E:190:ASN:HD22	5:E:192:TYR:HE1	1.69	0.41
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.56	0.41
6:F:297:LYS:HG3	6:F:301:GLU:CG	2.51	0.41
7:G:47:THR:HG23	7:G:51:GLN:HB2	2.03	0.41
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.86	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
10:P:198:ALA:O	10:P:199:ILE:C	2.61	0.41
17:X:137:LEU:HD12	17:X:138:PRO:HD2	2.03	0.41
18:Z:90:ASN:O	18:Z:94:GLU:HB2	2.21	0.41
23:s:66:SER:O	23:s:67:PRO:C	2.63	0.41
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.40
4:D:106:VAL:N	4:D:442:HIS:O	2.41	0.40
4:D:181:LEU:HD21	4:D:210:MET:CB	2.51	0.40
4:D:375:MET:HG2	7:G:121:LEU:HD22	2.02	0.40
6:F:76:ILE:O	6:F:80:MET:HG2	2.21	0.40
6:F:127:ASP:O	6:F:128:ARG:C	2.65	0.40
6:F:171:VAL:HG13	6:F:174:ARG:HH22	1.86	0.40
6:F:225:LEU:HB2	11:Q:160:TYR:HE2	1.75	0.40
6:F:294:VAL:HA	6:F:295:PRO:HD3	1.84	0.40
6:F:296:LEU:HB2	6:F:337:MET:HE3	2.03	0.40
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.40
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.54	0.40
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.49	0.40
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.40
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.86	0.40
30:H:403:3PE:N	20:b:18:VAL:HG23	2.36	0.40
13:S:22:HIS:CD2	13:S:66:TRP:HD1	2.39	0.40
17:X:130:LYS:NZ	20:b:63:MET:O	2.53	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.40
4:D:213:PHE:O	4:D:214:TYR:C	2.64	0.40
4:D:269:ARG:O	4:D:273:VAL:HG23	2.21	0.40
4:D:310:VAL:C	4:D:312:ASP:H	2.29	0.40
6:F:81:LYS:HD3	6:F:96:GLY:HA3	2.04	0.40
7:G:36:VAL:O	7:G:37:ASP:HB2	2.22	0.40
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.40
7:G:598:ASN:ND2	7:G:600:GLU:OE2	2.51	0.40
26:I:301:PC1:H112	18:Z:29:GLY:HA3	2.02	0.40
10:P:163:ARG:NH1	10:P:199:ILE:HD11	2.36	0.40
11:Q:57:GLU:O	11:Q:58:LYS:C	2.65	0.40
12:R:48:PHE:CD2	12:R:53:LYS:HB2	2.56	0.40
16:W:124:LYS:HE3	16:W:124:LYS:HB2	1.86	0.40
20:b:69:HIS:CD2	20:b:71:GLN:H	2.39	0.40
1:A:88:MET:HG3	1:A:92:PHE:CE2	2.56	0.40
3:C:55:LYS:HB3	3:C:55:LYS:HE2	1.83	0.40
5:E:68:ASN:OD1	23:s:56:ARG:NH1	2.54	0.40
5:E:139:CYS:HB3	5:E:144:SER:HB3	2.03	0.40
6:F:315:LEU:HA	6:F:359:ARG:CZ	2.52	0.40
7:G:64:CYS:SG	7:G:75:CYS:SG	3.14	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:160:VAL:CG1	7:G:161:GLU:N	2.83	0.40
7:G:169:VAL:HG12	7:G:231:LEU:HB2	2.03	0.40
7:G:283:GLU:O	7:G:283:GLU:CG	2.50	0.40
8:H:210:GLY:CA	8:H:213:VAL:HG23	2.50	0.40
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.80	0.40
9:I:201:ILE:O	9:I:205:ILE:HG12	2.21	0.40
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.40
13:S:36:PHE:HZ	13:S:44:LEU:CD1	2.26	0.40
13:S:59:SER:O	13:S:60:GLU:C	2.63	0.40
14:T:87:LEU:HD11	14:T:141:PRO:HG3	2.03	0.40
19:a:12:MET:HE2	19:a:12:MET:HB3	1.90	0.40
22:r:20:LEU:C	22:r:20:LEU:CD1	2.89	0.40
22:r:24:LEU:HD23	22:r:24:LEU:HA	1.85	0.40
23:s:44:THR:O	23:s:48:LEU:HG	2.21	0.40
1:A:55:PHE:HZ	8:H:282:TYR:HE2	1.56	0.40
2:B:106:HIS:O	2:B:109:ALA:HB3	2.22	0.40
2:B:114:MET:HG3	2:B:115:ASP:N	2.36	0.40
2:B:116:ARG:HG3	8:H:38:ASN:H	1.85	0.40
6:F:185:ASN:HA	6:F:189:SER:O	2.21	0.40
6:F:225:LEU:N	11:Q:160:TYR:HE2	2.16	0.40
6:F:335:VAL:HG12	6:F:336:LEU:N	2.36	0.40
8:H:130:PHE:CZ	8:H:134:ARG:HD3	2.56	0.40
8:H:293:PHE:O	8:H:294:LEU:C	2.63	0.40
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.40
10:P:54:VAL:O	10:P:78:SER:HB3	2.21	0.40
10:P:120:VAL:O	10:P:121:GLN:C	2.64	0.40
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.50	0.40
15:V:96:LYS:HE2	15:V:96:LYS:HB2	1.95	0.40
16:W:86:VAL:O	16:W:87:ILE:C	2.62	0.40
17:X:117:TRP:CD1	17:X:117:TRP:N	2.87	0.40
19:a:9:LEU:O	19:a:10:ALA:C	2.64	0.40
19:a:49:GLU:O	19:a:50:ARG:C	2.62	0.40
3:C:49:ARG:NH2	3:C:79:CYS:HA	2.36	0.40
3:C:234:LEU:O	4:D:387:GLU:HG3	2.22	0.40
3:C:241:PHE:O	3:C:242:PRO:C	2.62	0.40
4:D:116:LEU:O	4:D:118:ARG:HG3	2.22	0.40
4:D:128:THR:HG22	4:D:131:GLN:CG	2.52	0.40
4:D:158:LEU:O	4:D:392:PRO:HG2	2.21	0.40
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.54	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:272:ARG:NH2	11:Q:87:MET:HE3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:462:PHE:HD2	7:G:466:LEU:HG	1.86	0.40
8:H:187:ILE:CD1	30:H:403:3PE:H242	2.42	0.40
8:H:204:GLU:HA	8:H:204:GLU:OE1	2.22	0.40
30:H:403:3PE:O21	9:I:63:TRP:NE1	2.54	0.40
9:I:92:PRO:HB3	21:q:92:CYS:HB2	2.04	0.40
10:P:105:PHE:C	10:P:106:LEU:HD12	2.47	0.40
10:P:300:TRP:CE2	10:P:304:LEU:HD21	2.57	0.40
13:S:45:LYS:O	13:S:46:LYS:C	2.64	0.40
17:X:16:GLU:CD	17:X:68:LEU:HD13	2.46	0.40
17:X:38:LYS:O	17:X:42:GLU:HG3	2.22	0.40
17:X:60:GLY:O	17:X:63:VAL:HB	2.22	0.40
21:q:3:LEU:HD13	34:q:201:CDL:C51	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	87/115 (76%)	83 (95%)	4 (5%)	0	100	100
2	B	154/224 (69%)	142 (92%)	11 (7%)	1 (1%)	21	56
3	C	196/263 (74%)	187 (95%)	9 (5%)	0	100	100
4	D	383/463 (83%)	356 (93%)	27 (7%)	0	100	100
5	E	208/248 (84%)	193 (93%)	15 (7%)	0	100	100
6	F	422/464 (91%)	403 (96%)	19 (4%)	0	100	100
7	G	685/727 (94%)	632 (92%)	53 (8%)	0	100	100
8	H	313/318 (98%)	295 (94%)	18 (6%)	0	100	100
9	I	169/212 (80%)	169 (100%)	0	0	100	100
10	P	337/377 (89%)	314 (93%)	23 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	75 (93%)	6 (7%)	0	100	100
13	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
14	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
15	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
16	W	112/131 (86%)	111 (99%)	1 (1%)	0	100	100
17	X	140/172 (81%)	129 (92%)	11 (8%)	0	100	100
18	Z	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
19	a	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
20	b	77/84 (92%)	69 (90%)	8 (10%)	0	100	100
21	q	118/145 (81%)	115 (98%)	3 (2%)	0	100	100
22	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
23	s	27/104 (26%)	27 (100%)	0	0	100	100
All	All	4138/5036 (82%)	3906 (94%)	231 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	195	PRO

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 PDB entries followed by that with respect to all EM entries.

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	83/104 (80%)	83 (100%)	0	100	100
2	B	132/185 (71%)	131 (99%)	1 (1%)	73	82
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	332/395 (84%)	332 (100%)	0	100	100
5	E	182/206 (88%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	340/370 (92%)	340 (100%)	0	100 100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87 89
8	H	279/280 (100%)	278 (100%)	1 (0%)	84 86
9	I	147/178 (83%)	147 (100%)	0	100 100
10	P	296/325 (91%)	296 (100%)	0	100 100
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68 80
12	R	70/96 (73%)	69 (99%)	1 (1%)	59 77
13	S	74/80 (92%)	73 (99%)	1 (1%)	59 77
14	T	69/135 (51%)	68 (99%)	1 (1%)	59 77
15	V	100/102 (98%)	100 (100%)	0	100 100
16	W	108/114 (95%)	108 (100%)	0	100 100
17	X	129/154 (84%)	129 (100%)	0	100 100
18	Z	120/123 (98%)	119 (99%)	1 (1%)	73 82
19	a	57/60 (95%)	57 (100%)	0	100 100
20	b	70/73 (96%)	70 (100%)	0	100 100
21	q	110/131 (84%)	110 (100%)	0	100 100
22	r	44/96 (46%)	44 (100%)	0	100 100
23	s	28/95 (30%)	28 (100%)	0	100 100
All	All	3634/4292 (85%)	3626 (100%)	8 (0%)	85 89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	120	VAL
7	G	271	MET
8	H	250	ASN
11	Q	96	LYS
12	R	64	ILE
13	S	68	ARG
14	T	103	HIS
18	Z	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	106	HIS
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	54	HIS
3	C	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	88	HIS
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	245	GLN
6	F	168	ASN
6	F	270	ASN
6	F	283	ASN
6	F	303	HIS
6	F	346	GLN
7	G	59	GLN
7	G	74	ASN
7	G	105	ASN
7	G	164	ASN
7	G	205	GLN
7	G	359	ASN
7	G	388	ASN
7	G	495	ASN
7	G	498	GLN
7	G	540	ASN
7	G	569	GLN
7	G	571	HIS
7	G	605	GLN

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Mol	Chain	Res	Type
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	124	ASN
8	H	138	GLN
8	H	163	GLN
8	H	169	GLN
8	H	258	ASN
8	H	292	ASN
10	P	71	ASN
10	P	79	GLN
10	P	154	GLN
10	P	166	HIS
10	P	219	ASN
10	P	238	GLN
10	P	269	ASN
10	P	275	HIS
10	P	341	GLN
10	P	356	HIS
11	Q	51	GLN
11	Q	88	GLN
12	R	52	GLN
12	R	56	ASN
15	V	41	HIS
15	V	50	GLN
16	W	54	GLN
16	W	94	GLN
17	X	30	HIS
17	X	77	HIS
18	Z	76	GLN
19	a	31	ASN
20	b	69	HIS
20	b	71	GLN
20	b	83	ASN
21	q	13	GLN
21	q	31	ASN
21	q	52	ASN
21	q	54	GLN
21	q	87	HIS

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Mol	Chain	Res	Type
21	q	91	HIS
22	r	21	GLN
22	r	110	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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	$\#\|Z\| > 2$
30	3PE	H	402	-	45,45,50	0.97	2 (4%)	48,50,55	0.97	2 (4%)
27	FES	G	803	7	0,4,4	-	-	-		
28	FMN	F	501	-	33,33,33	1.39	5 (15%)	48,50,50	1.23	7 (14%)
29	UQ9	H	401	-	35,35,58	0.79	2 (5%)	42,45,73	0.50	0
31	NDP	P	401	-	49,52,52	1.21	5 (10%)	66,80,80	1.67	11 (16%)
24	SF4	B	301	2	0,12,12	-	-	-		
25	UQ1	B	302	-	18,18,18	2.00	2 (11%)	22,25,25	1.18	3 (13%)
24	SF4	G	801	7	0,12,12	-	-	-		
30	3PE	H	403	-	50,50,50	0.91	2 (4%)	53,55,55	1.01	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	SF4	I	303	9	0,12,12	-	-	-		
33	EHZ	W	201	-	27,31,37	1.89	7 (25%)	37,41,47	1.86	11 (29%)
34	CDL	q	201	-	56,56,99	1.21	4 (7%)	62,68,111	1.21	5 (8%)
24	SF4	G	802	7	0,12,12	-	-	-		
24	SF4	F	502	6	0,12,12	-	-	-		
26	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.16	4 (10%)
26	PC1	I	301	-	42,42,53	1.04	2 (4%)	48,50,61	1.04	3 (6%)
27	FES	E	301	5	0,4,4	-	-	-		
24	SF4	I	302	9	0,12,12	-	-	-		

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
27	FES	G	803	7	-	-	0/1/1/1
30	3PE	H	402	-	-	13/49/49/54	-
29	UQ9	H	401	-	-	17/30/54/81	0/1/1/1
28	FMN	F	501	-	-	1/18/18/18	0/3/3/3
31	NDP	P	401	-	-	4/34/77/77	0/5/5/5
34	CDL	q	201	-	-	20/67/67/110	-
30	3PE	H	403	-	-	11/54/54/54	-
33	EHZ	W	201	-	-	21/39/39/45	-
24	SF4	B	301	2	-	-	0/6/5/5
24	SF4	G	801	7	-	-	0/6/5/5
24	SF4	F	502	6	-	-	0/6/5/5
24	SF4	I	303	9	-	-	0/6/5/5
24	SF4	G	802	7	-	-	0/6/5/5
25	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
26	PC1	B	303	-	-	11/38/38/57	-
26	PC1	I	301	-	-	9/46/46/57	-
27	FES	E	301	5	-	-	0/1/1/1
24	SF4	I	302	9	-	-	0/6/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	302	UQ1	C6-C5	7.58	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	W	201	EHZ	C15-N2	5.39	1.45	1.33
33	W	201	EHZ	C12-N1	5.18	1.45	1.33
28	F	501	FMN	C9A-C5A	4.92	1.49	1.41
31	P	401	NDP	C5A-C4A	4.32	1.47	1.39
34	q	201	CDL	OA8-CA7	4.27	1.45	1.33
34	q	201	CDL	OB8-CB7	4.26	1.45	1.33
26	I	301	PC1	O31-C31	4.25	1.45	1.33
26	B	303	PC1	O31-C31	4.23	1.45	1.33
30	H	403	3PE	O31-C31	4.20	1.45	1.33
30	H	402	3PE	O31-C31	4.19	1.45	1.33
30	H	402	3PE	O21-C21	4.09	1.45	1.34
34	q	201	CDL	OB6-CB5	4.07	1.45	1.34
30	H	403	3PE	O21-C21	4.06	1.45	1.34
26	I	301	PC1	O21-C21	4.04	1.45	1.34
26	B	303	PC1	O21-C21	4.04	1.45	1.34
34	q	201	CDL	OA6-CA5	4.03	1.45	1.34
31	P	401	NDP	C6N-C5N	3.26	1.39	1.33
28	F	501	FMN	C8-C7	3.15	1.48	1.40
25	B	302	UQ1	C3-C2	3.05	1.48	1.36
29	H	401	UQ9	C3-C2	-2.69	1.41	1.48
31	P	401	NDP	C5A-C6A	2.67	1.48	1.41
33	W	201	EHZ	P1-O7	2.57	1.64	1.54
28	F	501	FMN	C4-N3	-2.52	1.34	1.38
29	H	401	UQ9	C4-C5	-2.49	1.41	1.48
33	W	201	EHZ	O4-C15	-2.45	1.18	1.23
31	P	401	NDP	C8A-N7A	2.45	1.36	1.31
33	W	201	EHZ	O3-C12	-2.42	1.18	1.23
33	W	201	EHZ	C9-S1	2.38	1.81	1.76
31	P	401	NDP	C5A-N7A	-2.24	1.34	1.39
33	W	201	EHZ	P1-OP3	-2.24	1.46	1.54
28	F	501	FMN	C5A-N5	-2.20	1.35	1.39
28	F	501	FMN	C4A-N5	2.14	1.34	1.30

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	W	201	EHZ	C8-C9-S1	6.35	121.48	113.63
31	P	401	NDP	C5A-C4A-N3A	-6.08	118.82	126.75
31	P	401	NDP	N3A-C4A-N9A	4.71	134.85	127.08
26	B	303	PC1	O21-C21-C22	4.24	120.65	111.50
26	I	301	PC1	O21-C21-C22	3.92	119.95	111.50
34	q	201	CDL	OB6-CB5-C51	3.86	119.82	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	q	201	CDL	OA6-CA5-C11	3.85	119.80	111.50
31	P	401	NDP	C2A-N3A-C4A	3.84	120.83	111.75
30	H	402	3PE	O21-C21-C22	3.62	119.31	111.50
31	P	401	NDP	PN-O3-PA	-3.42	121.08	132.83
31	P	401	NDP	C4A-C5A-N7A	-3.39	106.49	110.62
30	H	403	3PE	O21-C21-C22	3.36	118.74	111.50
31	P	401	NDP	N3A-C2A-N1A	-3.14	123.70	128.60
33	W	201	EHZ	C13-C12-N1	3.09	121.62	116.42
33	W	201	EHZ	C14-C13-C12	-3.04	107.29	112.36
31	P	401	NDP	C5A-N7A-C8A	2.91	107.64	103.51
31	P	401	NDP	C4A-N9A-C8A	2.91	108.88	105.73
33	W	201	EHZ	OP3-P1-O9	-2.90	99.31	110.68
33	W	201	EHZ	C7-C8-C9	-2.86	107.36	113.89
34	q	201	CDL	OB8-CB7-C71	2.73	120.46	111.91
30	H	403	3PE	O31-C31-C32	2.68	120.32	111.91
26	I	301	PC1	C2-O21-C21	-2.65	111.28	117.79
28	F	501	FMN	O4-C4-C4A	-2.64	119.60	126.60
28	F	501	FMN	C4A-C10-N1	-2.64	118.61	124.73
30	H	402	3PE	O31-C31-C32	2.59	120.05	111.91
26	I	301	PC1	O31-C31-C32	2.50	119.75	111.91
25	B	302	UQ1	C11-C9-C10	2.49	120.10	114.60
34	q	201	CDL	OA8-CA7-C31	2.49	119.72	111.91
25	B	302	UQ1	CM5-C5-C6	-2.43	120.44	124.40
26	B	303	PC1	O31-C31-C32	2.41	119.48	111.91
31	P	401	NDP	N9A-C8A-N7A	-2.38	110.66	113.91
33	W	201	EHZ	C5-C6-C7	-2.37	108.03	114.85
31	P	401	NDP	C6A-C5A-N7A	2.30	136.30	132.02
26	B	303	PC1	C2-O21-C21	-2.28	112.18	117.79
33	W	201	EHZ	C10-S1-C9	2.27	108.94	101.87
34	q	201	CDL	CA4-OA6-CA5	-2.27	112.21	117.79
28	F	501	FMN	C4-C4A-N5	2.21	121.38	118.23
28	F	501	FMN	C10-N1-C2	2.20	121.29	116.90
33	W	201	EHZ	C11-N1-C12	-2.17	118.81	122.84
33	W	201	EHZ	O2-C9-S1	-2.13	119.84	122.61
33	W	201	EHZ	O6-P1-O9	2.12	112.43	106.47
33	W	201	EHZ	O3-C12-N1	-2.12	119.01	123.01
28	F	501	FMN	C4A-C4-N3	2.11	118.54	113.19
28	F	501	FMN	O2-C2-N1	-2.09	118.37	121.83
31	P	401	NDP	C3D-C2D-C1D	2.08	105.38	101.43
26	B	303	PC1	O21-C21-O22	-2.03	118.80	123.70
25	B	302	UQ1	C7-C8-C9	-2.01	120.95	127.26
28	F	501	FMN	C4-N3-C2	-2.00	121.94	125.64

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	B	303	PC1	C1-O11-P-O12
26	B	303	PC1	C1-O11-P-O14
26	B	303	PC1	C1-O11-P-O13
26	B	303	PC1	O22-C21-O21-C2
29	H	401	UQ9	C17-C18-C19-C21
29	H	401	UQ9	C17-C18-C19-C20
29	H	401	UQ9	C12-C13-C14-C16
29	H	401	UQ9	C12-C13-C14-C15
29	H	401	UQ9	C9-C11-C12-C13
29	H	401	UQ9	C7-C8-C9-C11
29	H	401	UQ9	C7-C8-C9-C10
29	H	401	UQ9	C6-C7-C8-C9
30	H	402	3PE	C1-O11-P-O12
30	H	402	3PE	C1-O11-P-O14
30	H	402	3PE	C11-O13-P-O12
30	H	402	3PE	C11-O13-P-O14
30	H	402	3PE	O32-C31-O31-C3
30	H	402	3PE	C32-C31-O31-C3
30	H	403	3PE	C1-O11-P-O12
30	H	403	3PE	C1-O11-P-O13
30	H	403	3PE	C1-O11-P-O14
30	H	403	3PE	C11-O13-P-O14
31	P	401	NDP	C2B-O2B-P2B-O2X
31	P	401	NDP	C2N-C3N-C7N-N7N
33	W	201	EHZ	O1-C7-C8-C9
33	W	201	EHZ	C6-C7-C8-C9
33	W	201	EHZ	C7-C8-C9-S1
33	W	201	EHZ	S1-C10-C11-N1
33	W	201	EHZ	C11-C10-S1-C9
33	W	201	EHZ	C16-C17-C20-O6
33	W	201	EHZ	C20-O6-P1-O7
33	W	201	EHZ	C20-O6-P1-O9
33	W	201	EHZ	C20-O6-P1-OP3
34	q	201	CDL	CA2-OA2-PA1-OA3
34	q	201	CDL	OA7-CA5-OA6-CA4
34	q	201	CDL	C11-CA5-OA6-CA4
34	q	201	CDL	CB2-OB2-PB2-OB3
34	q	201	CDL	CB2-OB2-PB2-OB4
34	q	201	CDL	CB2-OB2-PB2-OB5
34	q	201	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
34	q	201	CDL	CB3-OB5-PB2-OB4
26	I	301	PC1	O22-C21-O21-C2
26	B	303	PC1	C22-C21-O21-C2
26	I	301	PC1	C22-C21-O21-C2
30	H	402	3PE	C22-C21-O21-C2
29	H	401	UQ9	C25-C24-C26-C27
29	H	401	UQ9	C23-C24-C26-C27
29	H	401	UQ9	C14-C16-C17-C18
30	H	403	3PE	C32-C31-O31-C3
34	q	201	CDL	C31-CA7-OA8-CA6
30	H	403	3PE	O32-C31-O31-C3
30	H	402	3PE	O22-C21-O21-C2
34	q	201	CDL	C51-CB5-OB6-CB4
34	q	201	CDL	OA9-CA7-OA8-CA6
34	q	201	CDL	OB7-CB5-OB6-CB4
26	I	301	PC1	C32-C31-O31-C3
30	H	402	3PE	C1-O11-P-O13
30	H	402	3PE	C11-O13-P-O11
30	H	403	3PE	C11-O13-P-O11
34	q	201	CDL	CA3-OA5-PA1-OA2
34	q	201	CDL	CB6-CB4-OB6-CB5
26	I	301	PC1	O32-C31-O31-C3
26	B	303	PC1	C32-C33-C34-C35
26	B	303	PC1	C23-C24-C25-C26
29	H	401	UQ9	C15-C14-C16-C17
29	H	401	UQ9	C13-C14-C16-C17
29	H	401	UQ9	C12-C11-C9-C8
29	H	401	UQ9	C12-C11-C9-C10
30	H	402	3PE	C31-C32-C33-C34
34	q	201	CDL	CA2-OA2-PA1-OA5
30	H	402	3PE	C2E-C2F-C2G-C2H
30	H	402	3PE	C3-C2-O21-C21
30	H	403	3PE	C3E-C3F-C3G-C3H
33	W	201	EHZ	N2-C15-C16-C17
30	H	403	3PE	C37-C38-C39-C3A
33	W	201	EHZ	C3-C4-C5-C6
33	W	201	EHZ	C5-C6-C7-O1
33	W	201	EHZ	O2-C9-S1-C10
31	P	401	NDP	PN-O3-PA-O2A
31	P	401	NDP	O4D-C1D-N1N-C6N
34	q	201	CDL	C1-CA2-OA2-PA1
26	I	301	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
26	I	301	PC1	C11-C12-N-C15
30	H	403	3PE	C11-O13-P-O12
34	q	201	CDL	CA3-OA5-PA1-OA3
34	q	201	CDL	CB3-OB5-PB2-OB3
33	W	201	EHZ	O4-C15-C16-O5
33	W	201	EHZ	C19-C17-C20-O6
28	F	501	FMN	C5'-O5'-P-O1P
26	I	301	PC1	C1-O11-P-O13
33	W	201	EHZ	C2-C3-C4-C5
29	H	401	UQ9	C20-C19-C21-C22
30	H	403	3PE	C24-C25-C26-C27
29	H	401	UQ9	C18-C19-C21-C22
26	B	303	PC1	C1-C2-C3-O31
26	I	301	PC1	C11-C12-N-C14
26	I	301	PC1	C32-C33-C34-C35
34	q	201	CDL	CA4-CA3-OA5-PA1
33	W	201	EHZ	N2-C15-C16-O5
33	W	201	EHZ	C18-C17-C20-O6
33	W	201	EHZ	C15-C16-C17-C18
33	W	201	EHZ	O5-C16-C17-C18
26	B	303	PC1	C32-C31-O31-C3
26	B	303	PC1	O32-C31-O31-C3
34	q	201	CDL	CB4-CB3-OB5-PB2
26	B	303	PC1	C3-C2-O21-C21
33	W	201	EHZ	O4-C15-C16-C17

There are no ring outliers.

15 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	H	402	3PE	7	0
27	G	803	FES	5	0
29	H	401	UQ9	28	0
31	P	401	NDP	5	0
24	B	301	SF4	3	0
25	B	302	UQ1	3	0
30	H	403	3PE	11	0
24	I	303	SF4	5	0
33	W	201	EHZ	4	0
34	q	201	CDL	22	0
24	G	802	SF4	2	0
24	F	502	SF4	5	0

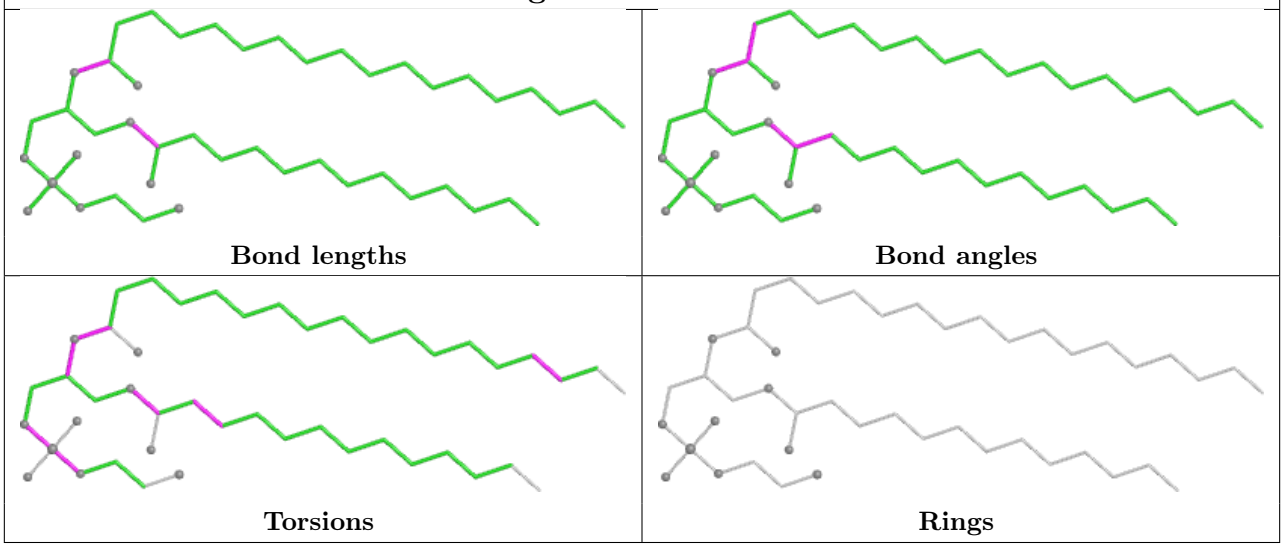
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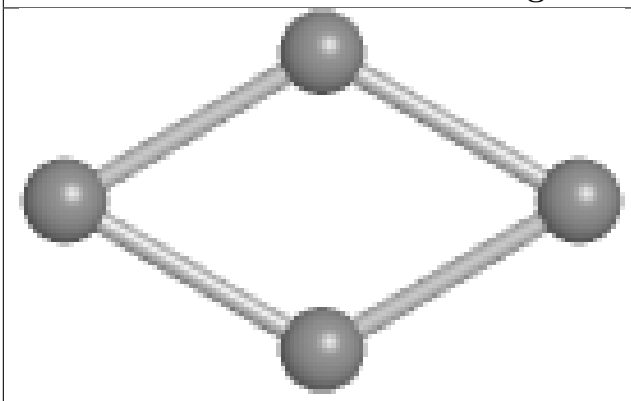
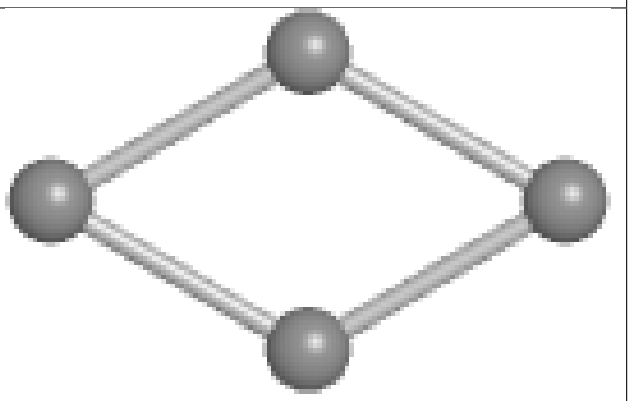
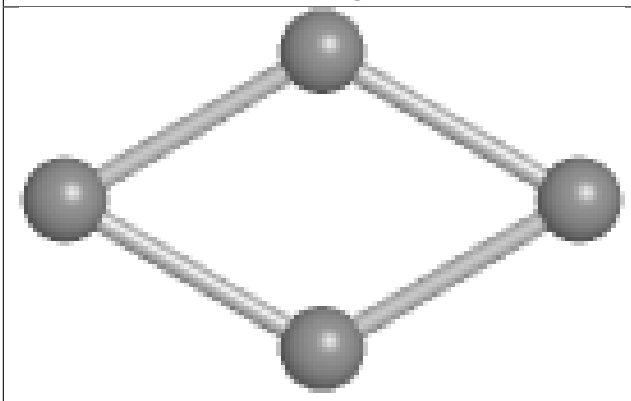
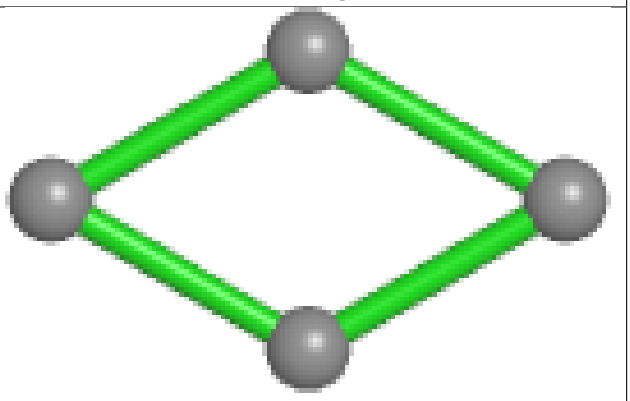
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	303	PC1	6	0
26	I	301	PC1	8	0
27	E	301	FES	4	0

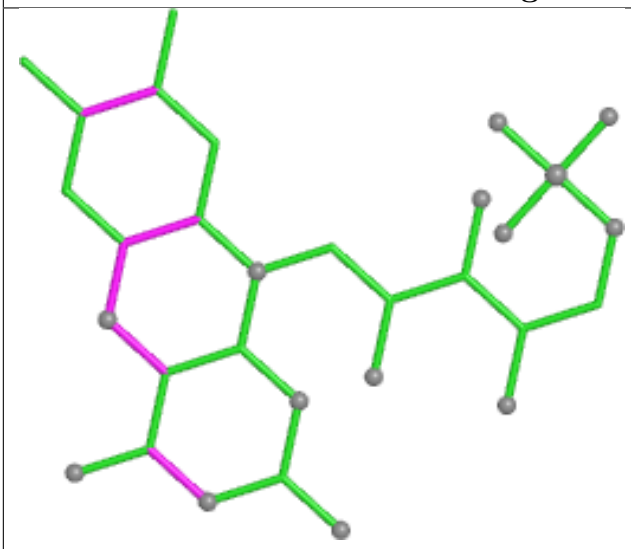
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 3PE H 402

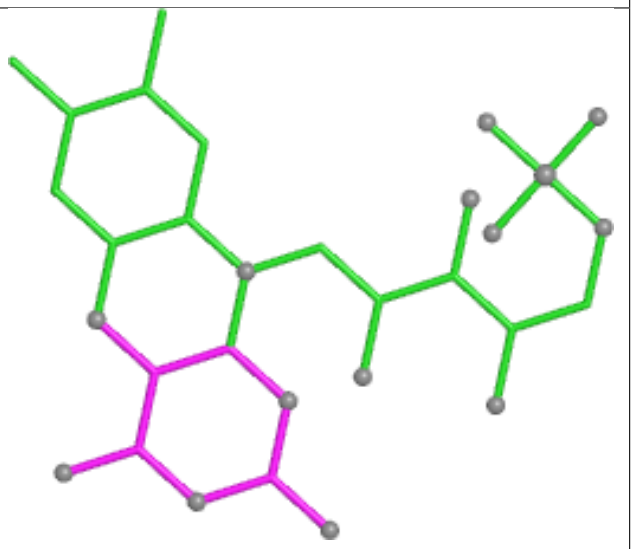


Ligand FES G 803	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

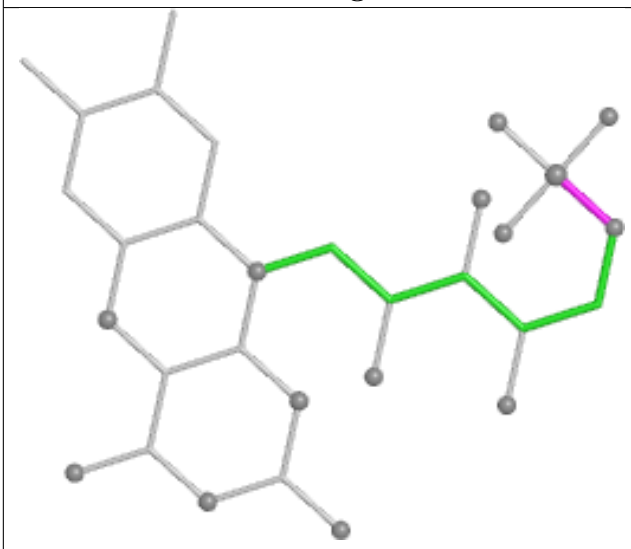
Ligand FMN F 501



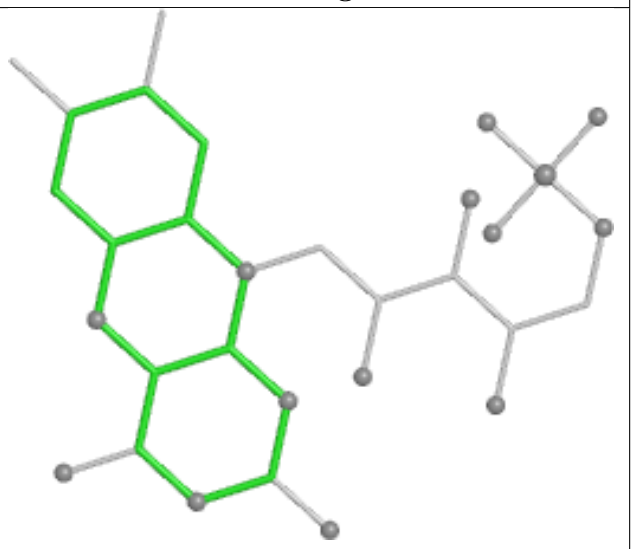
Bond lengths



Bond angles

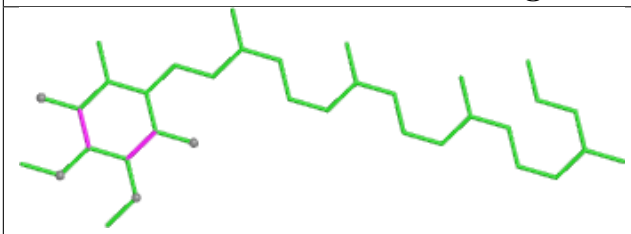


Torsions

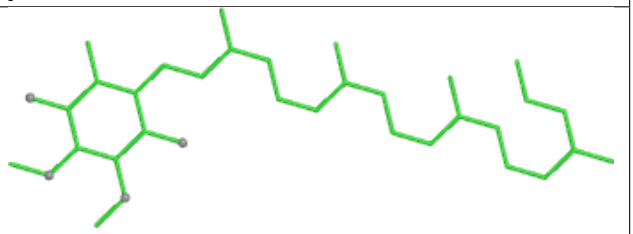


Rings

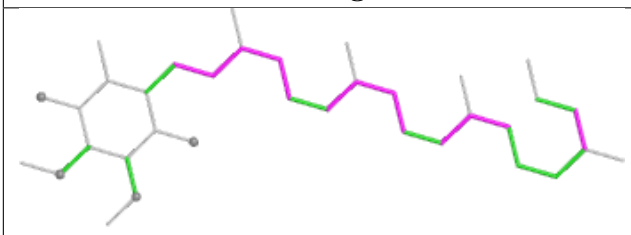
Ligand UQ9 H 401



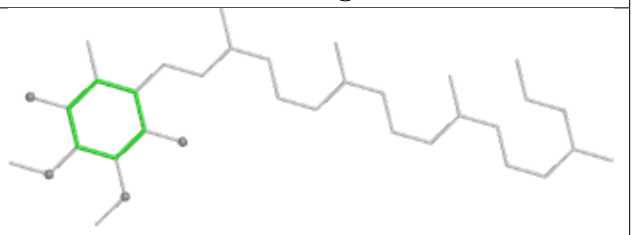
Bond lengths



Bond angles

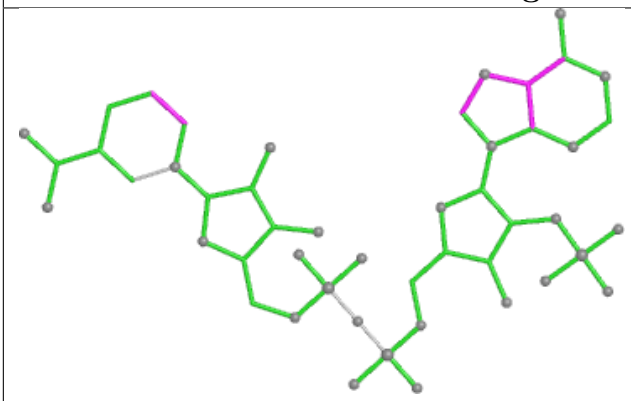


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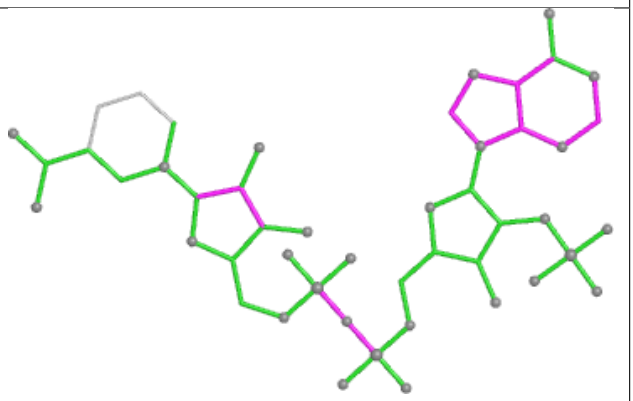


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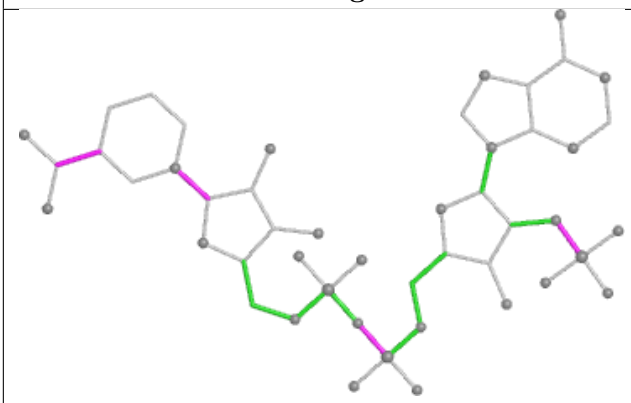
Ligand NDP P 401



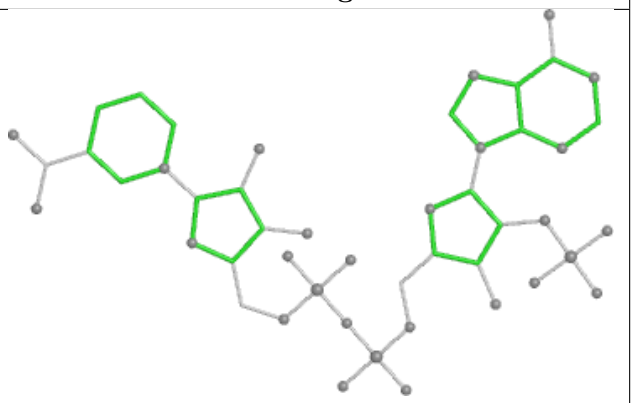
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Bond angles

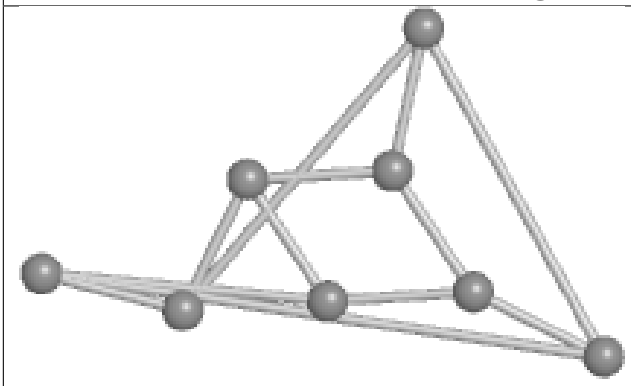


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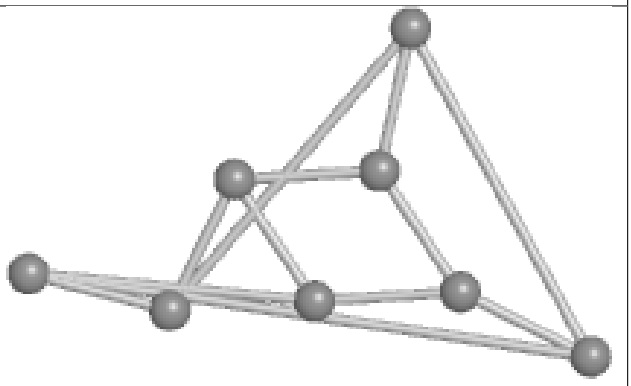


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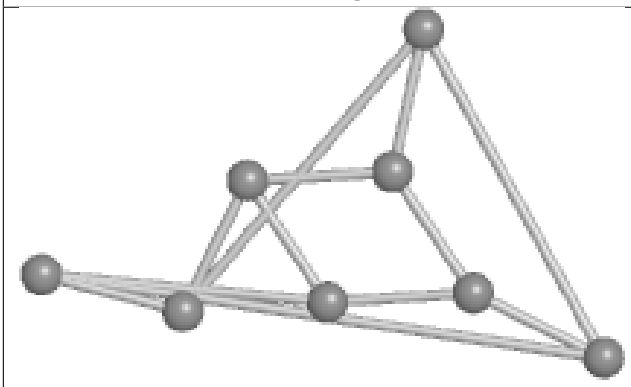
Ligand SF4 B 301



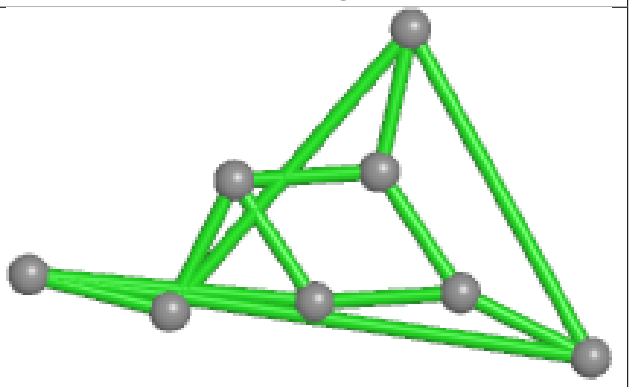
Bond lengths



Bond angles

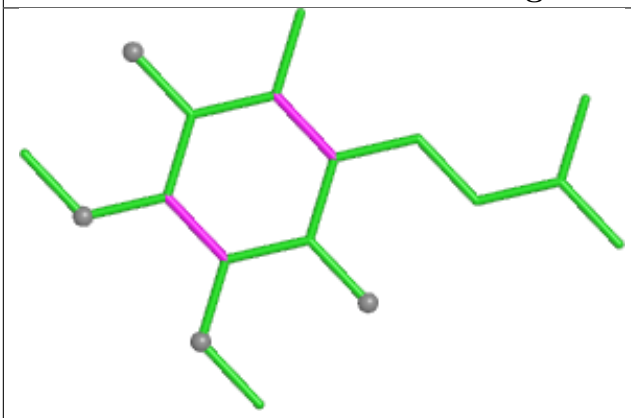


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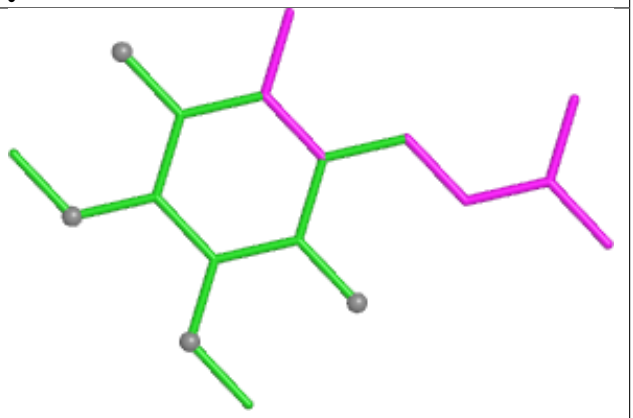


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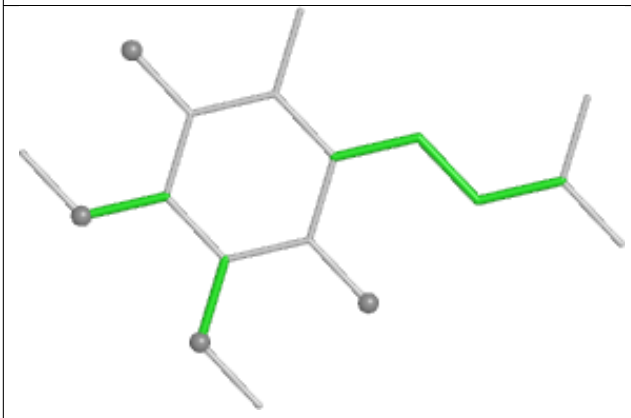
Ligand UQ1 B 302



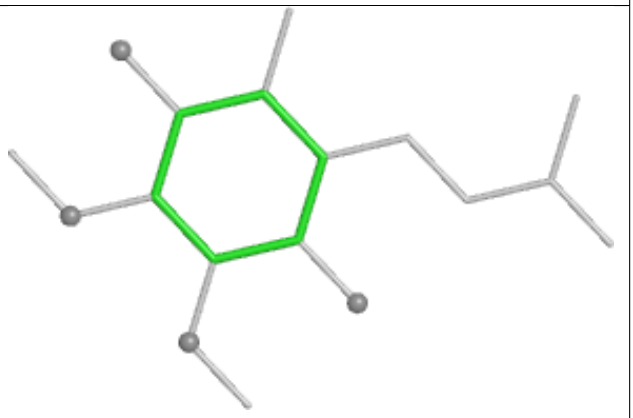
Bond lengths



Bond angles

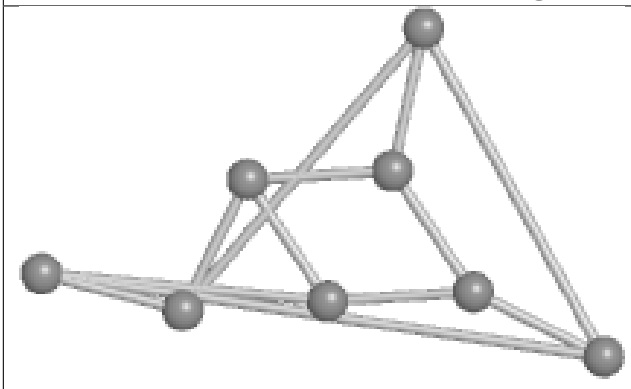


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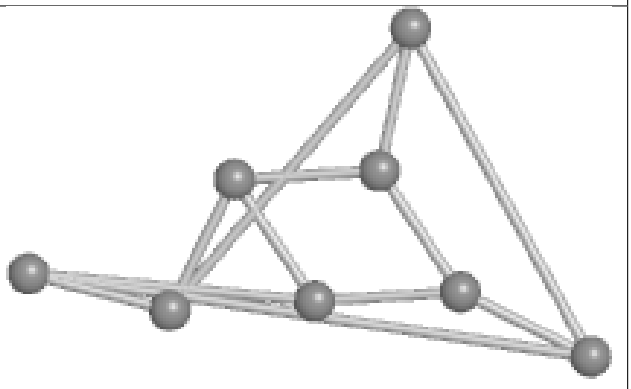


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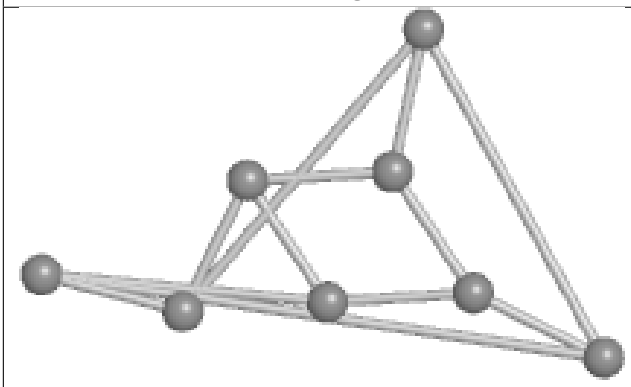
Ligand SF4 G 801



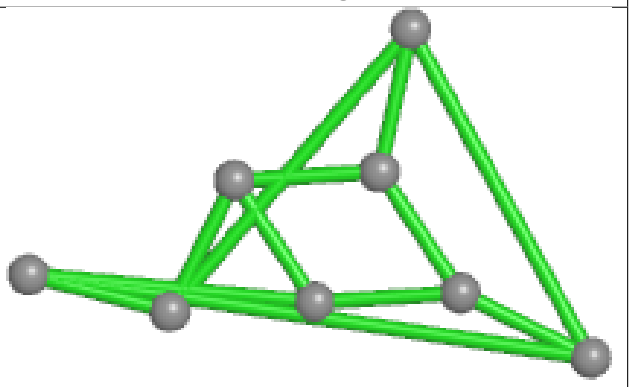
Bond lengths



Bond angles

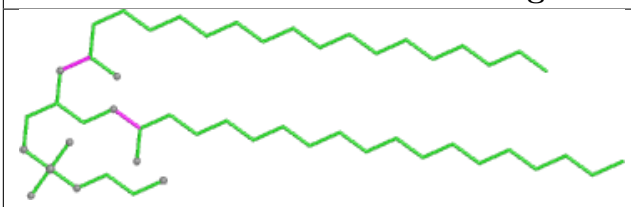


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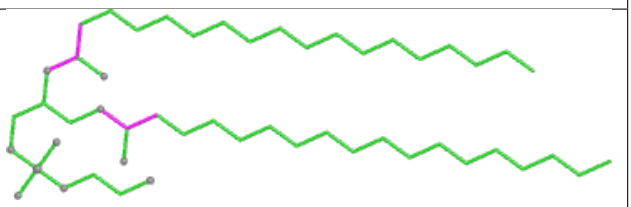


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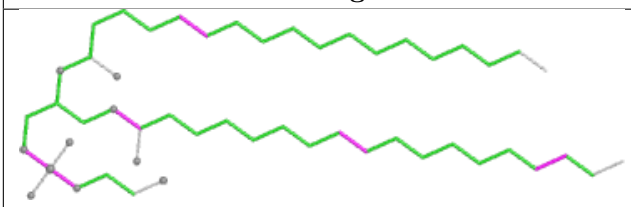
Ligand 3PE H 403



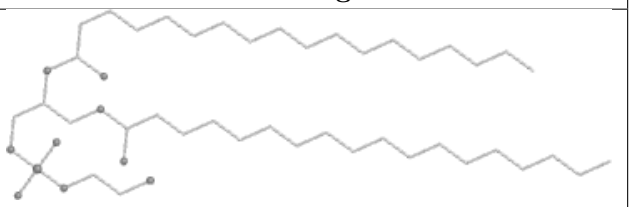
Bond lengths



Bond angles

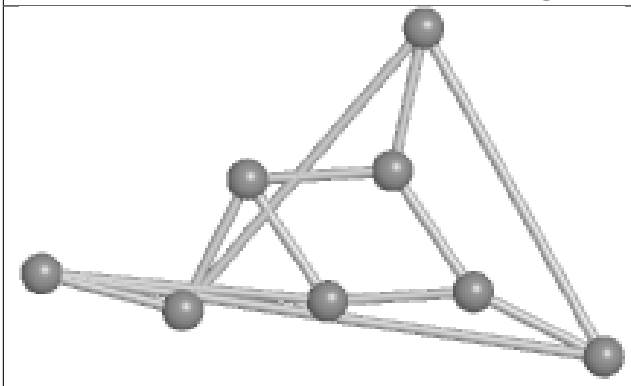


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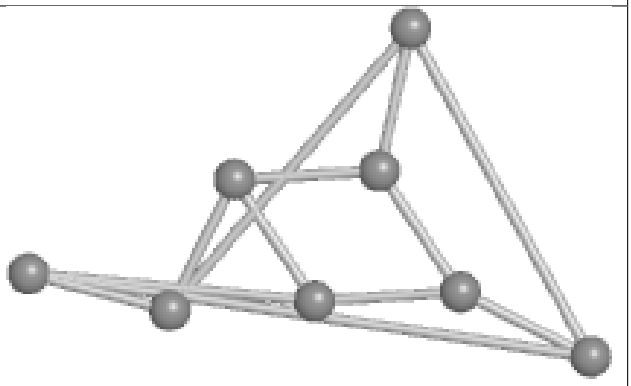


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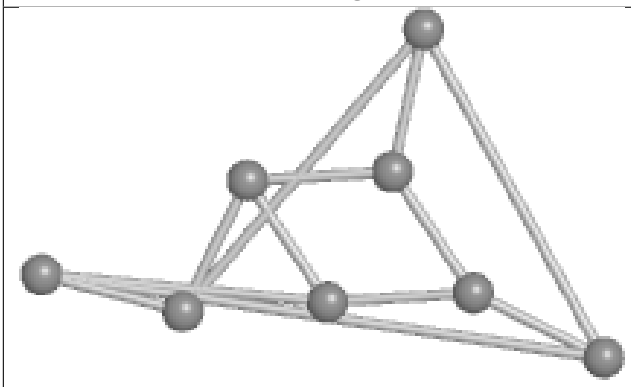
Ligand SF4 I 303



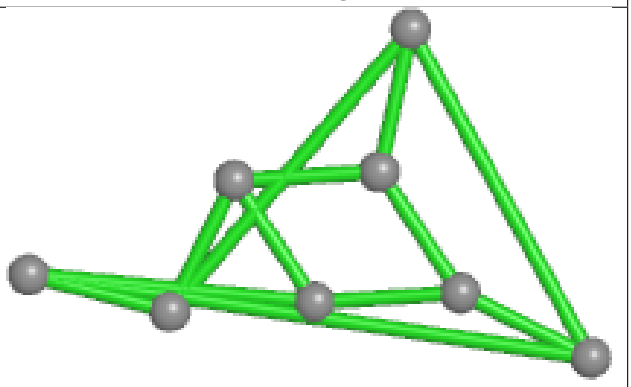
Bond lengths



Bond angles

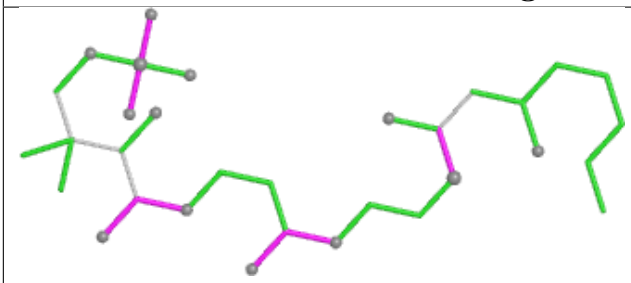


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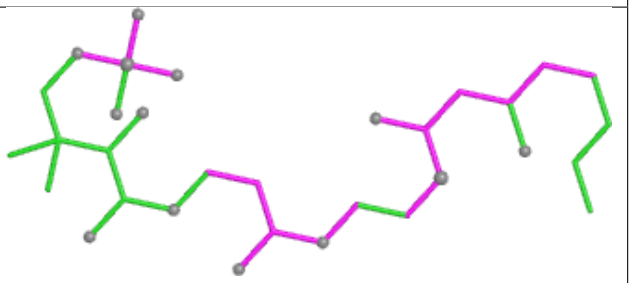


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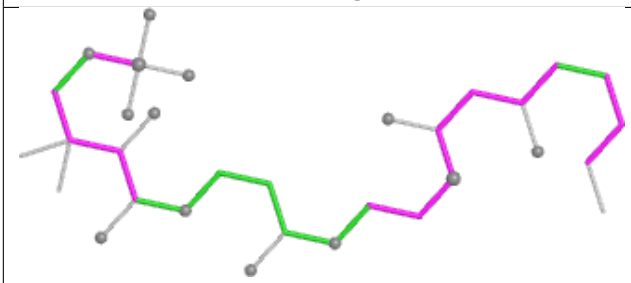
Ligand EHZ W 201



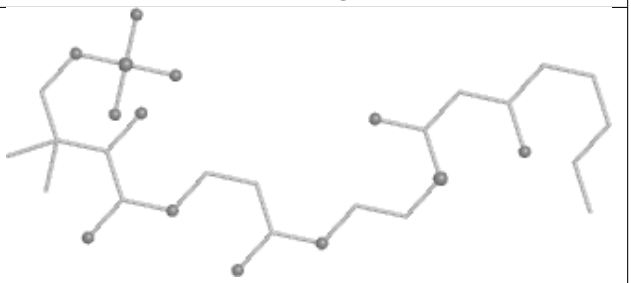
Bond lengths



Bond angles

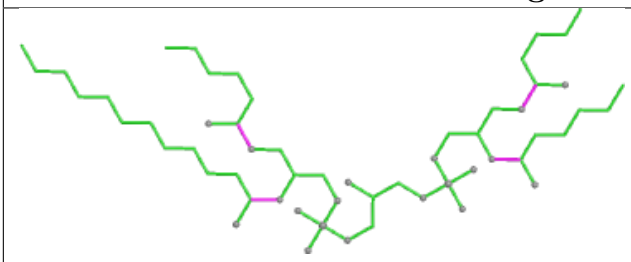


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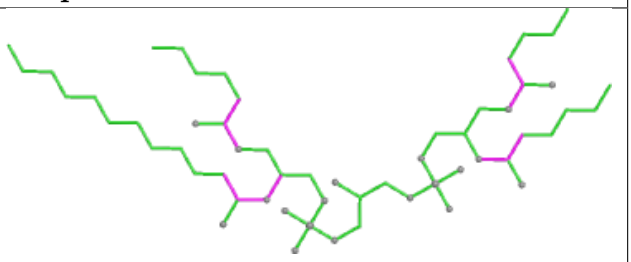


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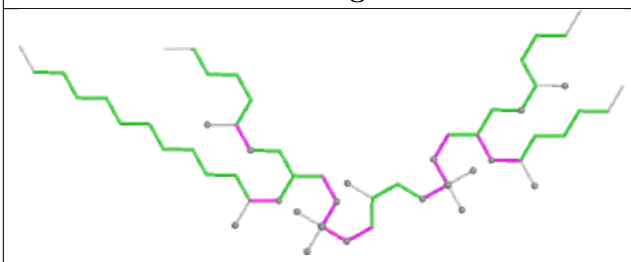
Ligand CDL q 201



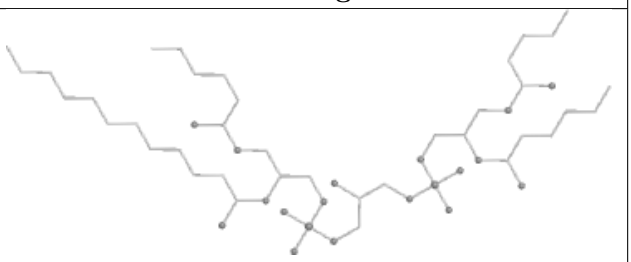
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Bond angles

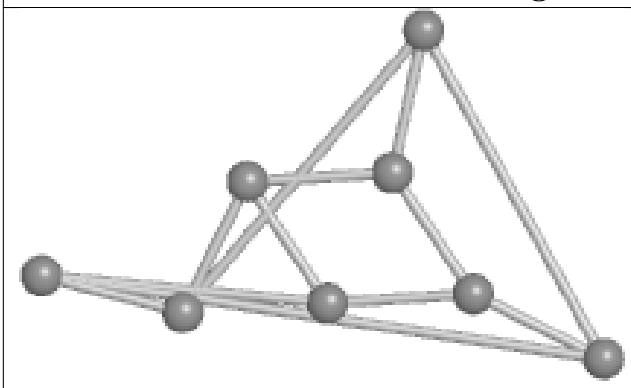


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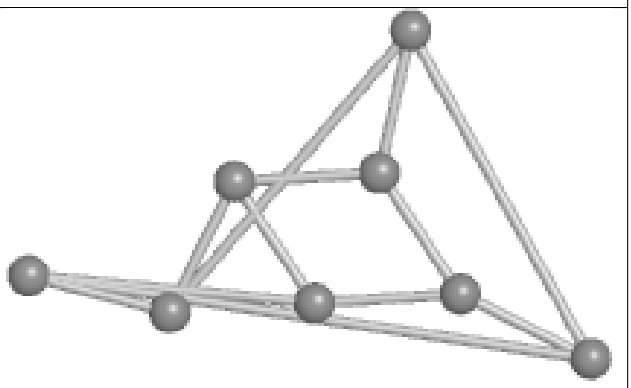


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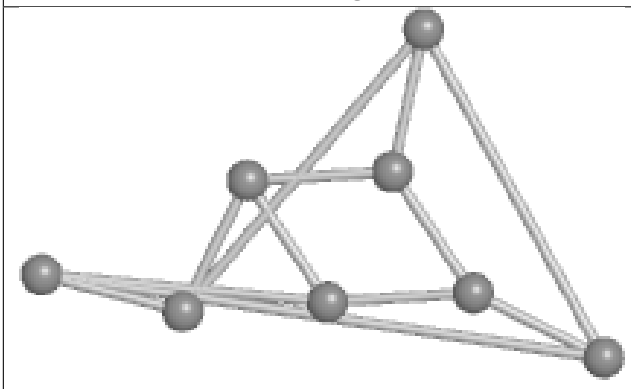
Ligand SF4 G 802



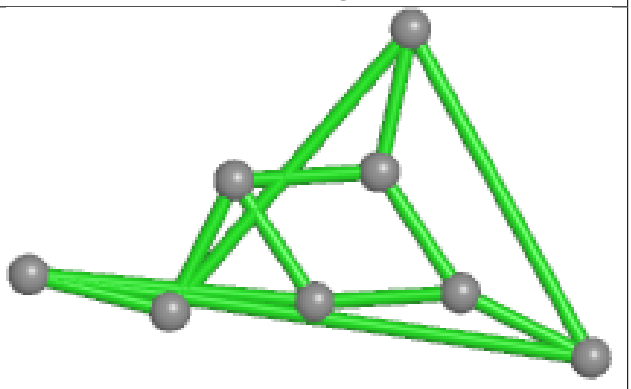
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Bond angles

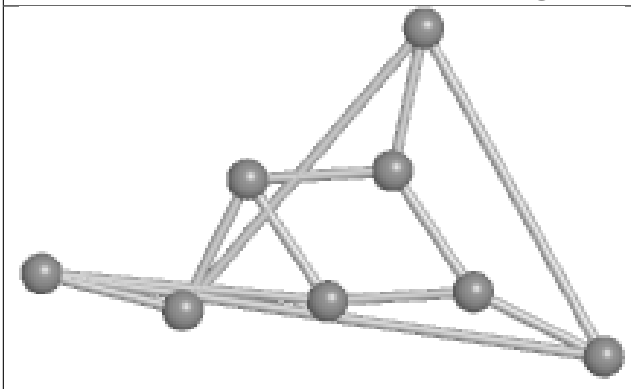


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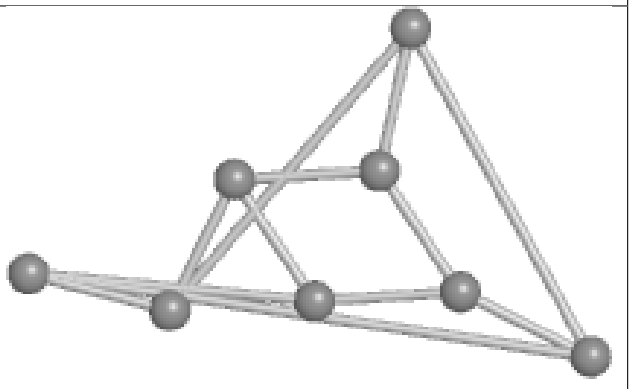


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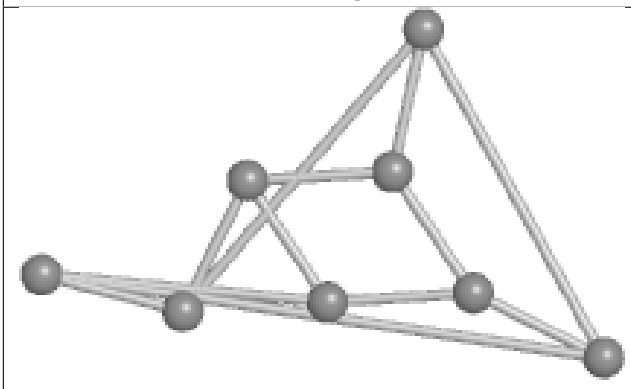
Ligand SF4 F 502



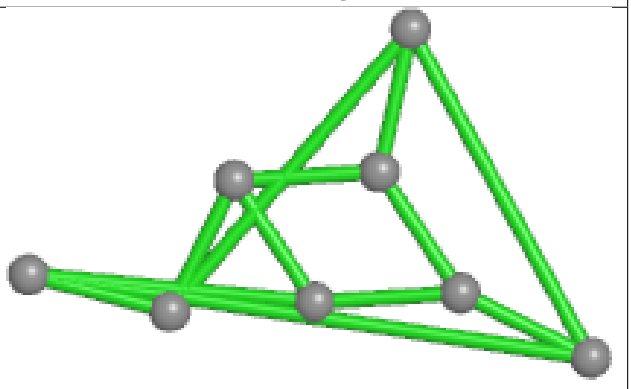
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Bond angles

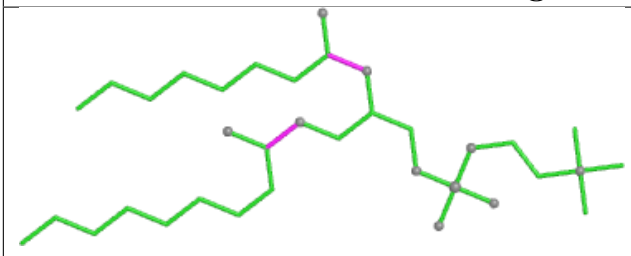


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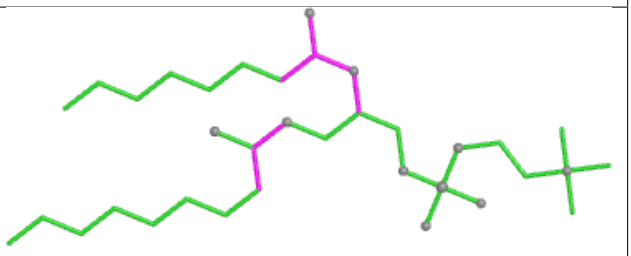


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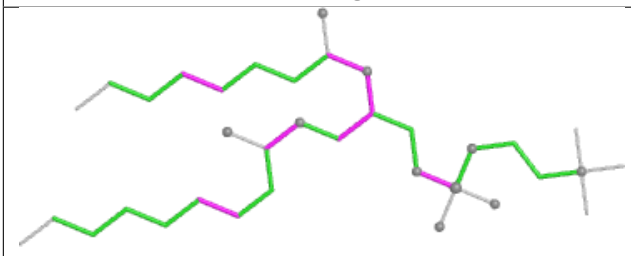
Ligand PC1 B 303



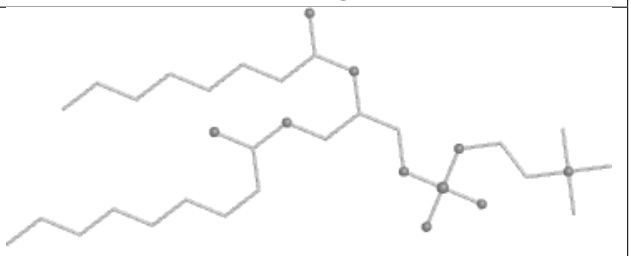
Bond lengths



Bond angles

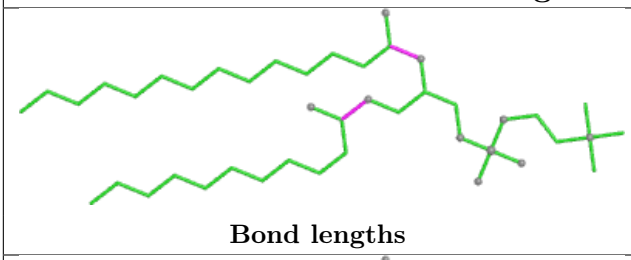


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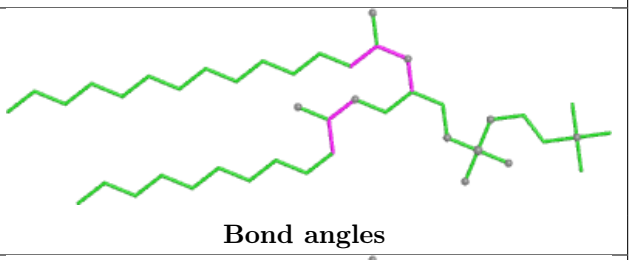


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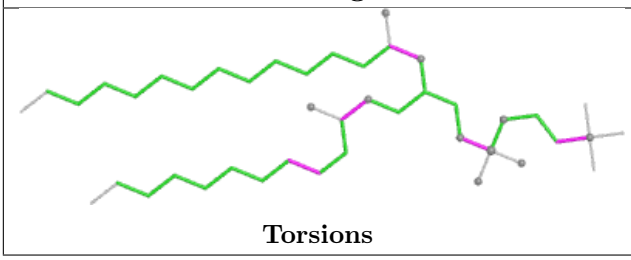
Ligand PC1 I 301



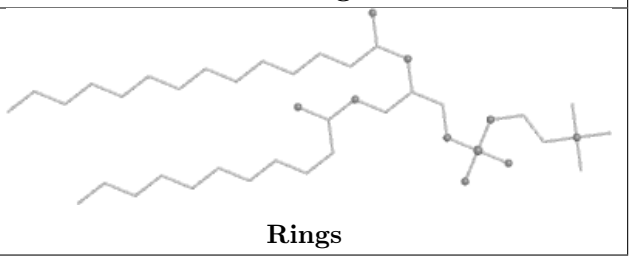
Bond lengths



Bond angles

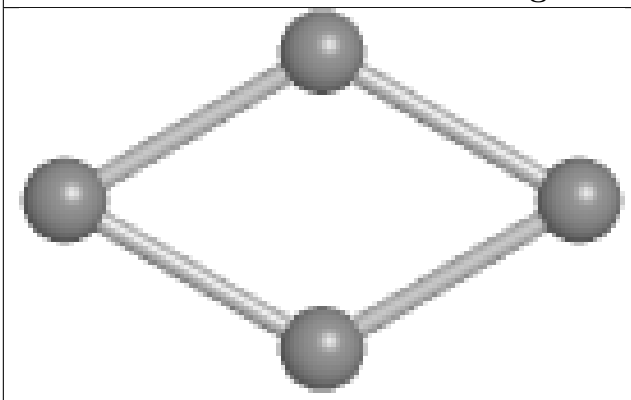


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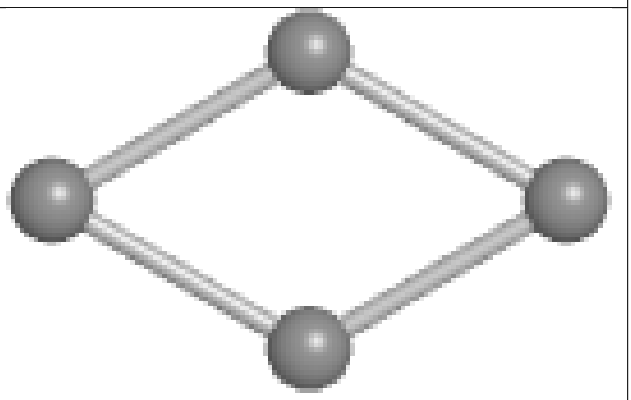


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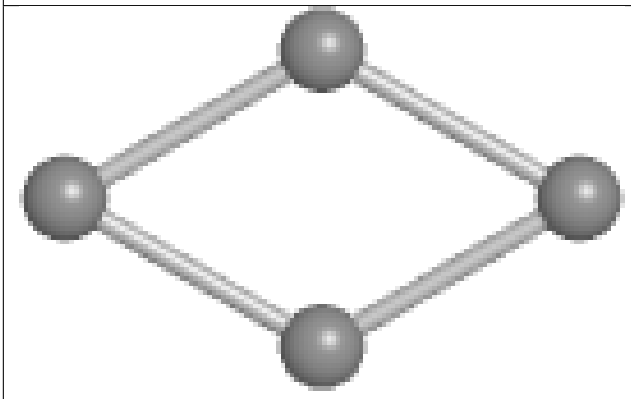
Ligand FES E 301



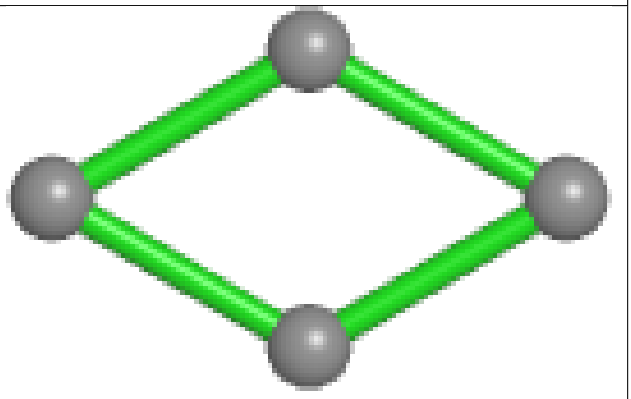
Bond lengths



Bond angles

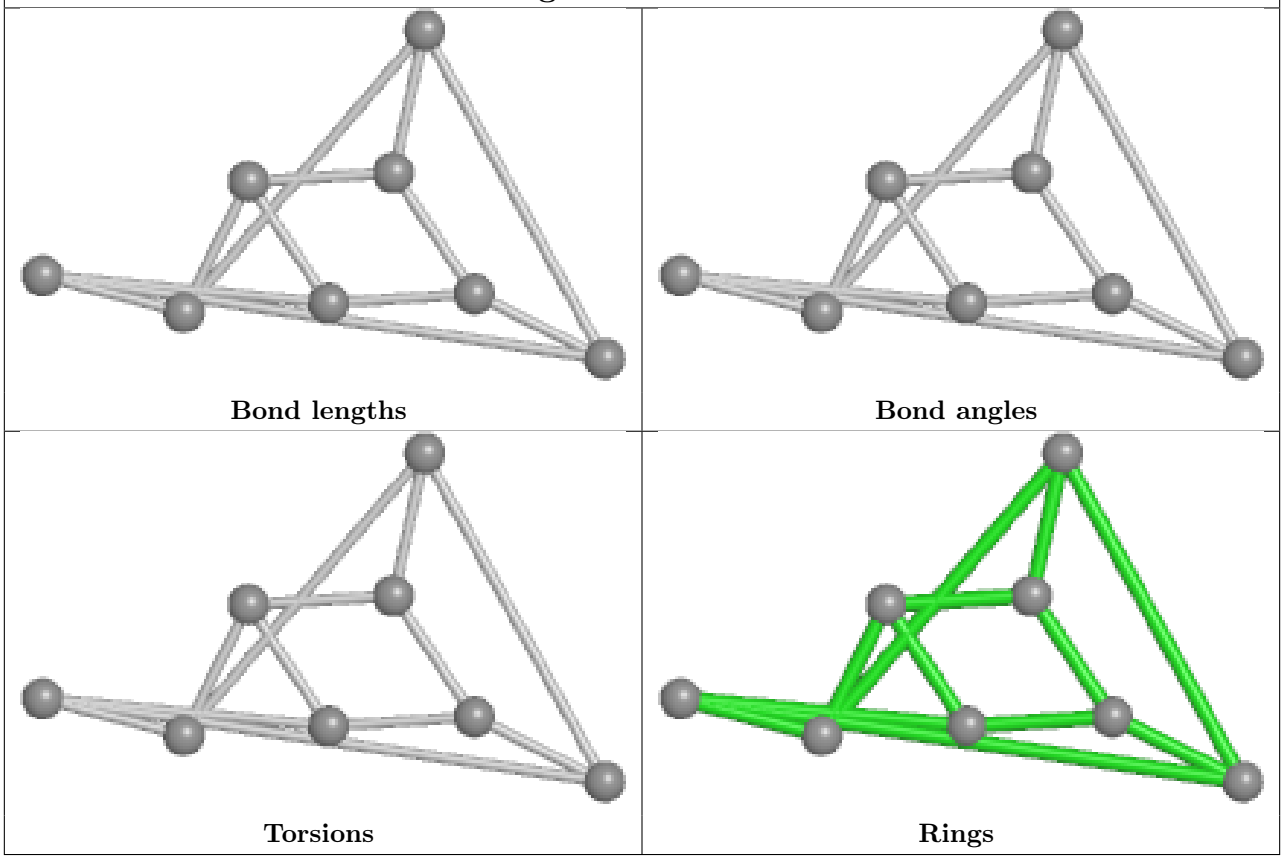


Torsions



Rings

Ligand SF4 I 302



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.

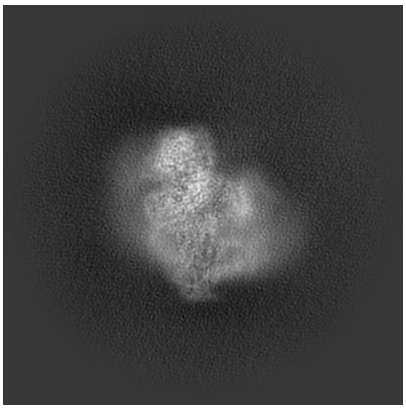
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35353. These allow visual inspection of the internal detail of the map and identification of artifacts.

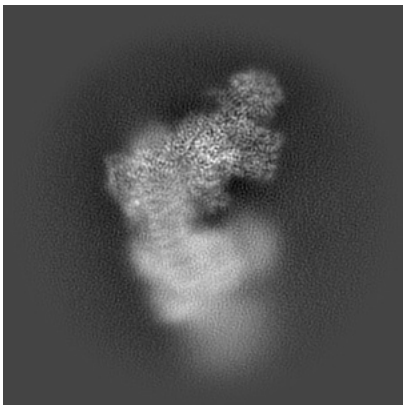
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

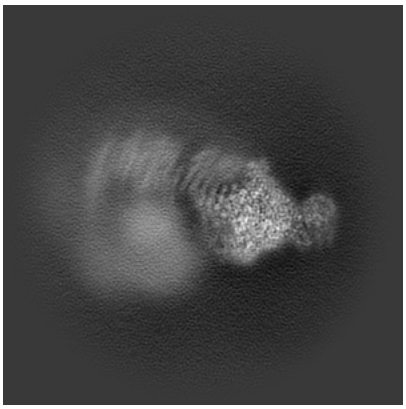
6.1.1 Primary map



X

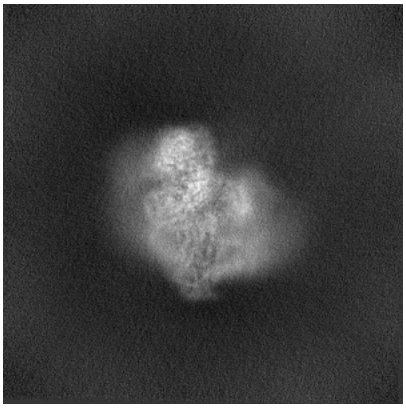


Y

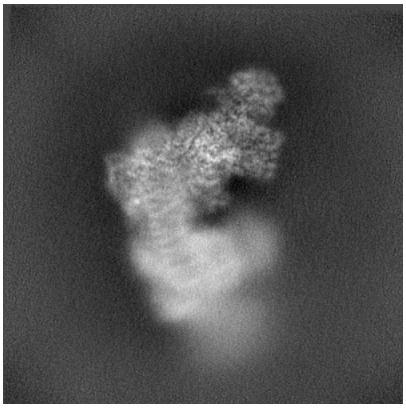


Z

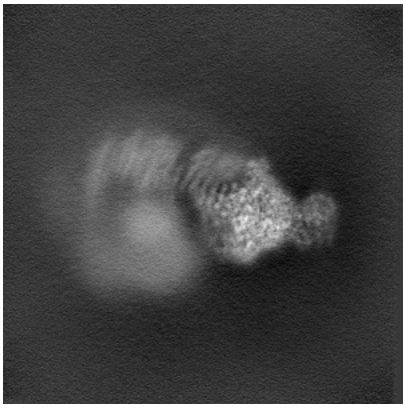
6.1.2 Raw map



X



Y

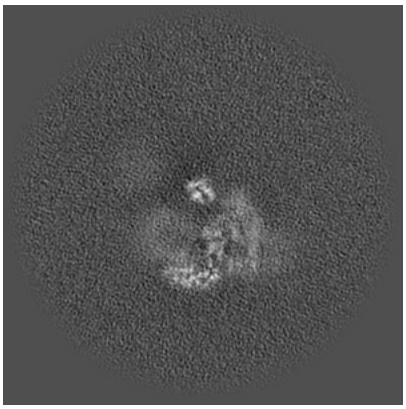


Z

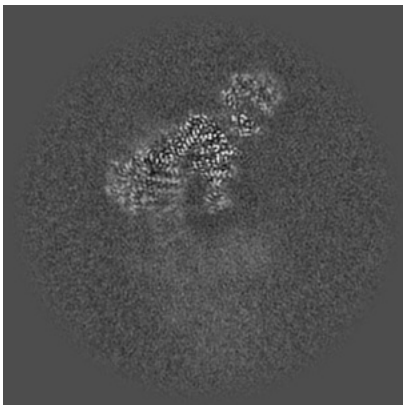
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

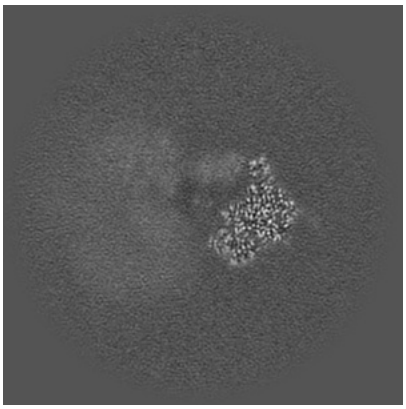
6.2.1 Primary map



X Index: 256

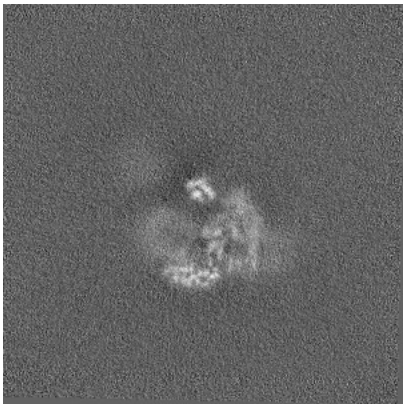


Y Index: 256

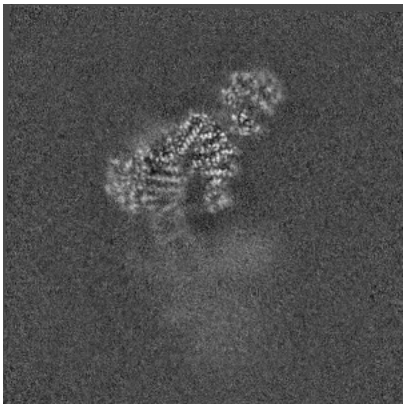


Z Index: 256

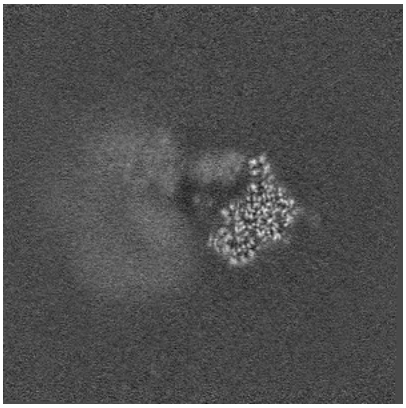
6.2.2 Raw map



X Index: 256



Y Index: 256

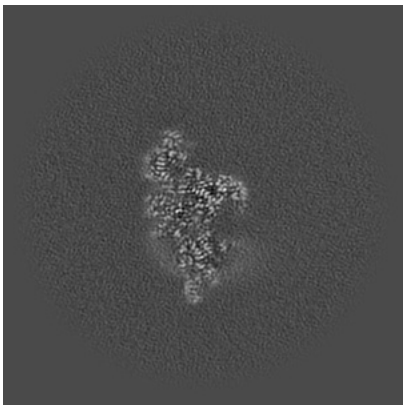


Z Index: 256

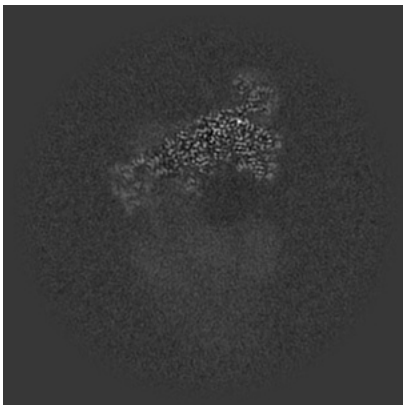
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

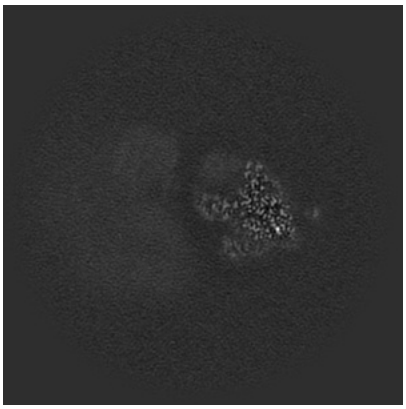
6.3.1 Primary map



X Index: 315

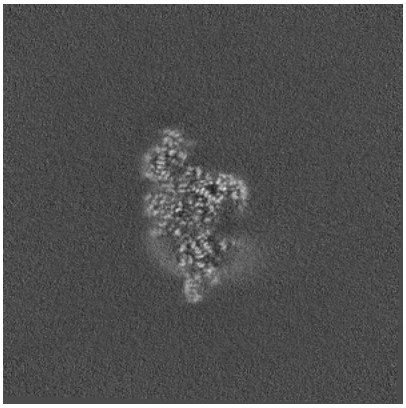


Y Index: 227

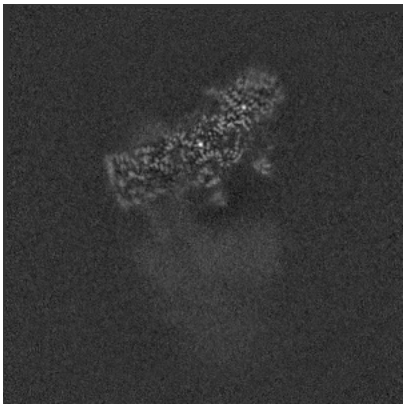


Z Index: 271

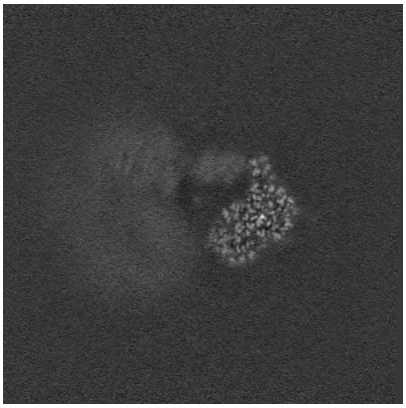
6.3.2 Raw map



X Index: 315



Y Index: 239

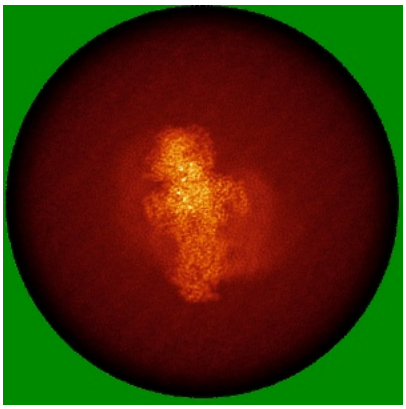


Z Index: 254

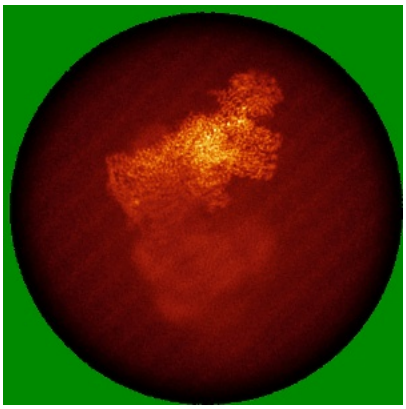
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

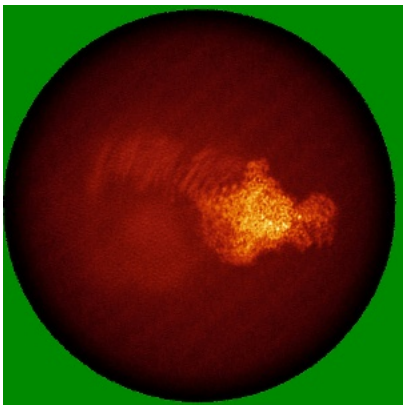
6.4.1 Primary map



X

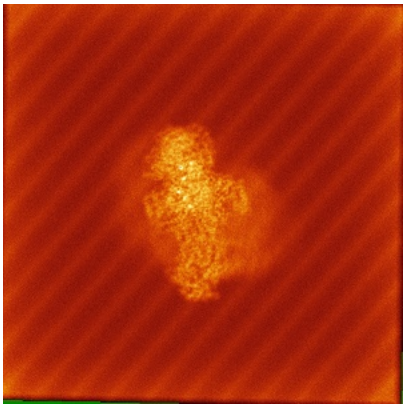


Y

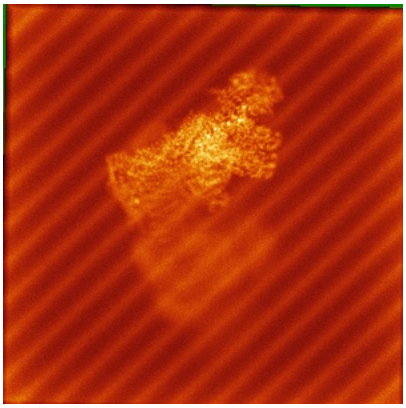


Z

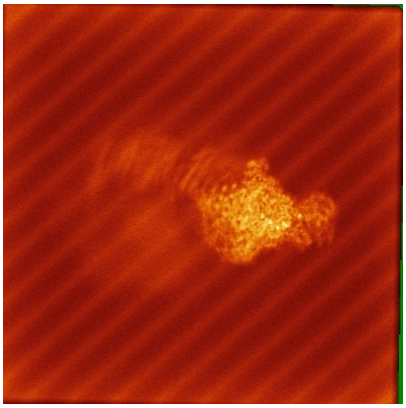
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

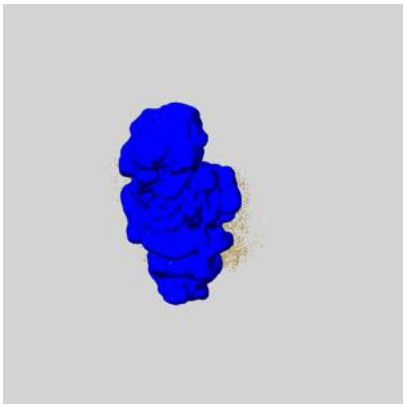
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

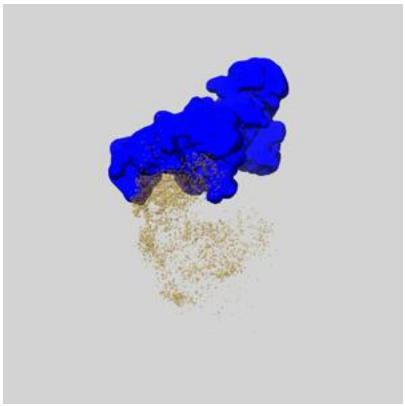
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

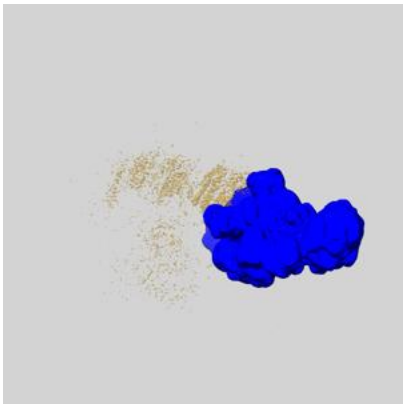
6.6.1 emd_35353_msk_1.map (i)



X



Y

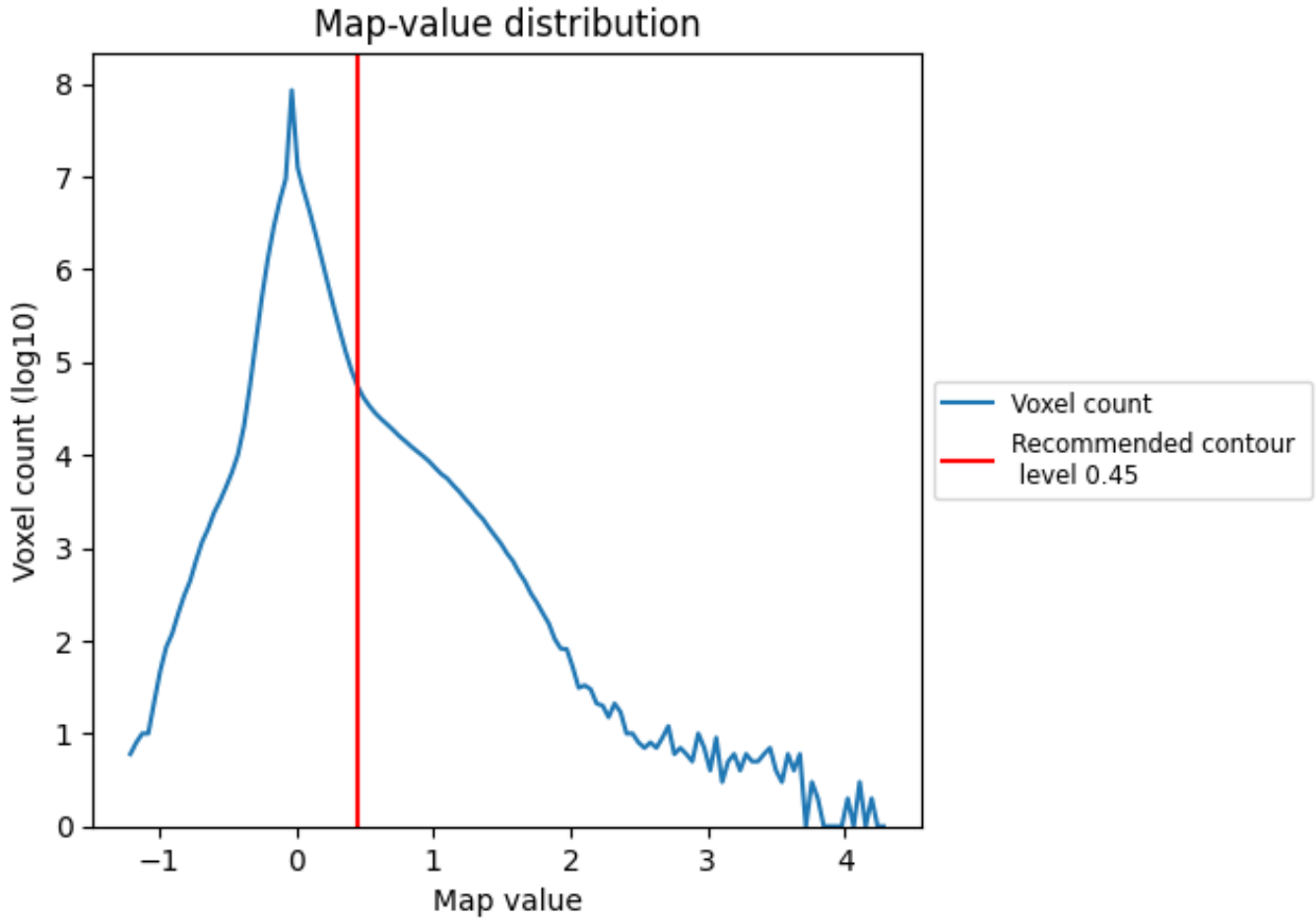


Z

7 Map analysis

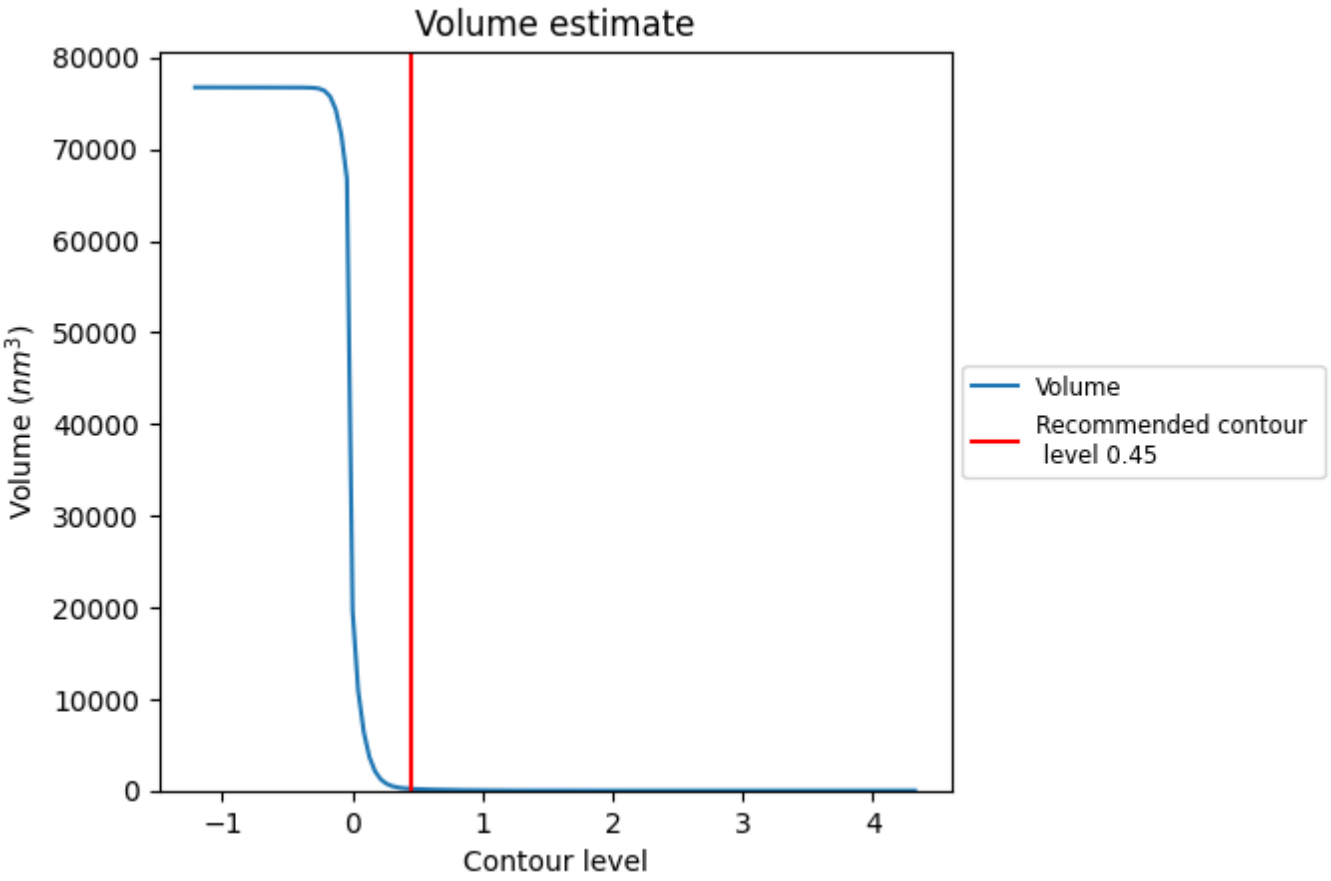
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

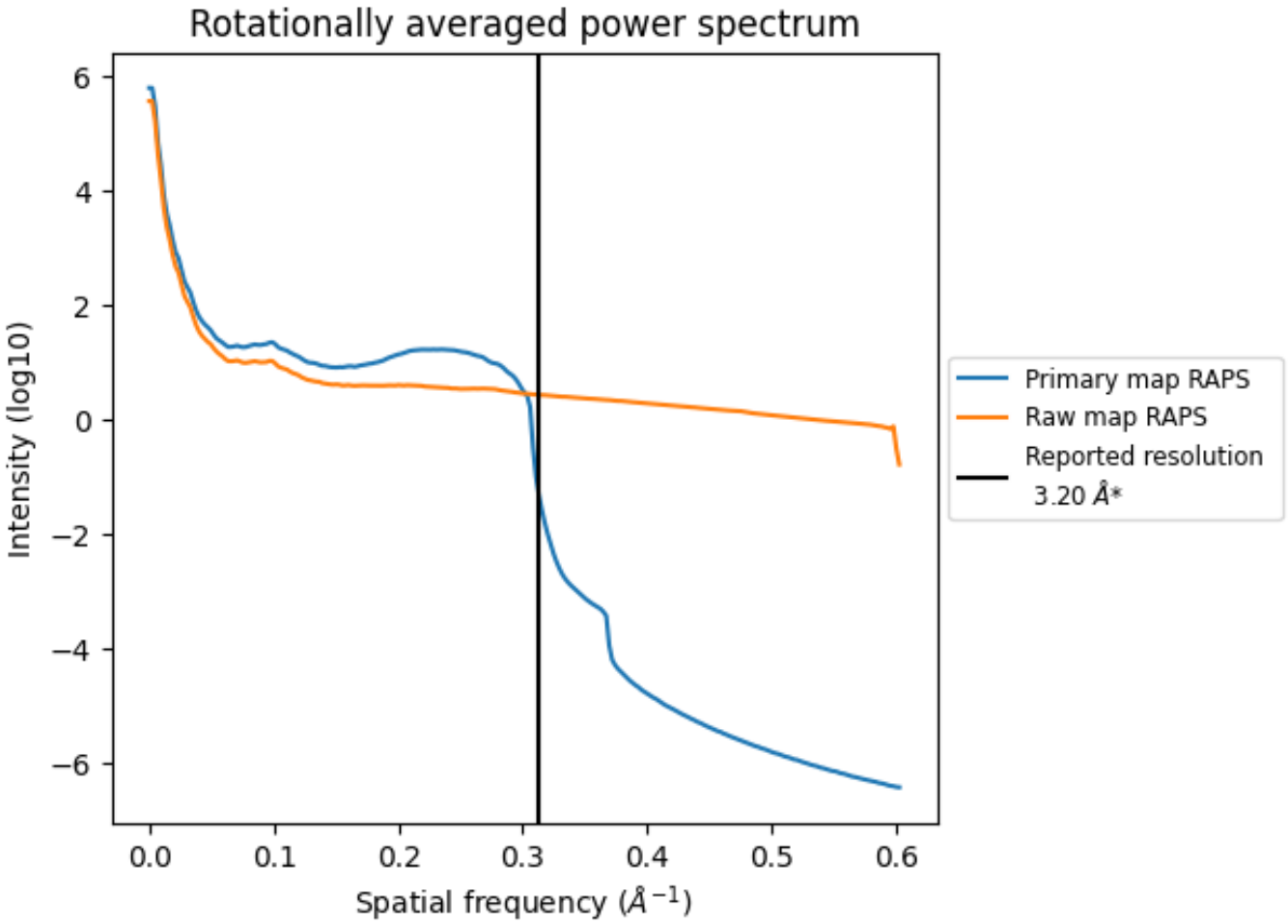
7.2 Volume estimate



The volume at the recommended contour level is 194 nm^3; this corresponds to an approximate mass of 175 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

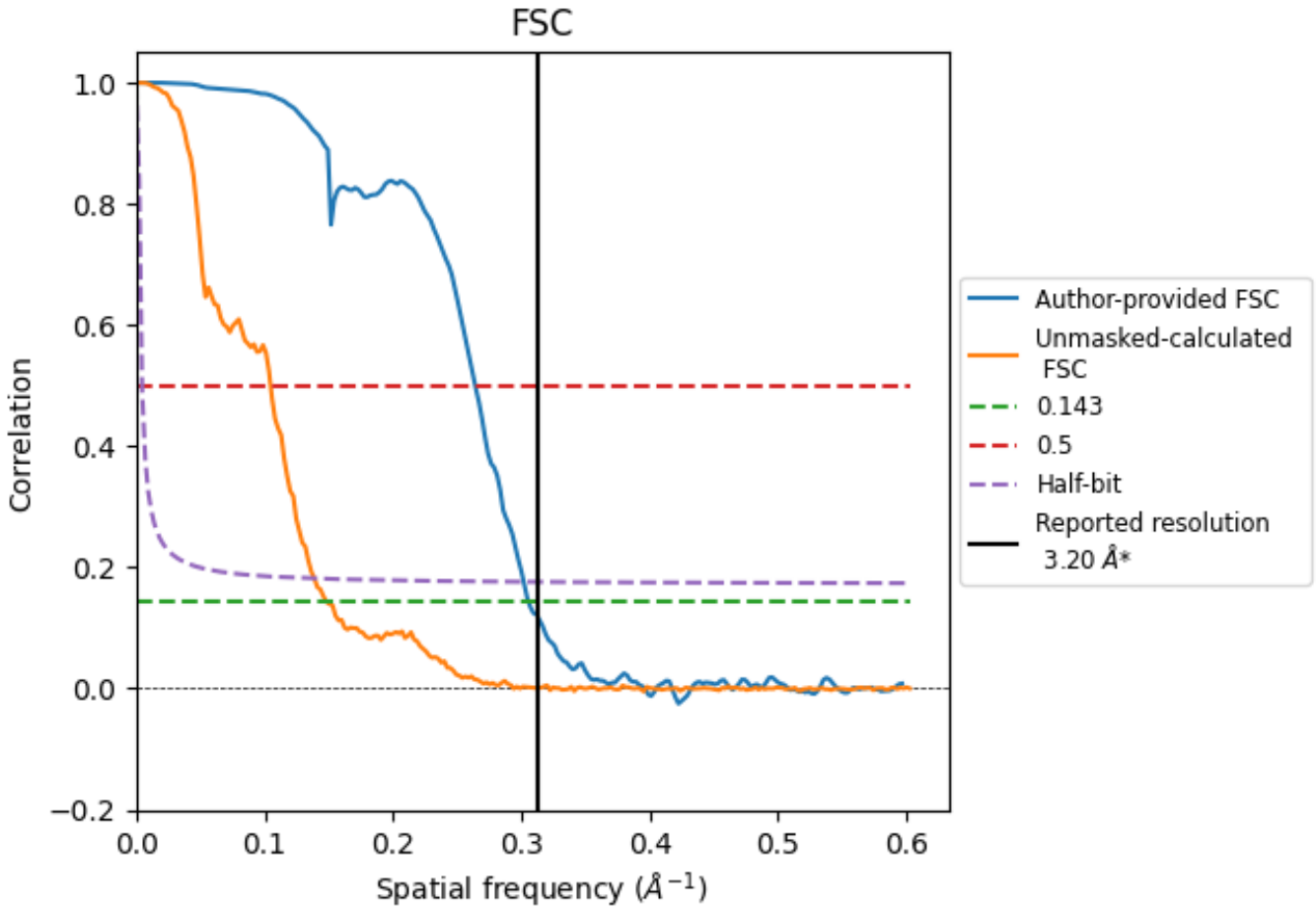


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8.2 Resolution estimates (i)

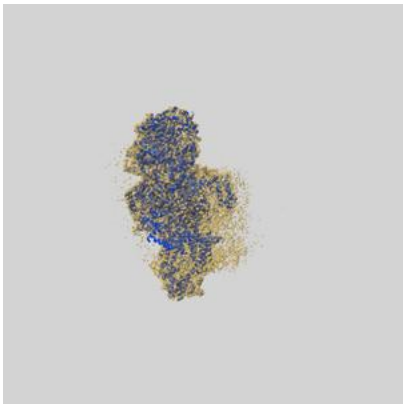
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.27	3.79	3.31
Unmasked-calculated*	6.74	9.54	7.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.74 differs from the reported value 3.2 by more than 10 %

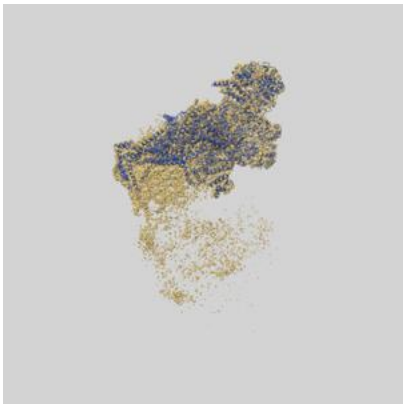
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35353 and PDB model 8IC3. Per-residue inclusion information can be found in section 3 on page 15.

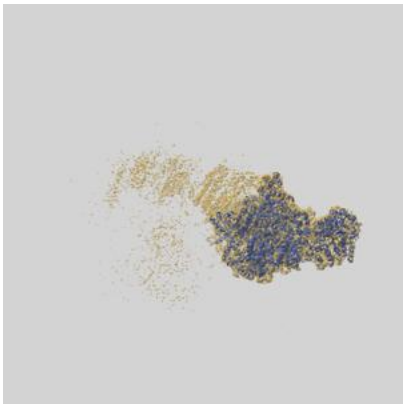
9.1 Map-model overlay



X



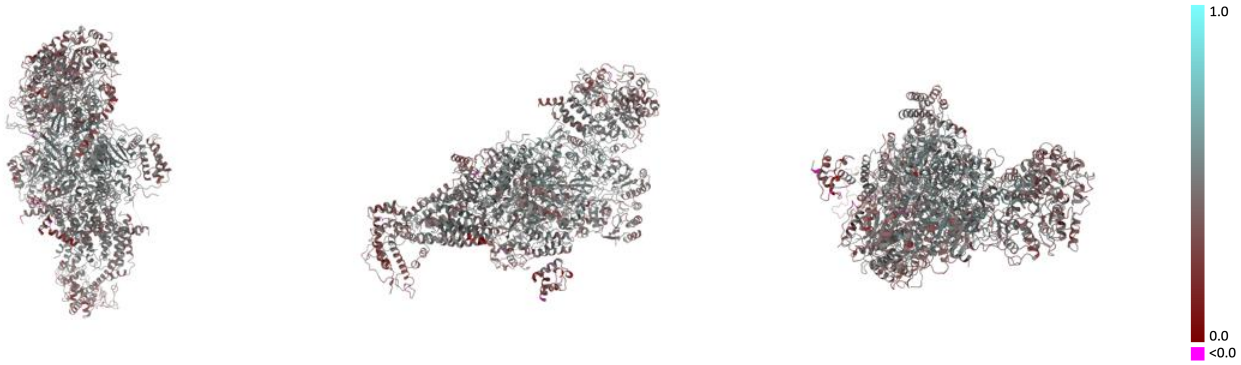
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

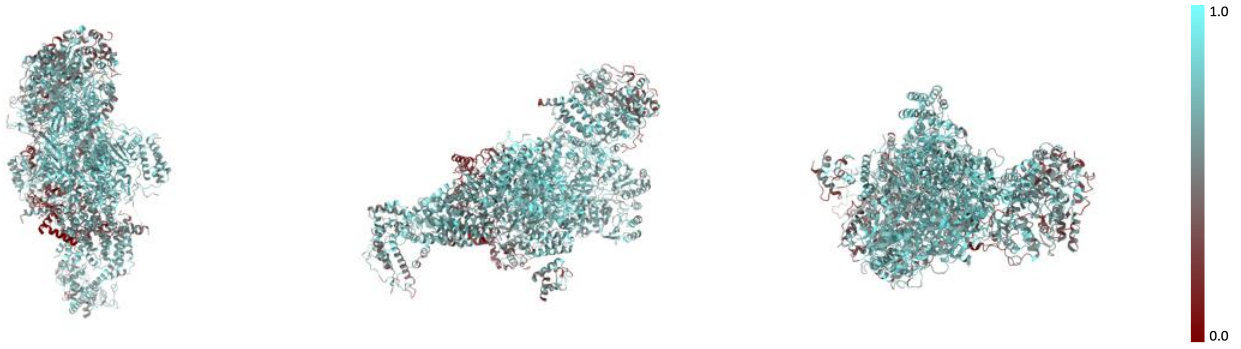
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

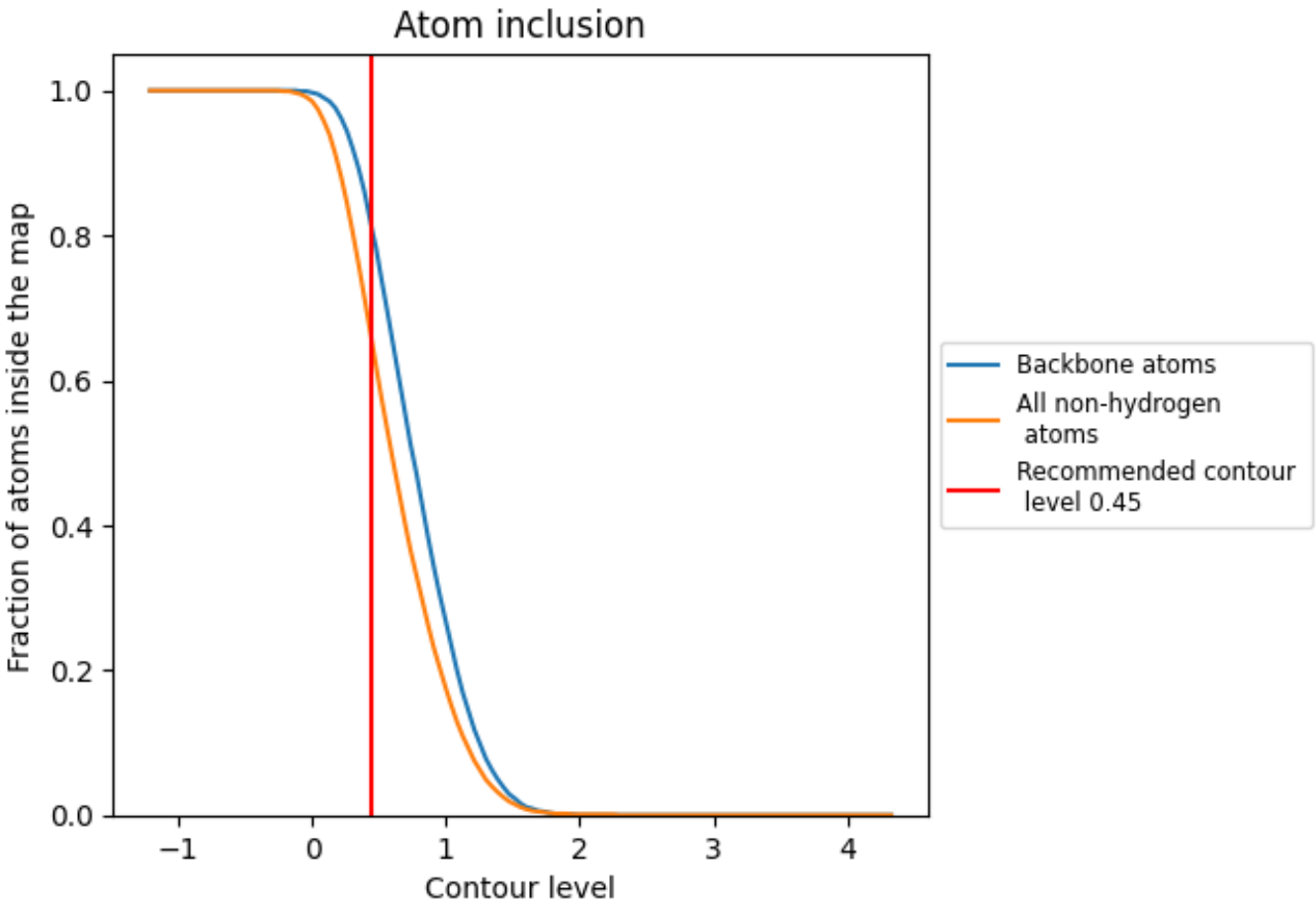
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6490	0.4310
A	0.5440	0.3950
B	0.7450	0.4920
C	0.7910	0.4990
D	0.7920	0.5020
E	0.5520	0.4000
F	0.6220	0.4100
G	0.7250	0.4520
H	0.6730	0.4690
I	0.7640	0.4910
P	0.5970	0.4040
Q	0.6690	0.4590
R	0.3970	0.3830
S	0.6500	0.3910
T	0.4840	0.2710
V	0.7140	0.4210
W	0.6780	0.4390
X	0.5800	0.3240
Z	0.6190	0.3670
a	0.6820	0.4180
b	0.6070	0.3870
q	0.2000	0.3530
r	0.3790	0.3680
s	0.2800	0.3680

