



Full wwPDB EM Validation Report ⓘ

Aug 7, 2026 – 01:54 AM JST

PDB ID : 8XNZ / pdb_00008xnz
EMDB ID : EMD-38520
Title : Respiratory complex Peripheral Arm of CI, close form A, focus-refined map of type I, PERK -/- mouse under Cold Acclimation
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-12-30
Resolution : 3.30 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:

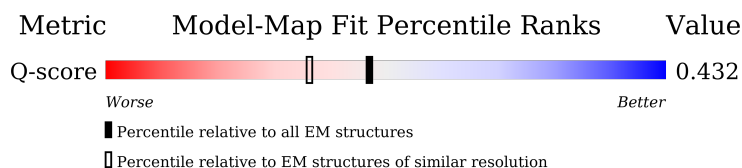
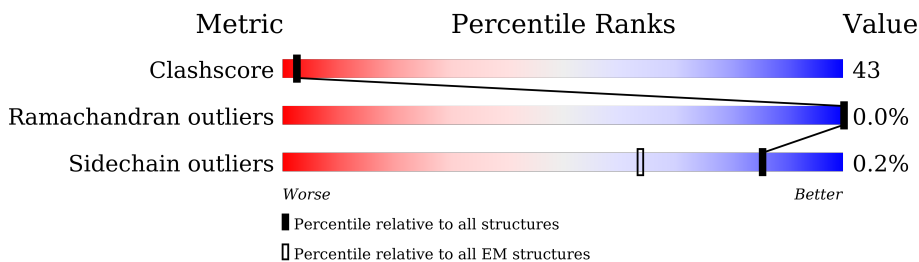
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 3.30 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.



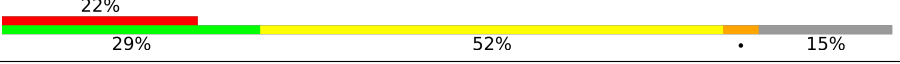
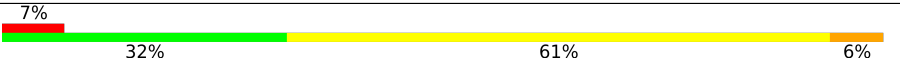
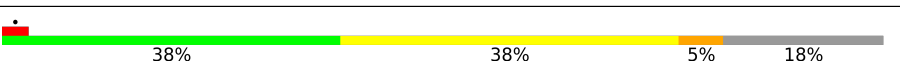
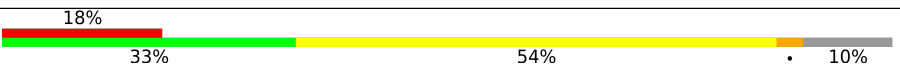
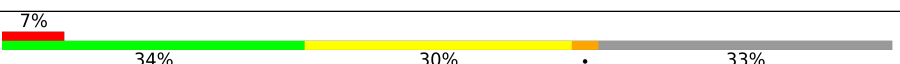
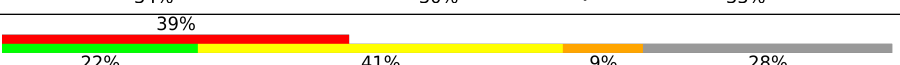
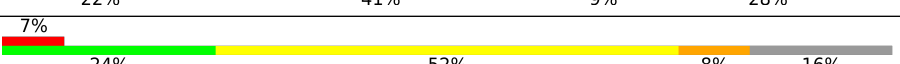
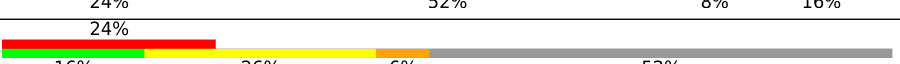
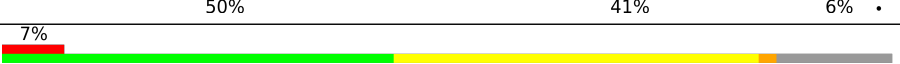
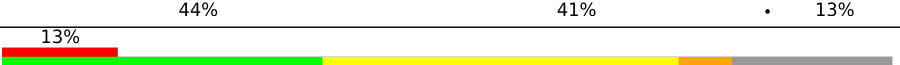
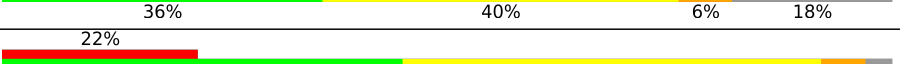
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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 $\leq 5\%$. 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	
2	B	224	
3	C	263	
4	D	463	

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Mol	Chain	Length	Quality of chain
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	P	377	
11	Q	175	
12	R	116	
13	S	99	
14	T	156	
15	V	116	
16	W	131	
17	X	172	
18	Z	144	
19	a	70	
20	b	84	
21	q	145	
22	r	113	
23	s	104	

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	-
25	UQ9	B	302	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	FES	E	301	-	-	X	-
27	FES	G	803	-	-	X	-
33	CDL	q	201	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 34090 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
1	A	112	Total	C	N	O	S	0	0
			901	612	129	153	7		

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

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

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

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

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

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

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

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

- 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	141	Total	C	N	O	S	0	0
			1153	730	205	208	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		

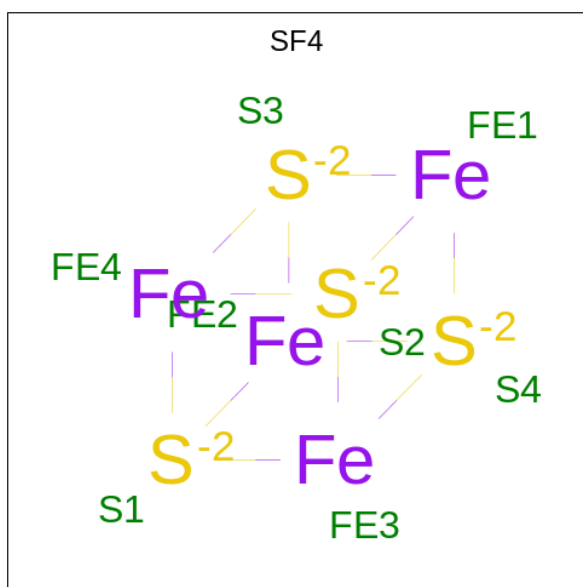
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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.

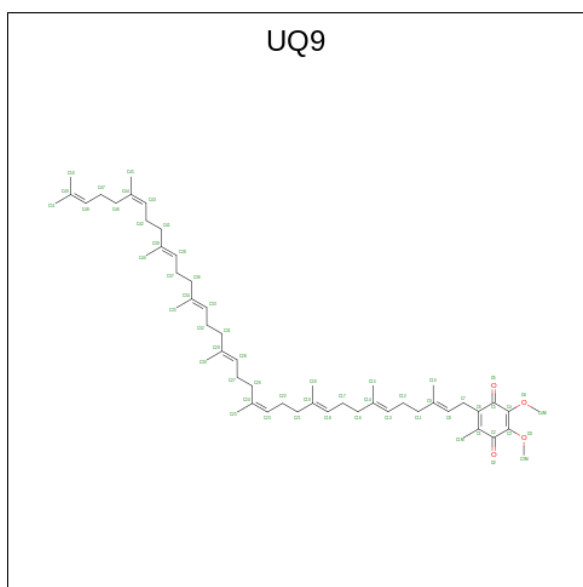
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	29	Total	C	N	O	0	0
			238	151	39	48		

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



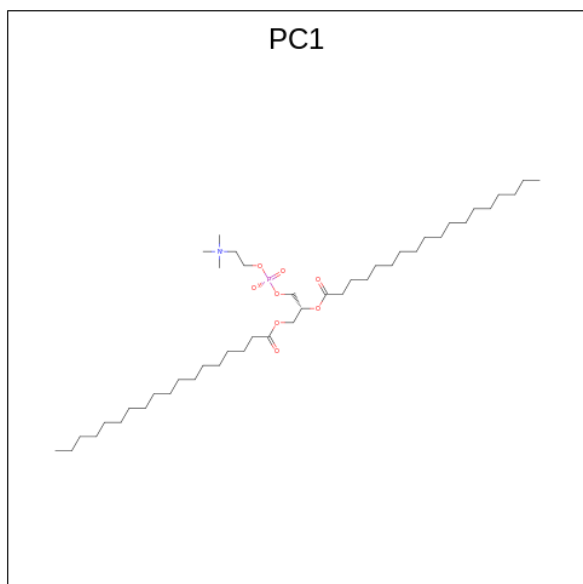
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	Fe	S	0
			8	4	4	
24	F	1	Total	Fe	S	0
			8	4	4	
24	G	1	Total	Fe	S	0
			8	4	4	
24	G	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 25 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
25	B	1	Total	C	O	0
			21	17	4	
25	H	1	Total	C	O	0
			35	31	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).



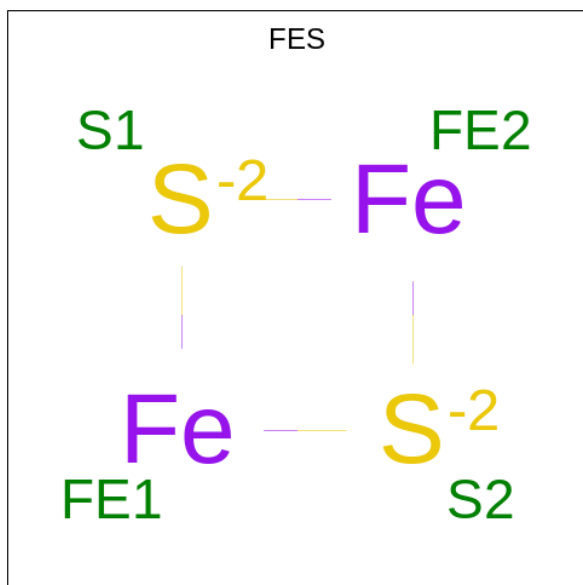
Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total	C	N	O	P	0
			35	25	1	8	1	

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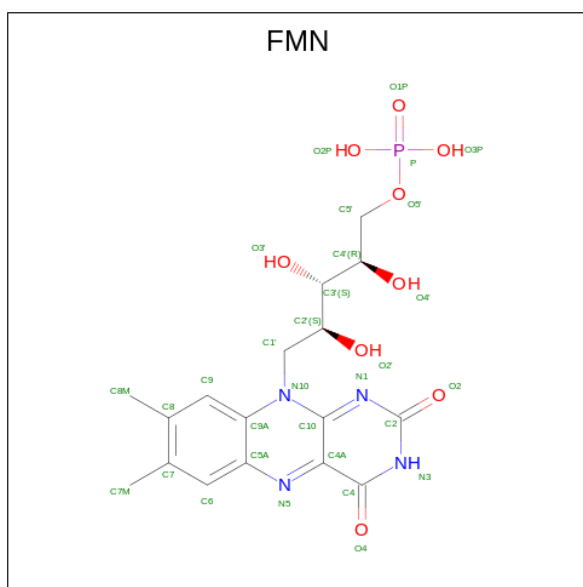
Mol	Chain	Residues	Atoms					AltConf
26	I	1	Total	C	N	O	P	0
			43	33	1	8	1	

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



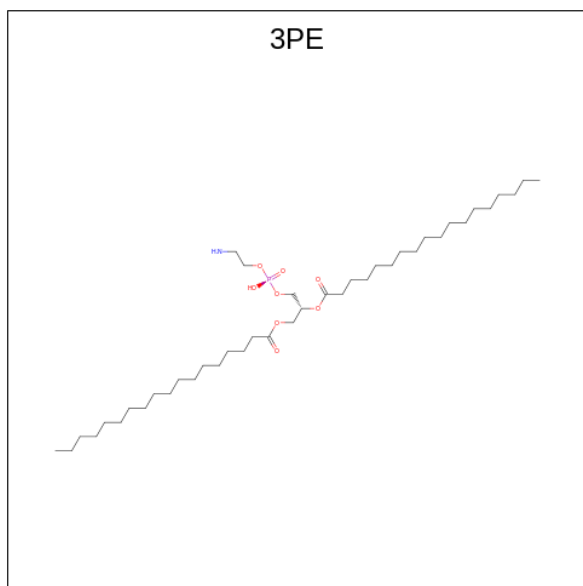
Mol	Chain	Residues	Atoms			AltConf
27	E	1	Total	Fe	S	0
			4	2	2	
27	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 28 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



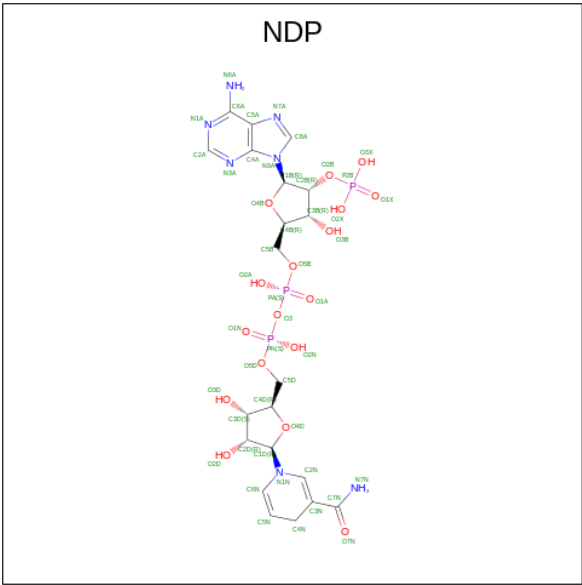
Mol	Chain	Residues	Atoms					AltConf
28	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 29 is 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
29	H	1	Total 46	C 36	N 1	O 8	P 1	0
29	H	1	Total 51	C 41	N 1	O 8	P 1	0

- Molecule 30 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).

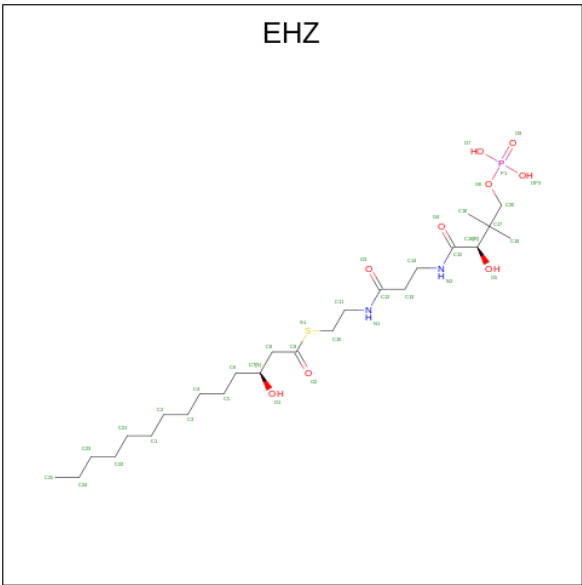


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
30	P	1	48	21	7	17	3	0

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

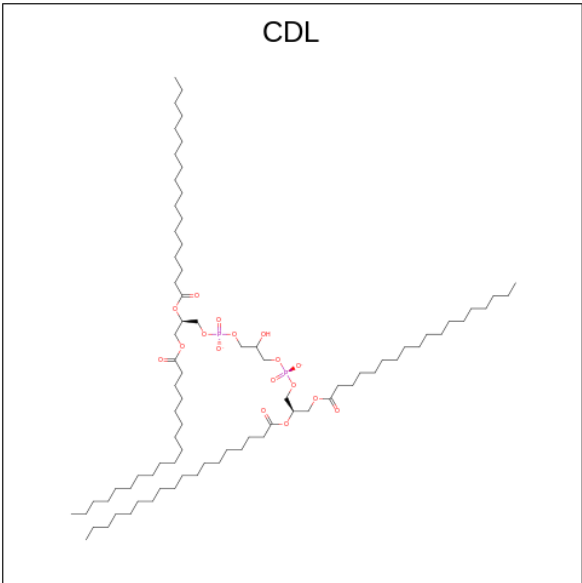
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
31	R	1	1	1	0

- Molecule 32 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).

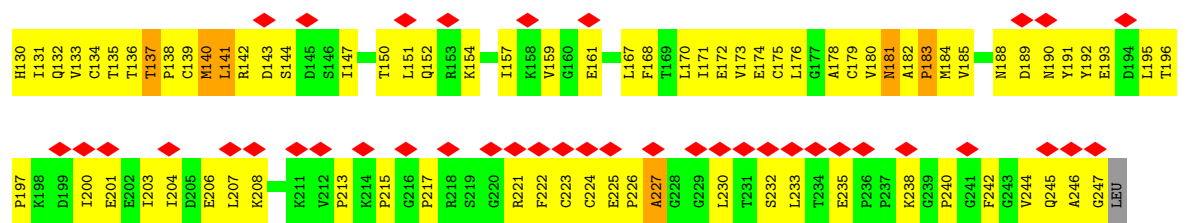


Mol	Chain	Residues	Atoms					AltConf	
32	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

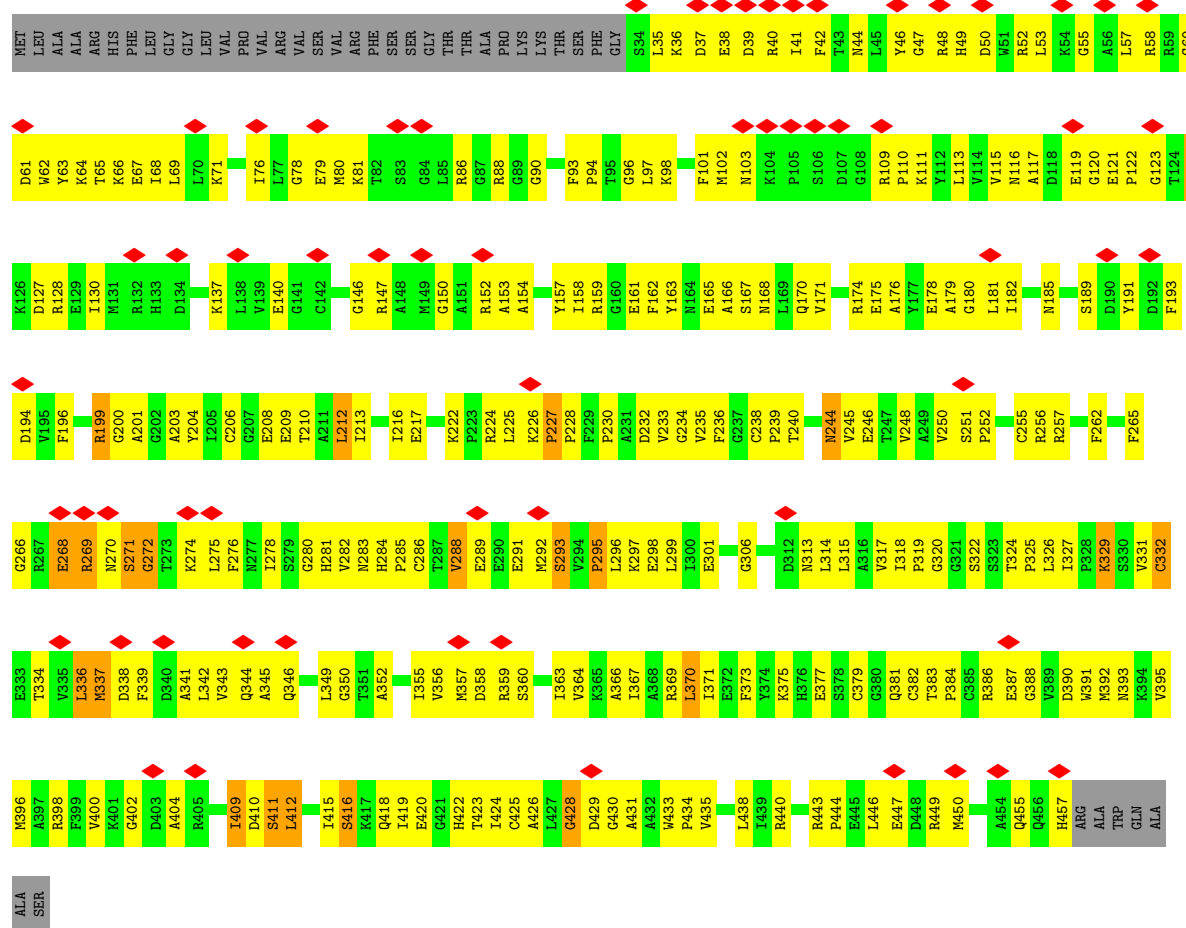
- Molecule 33 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



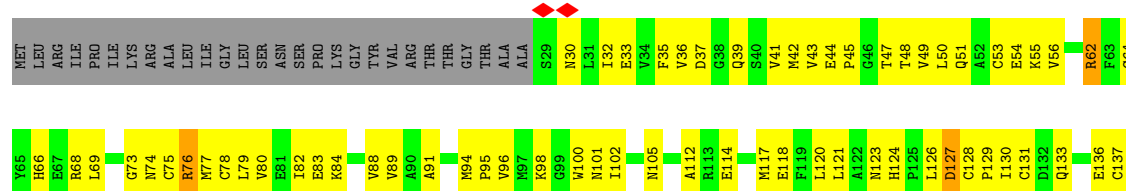
Mol	Chain	Residues	Atoms				AltConf
33	q	1	Total	C	O	P	0
			57	38	17	2	

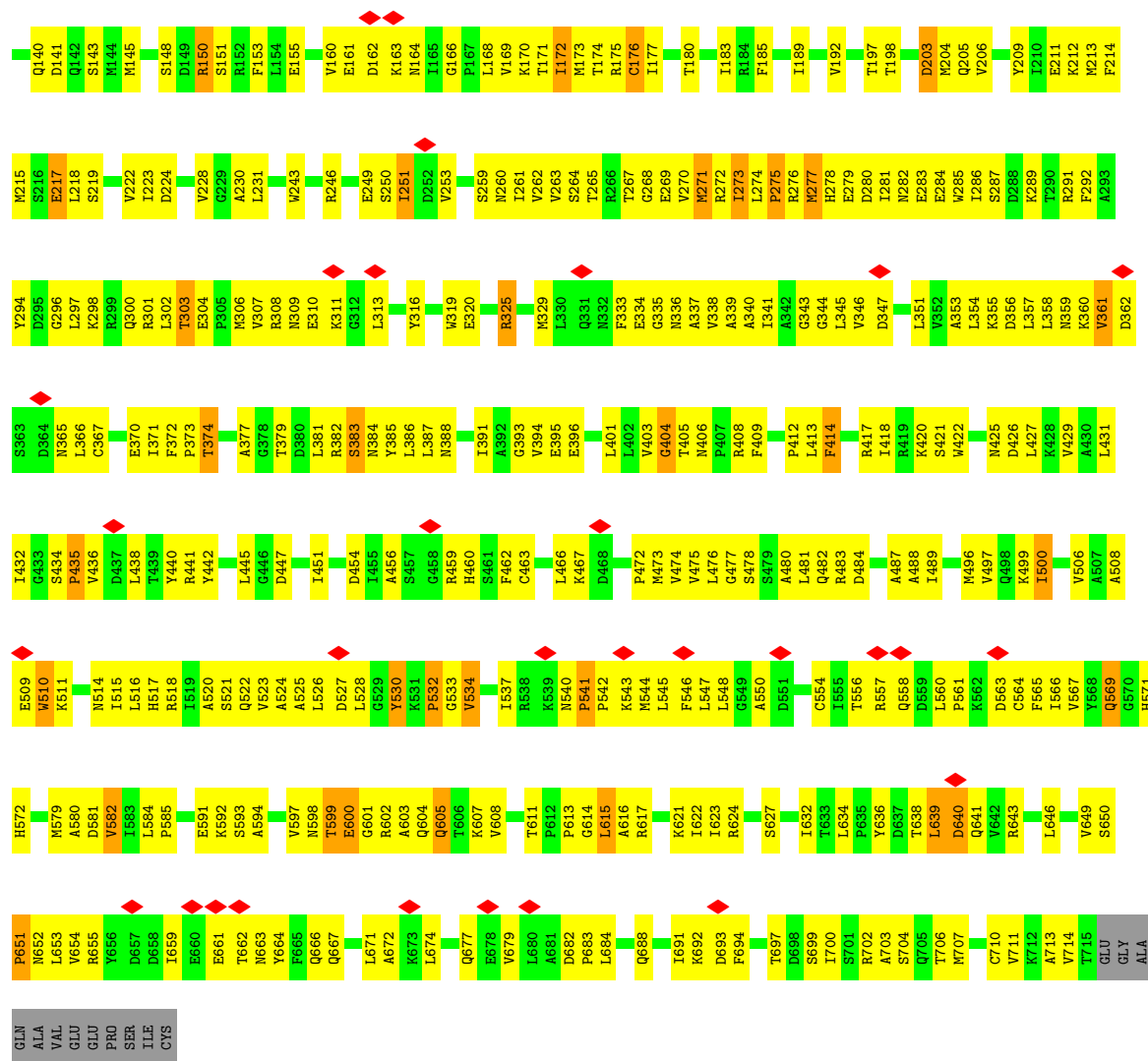


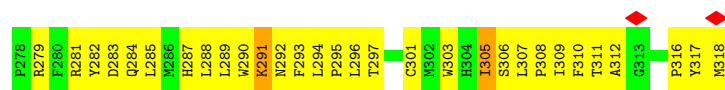
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



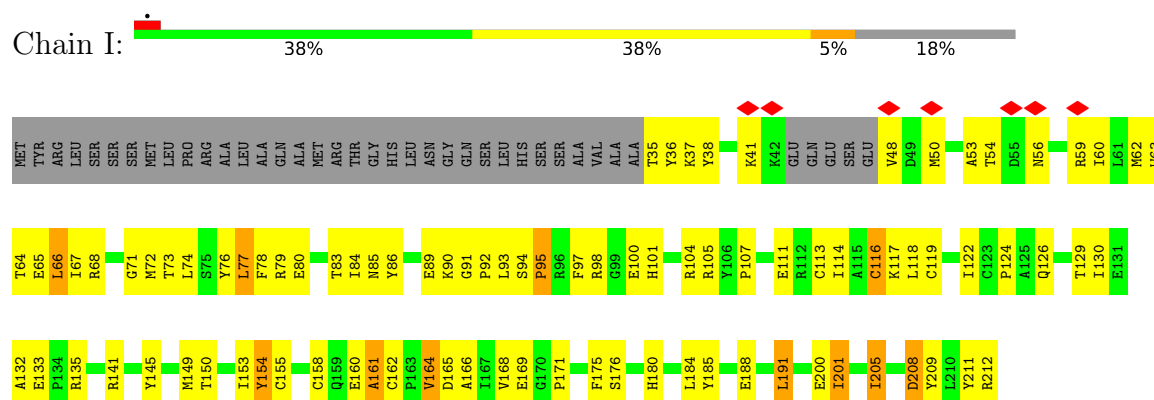
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



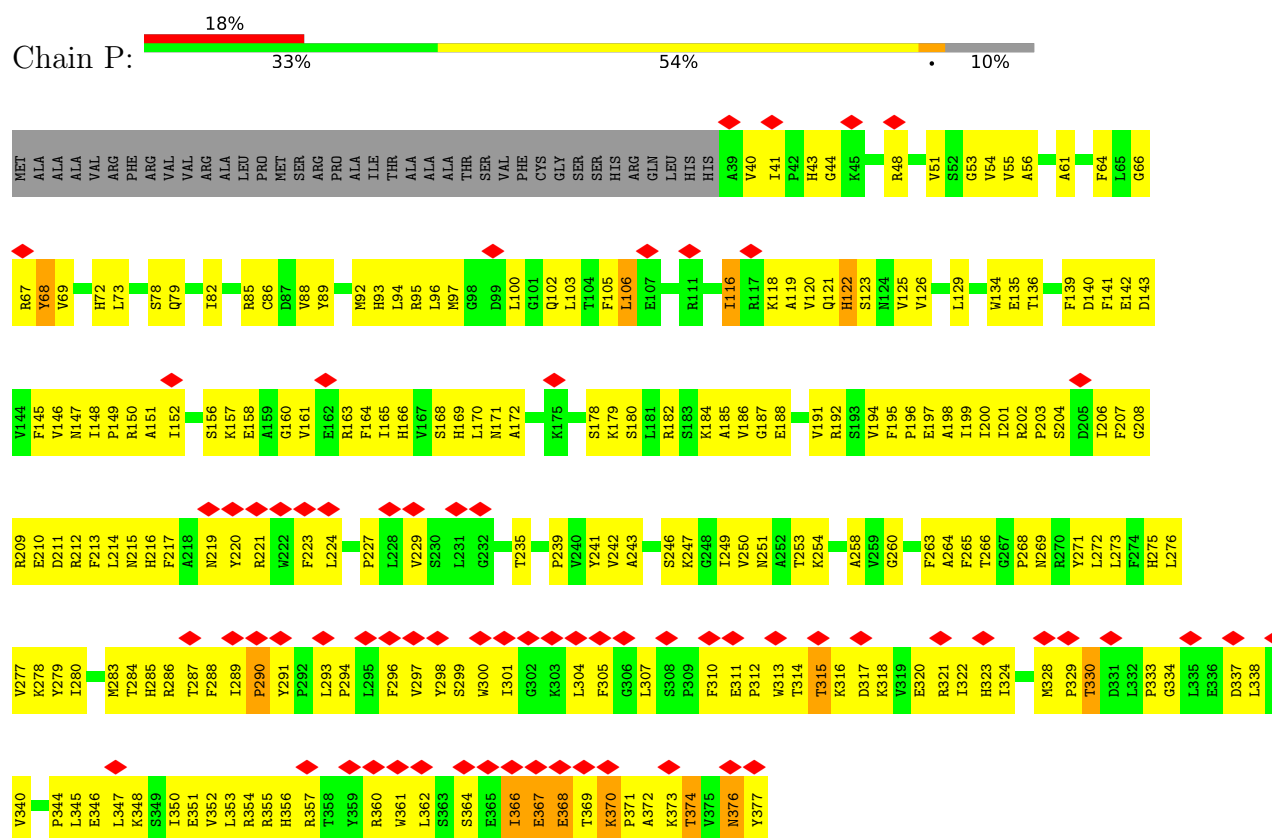




- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

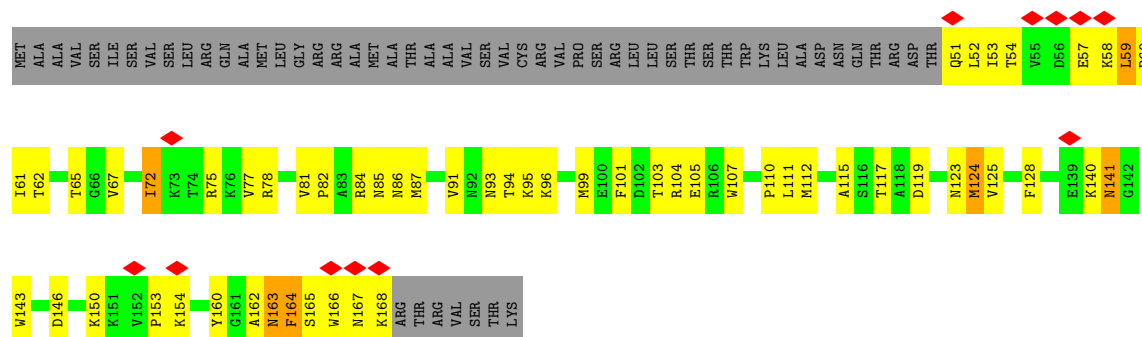


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

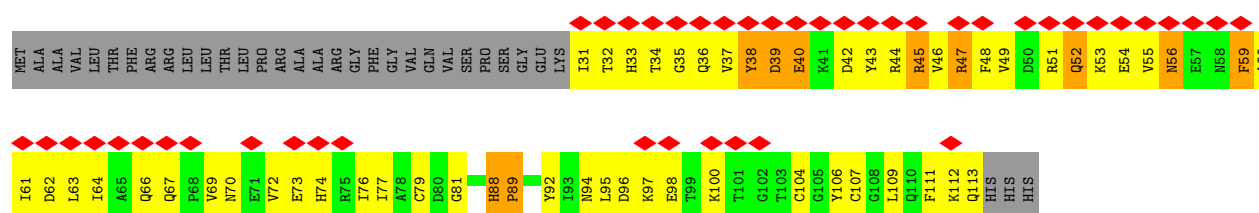
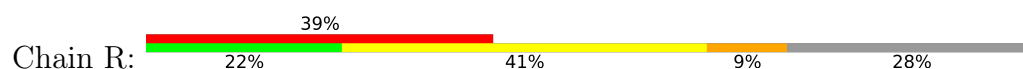


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

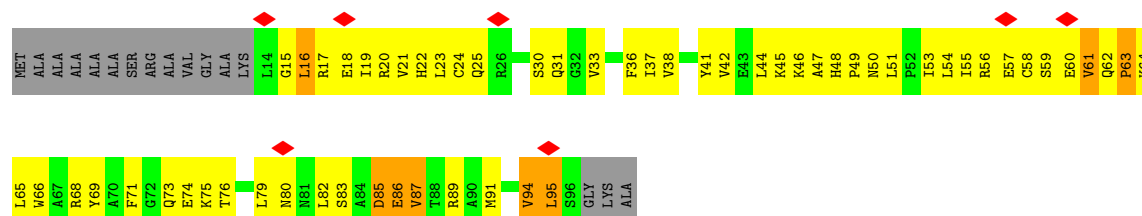




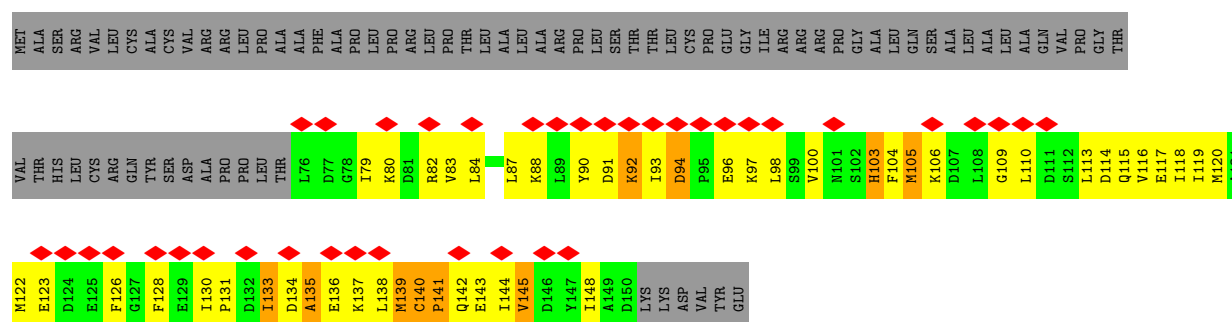
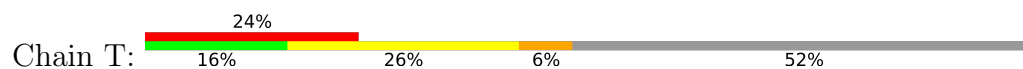
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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

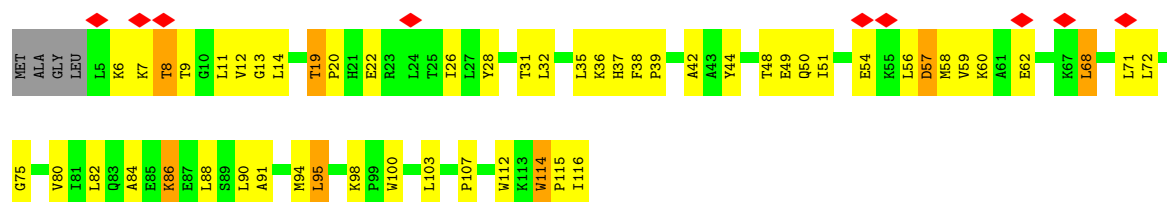


- Molecule 14: Acyl carrier protein, mitochondrial

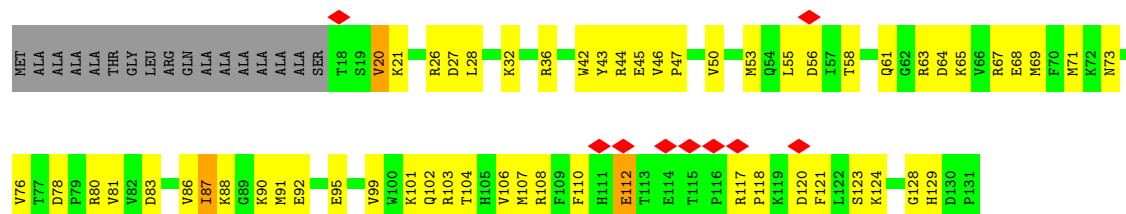
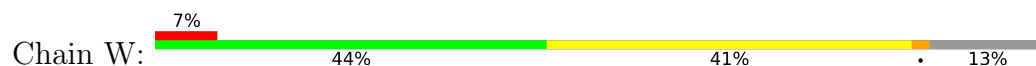


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

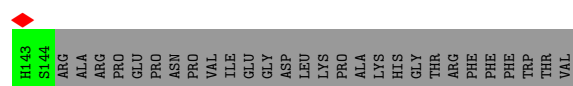
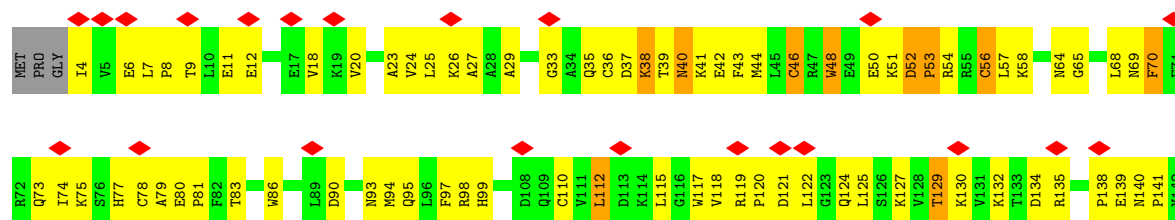




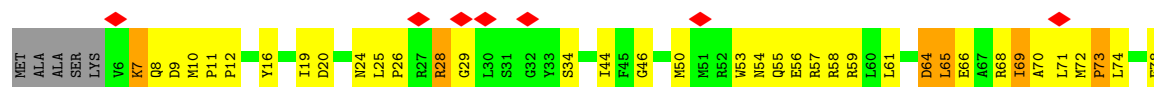
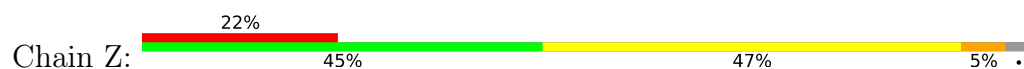
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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

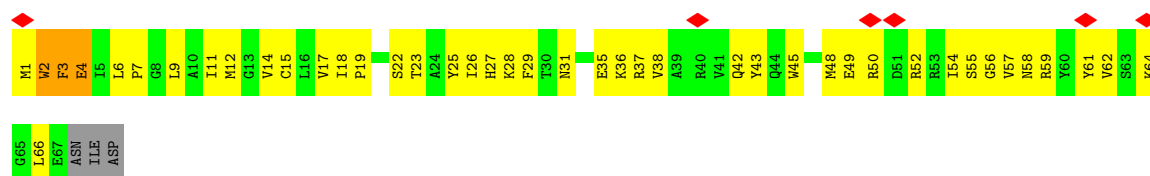


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

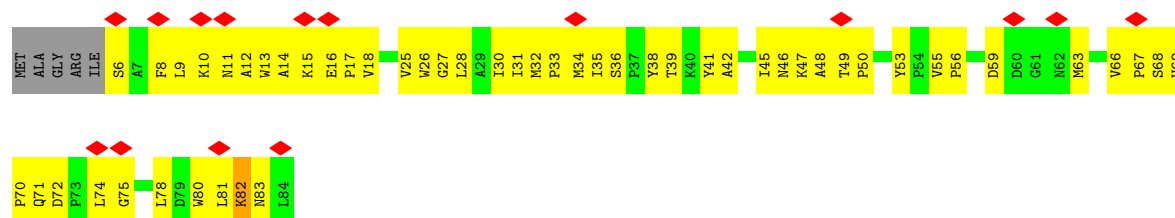


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

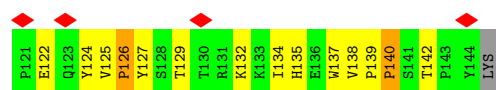
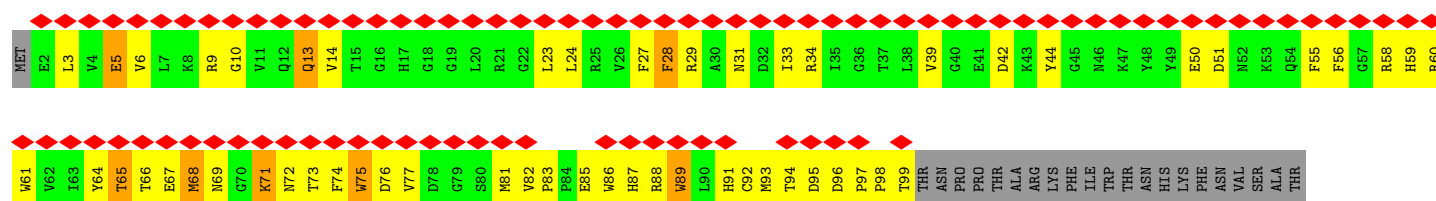




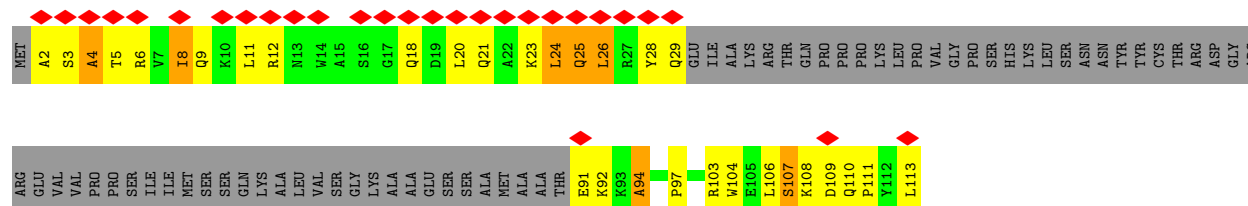
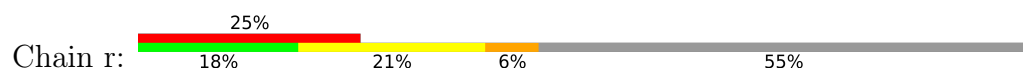
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



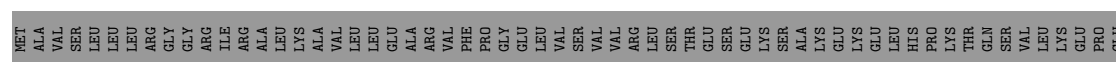
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

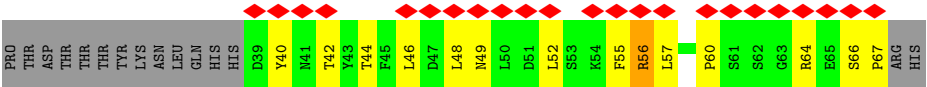


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19179	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 ($e^-/\text{\AA}^2$)	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	4.522	Depositor
Minimum map value	-1.281	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.55	Depositor
Map size ($\text{\AA}$)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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, PC1, FES, 3PE, ZN, UQ9, SF4, EHZ, FMN, 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	0.87	0/925	1.11	7/1262 (0.6%)
2	B	0.97	3/1278 (0.2%)	1.32	11/1730 (0.6%)
3	C	0.88	2/1687 (0.1%)	1.28	13/2297 (0.6%)
4	D	0.95	5/3162 (0.2%)	1.40	32/4276 (0.7%)
5	E	0.82	3/1675 (0.2%)	1.16	19/2282 (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	19/1915 (1.0%)
10	P	0.79	4/2793 (0.1%)	1.17	22/3787 (0.6%)
11	Q	0.88	1/980 (0.1%)	1.28	12/1324 (0.9%)
12	R	1.05	4/671 (0.6%)	1.38	12/903 (1.3%)
13	S	0.94	2/678 (0.3%)	1.47	11/915 (1.2%)
14	T	1.04	1/613 (0.2%)	1.56	13/826 (1.6%)
15	V	0.87	0/937	1.47	14/1270 (1.1%)
16	W	0.74	0/993	0.95	3/1335 (0.2%)
17	X	0.90	2/1180 (0.2%)	1.43	23/1591 (1.4%)
18	Z	0.84	1/1183 (0.1%)	1.24	11/1597 (0.7%)
19	a	0.88	0/561	1.38	8/755 (1.1%)
20	b	0.70	0/643	0.93	1/884 (0.1%)
21	q	1.05	3/1054 (0.3%)	1.53	20/1431 (1.4%)
22	r	1.17	3/426 (0.7%)	1.71	13/573 (2.3%)
23	s	0.46	0/244	1.09	2/331 (0.6%)
All	All	0.88	49/34429 (0.1%)	1.34	423/46648 (0.9%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	227	ALA	C-O	15.83	1.42	1.24
12	R	89	PRO	N-CD	-15.14	1.26	1.47
21	q	139	PRO	N-CD	-13.59	1.28	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	371	PRO	N-CD	12.93	1.65	1.47
7	G	532	PRO	N-CD	-12.63	1.30	1.47
14	T	141	PRO	N-CD	11.85	1.64	1.47
6	F	295	PRO	N-CD	-11.22	1.32	1.47
8	H	42	PRO	N-CD	10.78	1.62	1.47
22	r	91	GLU	N-CA	9.96	1.65	1.46
6	F	227	PRO	N-CD	9.88	1.61	1.47
10	P	290	PRO	N-CD	9.60	1.61	1.47
7	G	275	PRO	N-CD	-9.51	1.34	1.47
17	X	52	ASP	C-N	-9.44	1.25	1.33
5	E	44	PRO	N-CD	-9.41	1.34	1.47
6	F	319	PRO	N-CD	9.03	1.60	1.47
10	P	204	SER	C-O	-8.69	1.13	1.23
9	I	107	PRO	N-CD	8.65	1.59	1.47
4	D	163	PRO	N-CD	-8.32	1.36	1.47
18	Z	73	PRO	N-CD	8.02	1.58	1.47
13	S	63	PRO	N-CD	-7.99	1.36	1.47
12	R	39	ASP	CA-C	7.93	1.64	1.53
4	D	352	PRO	N-CD	-7.93	1.36	1.47
11	Q	53	ILE	C-O	7.89	1.33	1.24
12	R	40	GLU	N-CA	7.89	1.56	1.46
2	B	88	SER	C-N	-7.62	1.20	1.33
22	r	111	PRO	N-CD	-7.45	1.37	1.47
7	G	541	PRO	N-CD	-6.81	1.38	1.47
7	G	203	ASP	CA-C	6.71	1.62	1.52
7	G	600	GLU	CA-C	6.47	1.61	1.52
7	G	127	ASP	CA-C	6.34	1.62	1.52
3	C	66	GLU	C-N	6.34	1.41	1.33
2	B	153	PRO	N-CD	-6.33	1.38	1.47
4	D	266	ARG	C-O	-6.26	1.16	1.24
6	F	384	PRO	N-CD	-6.21	1.39	1.47
17	X	51	LYS	C-N	-6.13	1.25	1.33
2	B	110	PRO	C-O	-6.12	1.16	1.24
7	G	76	ARG	CA-C	6.10	1.61	1.53
5	E	93	PRO	N-CD	-5.91	1.39	1.47
22	r	25	GLN	CA-C	5.91	1.60	1.52
8	H	291	LYS	C-O	-5.88	1.16	1.24
12	R	59	PHE	CA-C	-5.68	1.45	1.52
10	P	204	SER	CA-C	-5.67	1.46	1.53
13	S	95	LEU	CA-C	5.42	1.59	1.52
7	G	683	PRO	N-CD	-5.39	1.40	1.47
4	D	392	PRO	C-O	-5.36	1.20	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	q	126	PRO	N-CD	5.31	1.55	1.47
4	D	266	ARG	CA-C	-5.19	1.45	1.52
21	q	69	ASN	CA-C	5.03	1.60	1.52
3	C	61	GLY	C-N	-5.01	1.27	1.33

All (423) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	142	VAL	N-CA-CB	19.26	132.41	110.65
4	D	142	VAL	N-CA-C	-19.07	92.50	110.42
7	G	174	THR	N-CA-C	-17.45	89.08	114.39
6	F	332	CYS	N-CA-C	15.56	130.00	111.02
22	r	91	GLU	N-CA-CB	14.54	135.23	110.50
21	q	139	PRO	N-CA-CB	-13.57	95.59	103.19
7	G	251	ILE	N-CA-C	13.21	126.66	108.17
9	I	164	VAL	N-CA-C	-12.71	100.25	112.83
7	G	77	MET	N-CA-C	-12.53	97.39	113.17
7	G	500	ILE	N-CA-C	-12.52	98.76	110.53
19	a	3	PHE	CB-CA-C	-12.38	89.64	110.68
10	P	106	LEU	N-CA-C	12.14	128.61	109.07
7	G	204	MET	N-CA-C	-11.69	91.36	109.25
6	F	449	ARG	N-CA-C	-11.55	98.77	111.36
6	F	288	VAL	N-CA-C	11.55	121.51	110.42
6	F	334	THR	N-CA-CB	11.43	127.19	109.82
7	G	599	THR	N-CA-C	11.35	126.22	112.38
11	Q	60	ASP	N-CA-C	-11.33	90.32	109.24
15	V	57	ASP	N-CA-C	-11.01	99.28	111.07
9	I	77	LEU	N-CA-C	-10.47	99.67	111.71
5	E	68	ASN	N-CA-C	-10.40	99.94	111.07
2	B	195	PRO	N-CA-C	-10.40	98.02	110.70
7	G	280	ASP	N-CA-C	10.38	122.60	111.28
14	T	139	MET	N-CA-C	-10.38	97.49	113.89
4	D	337	MET	N-CA-C	-10.23	100.12	111.07
4	D	140	ASP	CB-CA-C	-10.21	98.05	111.42
23	s	55	PHE	N-CA-C	10.19	125.71	112.26
7	G	414	PHE	N-CA-C	-10.17	101.37	113.88
10	P	366	ILE	N-CA-C	10.11	120.94	110.62
14	T	135	ALA	N-CA-C	-10.10	100.28	111.28
19	a	4	GLU	N-CA-C	10.09	124.84	112.54
9	I	161	ALA	N-CA-C	10.00	122.18	111.28
9	I	166	ALA	N-CA-C	-9.84	100.83	113.12
7	G	325	ARG	N-CA-C	-9.79	100.30	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	64	ALA	N-CA-C	-9.79	99.37	111.11
21	q	138	VAL	CA-C-N	-9.74	112.55	119.66
21	q	138	VAL	C-N-CA	-9.74	112.55	119.66
7	G	654	VAL	N-CA-C	9.70	123.22	111.09
16	W	87	ILE	N-CA-C	-9.66	101.15	110.42
19	a	2	TRP	N-CA-C	-9.65	101.51	113.28
10	P	371	PRO	N-CA-CB	9.62	111.83	103.36
6	F	418	GLN	N-CA-C	-9.60	100.77	111.14
8	H	91	MET	N-CA-C	-9.54	96.45	110.20
17	X	70	PHE	N-CA-C	-9.51	99.69	111.11
8	H	52	ALA	N-CA-C	-9.51	100.90	111.07
4	D	427	PRO	N-CA-C	-9.45	95.66	110.50
12	R	38	TYR	N-CA-C	-9.45	96.35	110.24
17	X	112	LEU	N-CA-C	-9.42	100.97	111.14
21	q	139	PRO	CA-N-CD	9.38	125.13	112.00
10	P	367	GLU	N-CA-C	9.38	122.70	111.82
7	G	694	PHE	N-CA-C	9.37	121.49	111.28
17	X	141	PRO	N-CA-C	-9.35	100.88	113.40
14	T	133	ILE	N-CA-C	9.34	119.88	110.82
7	G	692	LYS	N-CA-C	-9.23	100.60	112.23
18	Z	69	ILE	N-CA-C	-9.23	100.67	110.36
10	P	369	THR	N-CA-CB	9.22	123.45	110.17
5	E	85	ALA	N-CA-C	-9.21	101.32	111.36
7	G	640	ASP	N-CA-C	-9.16	101.37	111.36
6	F	103	ASN	N-CA-C	-9.12	101.08	113.30
19	a	57	VAL	N-CA-C	-9.00	105.16	113.71
6	F	411	SER	N-CA-C	-8.90	101.55	111.07
7	G	133	GLN	N-CA-CB	8.86	121.61	110.45
7	G	212	LYS	N-CA-C	-8.79	94.58	108.90
16	W	20	VAL	N-CA-C	8.69	120.79	108.36
9	I	154	TYR	N-CA-CB	-8.67	99.22	111.62
19	a	3	PHE	CA-CB-CG	8.64	122.44	113.80
13	S	18	GLU	N-CA-C	8.61	123.43	109.40
13	S	86	GLU	N-CA-C	-8.55	102.04	111.36
2	B	100	CYS	N-CA-C	-8.52	102.64	113.72
3	C	70	LYS	N-CA-C	8.51	121.63	111.33
10	P	373	LYS	N-CA-C	8.49	121.89	110.35
17	X	48	TRP	N-CA-C	8.45	120.57	111.36
3	C	108	LYS	N-CA-C	8.43	120.08	111.07
11	Q	54	THR	N-CA-C	8.38	123.36	109.46
7	G	532	PRO	CA-N-CD	8.36	123.70	112.00
17	X	99	HIS	N-CA-C	-8.32	102.29	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	558	GLN	N-CA-C	-8.29	102.20	111.07
8	H	196	ALA	N-CA-C	8.26	128.05	109.81
3	C	196	PRO	N-CA-C	8.22	124.96	113.53
7	G	484	ASP	N-CA-C	8.18	121.12	111.71
7	G	691	ILE	N-CA-C	8.18	123.67	111.89
15	V	86	LYS	N-CA-C	-8.15	102.34	111.14
6	F	411	SER	N-CA-CB	8.14	121.81	110.01
17	X	43	PHE	N-CA-C	-8.09	102.41	111.07
7	G	62	ARG	N-CA-C	8.06	121.55	108.32
7	G	500	ILE	N-CA-CB	8.05	120.88	110.57
7	G	534	VAL	N-CA-C	-8.04	104.75	111.91
9	I	201	ILE	N-CA-C	-8.02	102.62	110.72
13	S	76	THR	N-CA-C	7.95	121.86	108.90
21	q	67	GLU	CB-CA-C	-7.93	99.60	112.06
7	G	651	PRO	CB-CA-C	-7.93	98.48	111.56
2	B	110	PRO	N-CA-C	7.92	124.35	113.65
15	V	6	LYS	N-CA-C	-7.92	100.08	110.53
17	X	46	CYS	N-CA-C	-7.91	102.74	111.36
1	A	9	ILE	N-CA-C	-7.90	102.56	110.62
8	H	271	LEU	N-CA-C	-7.87	102.65	111.14
9	I	160	GLU	N-CA-C	7.84	124.22	111.37
17	X	58	LYS	N-CA-C	-7.83	102.70	111.07
9	I	74	LEU	N-CA-C	-7.81	102.76	111.28
7	G	270	VAL	N-CA-CB	-7.80	100.71	110.31
4	D	141	TYR	CA-C-N	7.75	130.18	120.72
4	D	141	TYR	C-N-CA	7.75	130.18	120.72
6	F	334	THR	N-CA-C	-7.74	101.58	111.02
21	q	44	TYR	N-CA-C	-7.72	98.85	110.28
21	q	89	TRP	N-CA-C	-7.69	102.84	111.14
12	R	74	HIS	N-CA-C	7.62	121.25	110.50
4	D	361	ALA	N-CA-C	-7.60	103.11	112.38
7	G	569	GLN	N-CA-C	7.60	121.99	108.24
12	R	47	ARG	N-CA-C	7.60	120.52	111.33
9	I	119	CYS	N-CA-C	-7.57	103.11	111.36
2	B	183	ARG	N-CA-C	-7.57	104.29	113.97
5	E	68	ASN	N-CA-CB	7.55	120.97	110.01
9	I	158	CYS	N-CA-C	-7.52	103.08	111.28
6	F	295	PRO	CA-N-CD	7.52	122.53	112.00
14	T	141	PRO	N-CA-C	-7.52	103.08	113.53
8	H	223	PHE	CB-CA-C	-7.51	99.09	110.88
18	Z	73	PRO	N-CA-C	-7.47	103.14	113.53
6	F	125	CYS	N-CA-C	-7.46	103.75	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	57	ASP	N-CA-CB	7.42	120.77	110.01
7	G	277	MET	N-CA-C	7.41	120.48	109.59
4	D	350	LYS	CB-CA-C	-7.41	100.96	111.85
7	G	510	TRP	N-CA-CB	7.38	120.84	109.85
7	G	661	GLU	N-CA-C	7.35	118.99	110.97
6	F	430	GLY	N-CA-C	7.34	121.54	112.73
7	G	374	THR	CB-CA-C	-7.33	99.70	111.28
7	G	303	THR	N-CA-C	7.32	122.92	113.18
13	S	94	VAL	N-CA-C	7.30	117.43	110.42
7	G	384	ASN	N-CA-C	-7.30	103.35	111.82
21	q	24	LEU	N-CA-C	-7.29	103.33	111.28
3	C	195	HIS	CB-CA-C	7.29	117.39	110.17
14	T	105	MET	N-CA-C	7.26	119.27	111.36
12	R	39	ASP	N-CA-C	7.26	121.12	110.59
8	H	50	ALA	N-CA-C	7.22	118.79	111.07
15	V	68	LEU	N-CA-C	-7.21	103.42	111.28
8	H	176	LEU	CA-C-N	-7.20	113.39	120.52
8	H	176	LEU	C-N-CA	-7.20	113.39	120.52
6	F	295	PRO	N-CA-CB	-7.20	96.71	103.19
6	F	269	ARG	N-CA-C	7.17	118.74	111.07
11	Q	162	ALA	N-CA-C	7.17	119.09	111.28
7	G	497	VAL	N-CA-C	-7.12	103.35	110.62
15	V	95	LEU	N-CA-C	-7.12	103.52	111.28
7	G	150	ARG	N-CA-C	7.06	119.66	109.14
4	D	99	LEU	N-CA-C	7.06	121.02	109.24
6	F	428	GLY	N-CA-C	-7.01	103.80	112.77
2	B	166	ASN	N-CA-C	-7.00	103.34	110.97
6	F	246	GLU	N-CA-C	-6.99	103.66	111.28
23	s	56	ARG	N-CA-C	6.98	120.55	108.76
7	G	217	GLU	N-CA-C	-6.97	101.83	110.41
6	F	455	GLN	N-CA-C	6.97	118.53	111.07
7	G	294	TYR	N-CA-C	-6.97	104.58	113.23
21	q	77	VAL	N-CA-C	-6.96	99.74	109.21
6	F	418	GLN	N-CA-CB	6.94	120.14	110.07
6	F	103	ASN	N-CA-CB	6.92	121.06	110.61
7	G	582	VAL	N-CA-C	6.92	118.44	108.48
18	Z	34	SER	N-CA-C	-6.91	103.68	111.07
12	R	45	ARG	N-CA-C	-6.89	104.74	113.01
14	T	145	VAL	N-CA-C	-6.87	103.79	110.72
7	G	268	GLY	N-CA-C	6.86	124.84	115.30
7	G	300	GLN	N-CA-CB	6.85	122.42	112.08
6	F	329	LYS	N-CA-C	6.84	119.60	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Z	28	ARG	N-CA-C	6.82	119.64	108.52
12	R	56	ASN	N-CA-C	6.82	120.01	108.90
8	H	8	THR	N-CA-C	-6.80	101.10	110.35
5	E	140	MET	N-CA-C	-6.80	103.80	111.07
22	r	11	LEU	N-CA-C	-6.76	103.99	111.36
6	F	244	ASN	N-CA-C	-6.75	100.98	110.50
7	G	133	GLN	N-CA-C	-6.74	101.31	110.68
15	V	114	TRP	N-CA-CB	6.71	120.29	110.30
7	G	434	SER	N-CA-C	-6.70	101.05	110.29
10	P	371	PRO	CA-N-CD	-6.68	102.65	112.00
7	G	640	ASP	N-CA-CB	6.68	120.04	110.16
9	I	208	ASP	N-CA-C	6.67	121.58	113.17
7	G	601	GLY	N-CA-C	6.67	124.90	115.30
15	V	8	THR	N-CA-C	6.66	118.98	108.79
17	X	129	THR	N-CA-C	6.64	120.86	110.17
4	D	184	ILE	N-CA-C	-6.63	103.86	110.62
8	H	182	ALA	N-CA-C	-6.63	103.98	111.07
6	F	344	GLN	N-CA-C	-6.63	104.06	111.28
15	V	86	LYS	N-CA-CB	6.62	119.67	110.07
7	G	287	SER	N-CA-C	6.62	119.26	110.53
7	G	435	PRO	N-CA-C	-6.61	100.12	110.50
3	C	125	PHE	N-CA-CB	-6.60	100.66	110.17
5	E	44	PRO	CA-N-CD	6.60	121.24	112.00
14	T	141	PRO	N-CA-CB	6.59	110.58	103.33
6	F	196	PHE	N-CA-C	6.59	119.89	109.81
10	P	116	ILE	N-CA-C	-6.58	104.07	110.72
6	F	228	PRO	N-CA-C	-6.58	98.92	112.47
6	F	336	LEU	N-CA-CB	-6.58	100.97	111.43
8	H	223	PHE	N-CA-C	-6.57	104.04	111.07
3	C	69	PRO	N-CA-C	-6.57	104.40	113.53
11	Q	141	ASN	N-CA-CB	6.56	120.76	110.46
8	H	208	VAL	N-CA-CB	-6.55	104.19	111.66
8	H	267	SER	N-CA-C	-6.54	104.23	111.36
4	D	388	GLY	N-CA-C	6.53	119.66	110.38
18	Z	65	LEU	N-CA-C	-6.53	104.24	111.36
22	r	24	LEU	N-CA-C	6.53	119.71	110.50
7	G	275	PRO	CA-N-CD	6.52	121.13	112.00
13	S	16	LEU	N-CA-C	-6.51	98.28	108.90
7	G	250	SER	N-CA-C	6.51	116.87	108.34
17	X	98	ARG	N-CA-C	6.51	120.49	112.54
15	V	49	GLU	N-CA-C	-6.50	104.19	111.28
7	G	361	VAL	N-CA-C	-6.48	105.01	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	q	75	TRP	N-CA-C	6.47	121.45	112.45
7	G	275	PRO	CB-CA-C	-6.46	102.51	110.98
12	R	81	GLY	N-CA-C	-6.46	106.81	115.21
6	F	370	LEU	N-CA-C	-6.45	104.33	111.36
3	C	125	PHE	N-CA-C	6.45	119.59	110.50
6	F	78	GLY	N-CA-C	-6.43	104.54	112.77
7	G	605	GLN	N-CA-C	6.43	119.00	108.52
8	H	177	PRO	N-CA-C	-6.42	101.56	111.13
14	T	141	PRO	CA-N-CD	-6.41	103.02	112.00
4	D	140	ASP	N-CA-C	-6.40	96.54	107.23
5	E	141	LEU	N-CA-C	-6.37	101.68	110.35
7	G	95	PRO	N-CA-C	-6.37	101.19	110.80
7	G	273	ILE	N-CA-C	-6.36	98.35	107.77
21	q	28	PHE	N-CA-C	6.35	117.87	111.07
6	F	416	SER	N-CA-C	6.34	117.86	111.07
6	F	415	ILE	N-CA-C	-6.34	104.32	110.72
11	Q	59	LEU	N-CA-C	-6.34	100.79	110.30
7	G	176	CYS	N-CA-C	6.34	119.67	110.42
15	V	71	LEU	N-CA-C	6.33	118.18	111.28
8	H	271	LEU	N-CA-CB	6.33	119.25	110.07
15	V	91	ALA	N-CA-C	-6.33	104.39	111.28
4	D	141	TYR	N-CA-C	6.32	120.99	113.16
9	I	205	ILE	N-CA-C	-6.31	104.34	110.72
7	G	383	SER	N-CA-C	-6.29	106.83	114.75
19	a	26	ILE	N-CA-C	-6.29	104.52	113.07
10	P	315	THR	N-CA-C	6.27	118.94	109.23
22	r	26	LEU	N-CA-CB	-6.26	101.02	110.35
5	E	64	ALA	N-CA-CB	6.26	119.27	109.94
8	H	269	THR	N-CA-C	6.25	118.09	111.28
8	H	52	ALA	N-CA-CB	6.24	119.06	110.01
4	D	233	HIS	N-CA-C	6.24	119.01	111.40
17	X	99	HIS	N-CA-CB	6.22	119.37	110.16
11	Q	141	ASN	N-CA-C	-6.21	105.70	113.28
2	B	113	ASP	N-CA-CB	6.21	119.47	109.28
22	r	8	ILE	N-CA-C	-6.21	104.45	110.72
6	F	409	ILE	N-CA-C	6.17	116.34	110.42
7	G	325	ARG	N-CA-CB	6.17	118.92	109.91
8	H	101	GLY	N-CA-C	6.17	120.11	112.64
18	Z	69	ILE	N-CA-CB	6.17	117.36	110.51
21	q	69	ASN	N-CA-CB	6.17	121.28	111.66
6	F	212	LEU	N-CA-C	-6.17	104.56	111.28
8	H	276	SER	N-CA-C	6.16	118.97	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	291	VAL	N-CA-C	-6.14	103.41	111.09
7	G	418	ILE	N-CA-C	-6.13	103.45	112.04
7	G	420	LYS	N-CA-C	6.12	118.74	111.33
10	P	118	LYS	N-CA-C	6.12	118.92	111.82
13	S	87	VAL	N-CA-C	-6.12	104.38	110.62
10	P	368	GLU	N-CA-CB	6.12	119.72	110.30
13	S	61	VAL	N-CA-C	-6.12	99.67	108.42
7	G	508	ALA	N-CA-C	6.08	117.91	111.28
6	F	272	GLY	N-CA-C	6.07	122.30	111.01
7	G	638	THR	N-CA-C	-6.07	100.08	109.24
18	Z	65	LEU	N-CA-CB	6.07	119.14	110.16
17	X	51	LYS	N-CA-C	6.05	117.57	110.97
2	B	196	PRO	N-CA-C	-6.03	101.74	111.03
8	H	24	GLU	N-CA-C	-6.03	104.07	112.45
7	G	353	ALA	N-CA-C	-6.03	104.64	112.23
7	G	532	PRO	N-CA-CB	-6.01	97.07	103.38
12	R	34	THR	N-CA-C	-6.00	106.61	112.97
8	H	185	TRP	N-CA-C	-5.99	104.12	112.45
10	P	370	LYS	N-CA-C	5.99	119.19	108.47
8	H	7	LEU	N-CA-C	-5.99	104.39	111.03
9	I	66	LEU	N-CA-C	-5.98	104.33	111.69
4	D	352	PRO	N-CA-CB	-5.96	97.30	103.08
22	r	92	LYS	N-CA-CB	-5.94	101.61	110.17
10	P	330	THR	CB-CA-C	-5.92	109.74	116.54
22	r	108	LYS	N-CA-C	5.92	117.81	111.36
7	G	639	LEU	N-CA-C	5.90	118.67	111.82
7	G	480	ALA	N-CA-C	-5.90	104.93	111.36
5	E	66	VAL	N-CA-C	5.89	116.55	110.36
13	S	86	GLU	N-CA-CB	5.89	118.88	110.16
14	T	94	ASP	N-CA-CB	-5.88	105.13	111.66
17	X	38	LYS	N-CA-C	-5.88	104.78	111.07
7	G	275	PRO	N-CA-CB	-5.85	97.89	103.33
7	G	672	ALA	N-CA-C	-5.85	104.91	111.28
21	q	5	GLU	N-CA-C	-5.85	104.99	111.36
18	Z	44	ILE	N-CA-C	-5.84	104.81	110.42
9	I	116	CYS	N-CA-C	-5.84	105.65	112.89
15	V	19	THR	N-CA-CB	5.84	120.76	110.37
21	q	65	THR	N-CA-C	5.83	119.18	110.14
11	Q	164	PHE	N-CA-CB	5.83	119.86	110.42
8	H	208	VAL	N-CA-C	5.83	116.06	107.15
10	P	367	GLU	CB-CA-C	-5.81	99.51	110.67
5	E	223	CYS	CB-CA-C	-5.81	109.33	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	209	LEU	N-CA-CB	-5.81	100.72	110.83
17	X	36	CYS	CB-CA-C	-5.80	102.52	111.74
6	F	393	ASN	N-CA-C	-5.79	104.88	111.07
10	P	122	HIS	N-CA-C	5.79	120.03	112.92
7	G	289	LYS	N-CA-C	5.78	117.58	111.28
19	a	3	PHE	N-CA-CB	5.76	118.70	110.06
17	X	97	PHE	N-CA-C	5.75	118.49	111.82
5	E	137	THR	CA-C-N	-5.74	113.00	118.97
5	E	137	THR	C-N-CA	-5.74	113.00	118.97
10	P	272	LEU	N-CA-C	-5.74	101.78	110.28
4	D	414	ASP	N-CA-C	-5.74	101.46	110.36
4	D	258	VAL	N-CA-C	-5.72	104.10	110.62
9	I	191	LEU	N-CA-C	-5.69	105.16	111.36
10	P	119	ALA	N-CA-C	-5.68	105.00	111.14
13	S	73	GLN	N-CA-C	-5.68	100.44	109.59
13	S	63	PRO	CA-N-CD	5.67	119.94	112.00
6	F	457	HIS	N-CA-CB	-5.67	100.87	110.50
21	q	140	PRO	N-CA-C	-5.66	102.25	110.80
11	Q	124	MET	CA-C-N	-5.65	114.96	122.98
11	Q	124	MET	C-N-CA	-5.65	114.96	122.98
2	B	135	GLY	N-CA-C	5.64	118.62	111.85
12	R	52	GLN	N-CA-C	5.63	117.97	110.53
2	B	112	TYR	N-CA-C	5.63	122.80	110.80
7	G	615	LEU	N-CA-C	-5.62	106.19	113.16
17	X	53	PRO	N-CA-C	-5.62	106.83	114.80
2	B	201	LEU	N-CA-C	-5.61	105.16	111.28
17	X	40	ASN	N-CA-C	-5.61	104.85	110.97
6	F	268	GLU	CB-CA-C	-5.60	110.10	116.54
12	R	35	GLY	N-CA-C	5.59	121.65	113.48
7	G	599	THR	CA-C-N	-5.59	114.22	122.83
7	G	599	THR	C-N-CA	-5.59	114.22	122.83
5	E	119	THR	N-CA-C	-5.59	105.96	112.89
21	q	68	MET	N-CA-C	5.59	119.36	112.54
4	D	352	PRO	N-CA-C	5.58	117.51	110.70
7	G	530	TYR	N-CA-C	-5.58	102.02	110.28
17	X	56	CYS	N-CA-C	5.58	119.79	112.92
17	X	52	ASP	CA-C-N	5.57	127.63	120.89
17	X	52	ASP	C-N-CA	5.57	127.63	120.89
5	E	183	PRO	N-CA-C	-5.57	102.19	111.26
18	Z	64	ASP	N-CA-C	5.56	119.79	112.89
12	R	89	PRO	N-CA-CB	-5.55	98.28	103.27
4	D	163	PRO	N-CA-CB	-5.53	97.72	103.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	127	ASP	CA-C-O	5.53	129.02	121.89
21	q	142	THR	N-CA-CB	5.52	119.78	109.68
4	D	132	ALA	N-CA-C	-5.51	106.56	113.72
22	r	94	ALA	N-CA-C	-5.50	101.70	109.96
14	T	135	ALA	N-CA-CB	5.49	118.19	110.12
19	a	25	TYR	N-CA-C	-5.48	107.84	114.75
4	D	231	GLY	N-CA-C	-5.47	103.04	110.43
10	P	86	CYS	N-CA-C	-5.47	103.16	110.55
21	q	71	LYS	N-CA-C	5.46	119.94	113.16
7	G	404	GLY	N-CA-C	5.45	121.43	113.48
22	r	111	PRO	N-CA-C	-5.44	106.44	113.57
7	G	150	ARG	N-CA-CB	-5.43	102.82	111.62
5	E	74	GLN	N-CA-C	-5.43	107.31	114.04
4	D	201	PHE	N-CA-C	-5.42	105.45	111.36
7	G	556	THR	N-CA-C	-5.42	101.52	109.81
12	R	88	HIS	CB-CA-C	5.41	117.35	109.08
10	P	374	THR	N-CA-C	5.40	117.53	108.73
6	F	199	ARG	N-CA-C	5.40	117.53	109.59
7	G	682	ASP	CA-C-N	-5.39	114.21	119.76
7	G	682	ASP	C-N-CA	-5.39	114.21	119.76
7	G	420	LYS	N-CA-CB	-5.39	101.98	110.06
18	Z	55	GLN	N-CA-C	-5.39	105.41	111.28
11	Q	164	PHE	N-CA-C	-5.38	106.69	113.20
6	F	180	GLY	N-CA-C	-5.38	108.22	115.21
4	D	109	CYS	N-CA-C	5.38	118.50	107.69
17	X	27	ALA	N-CA-C	-5.38	105.08	111.69
4	D	391	VAL	CA-C-N	-5.38	115.79	119.66
4	D	391	VAL	C-N-CA	-5.38	115.79	119.66
4	D	200	PHE	CA-CB-CG	5.37	119.17	113.80
11	Q	163	ASN	CB-CA-C	-5.36	99.29	109.95
17	X	33	GLY	N-CA-C	-5.36	107.68	114.16
2	B	101	ALA	N-CA-C	-5.36	105.44	111.28
14	T	92	LYS	N-CA-C	-5.34	106.35	112.92
4	D	141	TYR	N-CA-CB	-5.33	102.28	110.44
5	E	143	ASP	N-CA-C	5.33	118.98	111.52
18	Z	50	MET	N-CA-C	-5.32	105.48	111.28
7	G	510	TRP	N-CA-C	-5.32	101.98	109.96
10	P	68	TYR	N-CA-C	5.31	117.15	111.36
5	E	44	PRO	N-CA-CB	-5.31	97.66	103.39
7	G	435	PRO	CB-CA-C	-5.29	105.79	111.56
11	Q	72	ILE	N-CA-C	-5.28	108.35	113.53
9	I	160	GLU	N-CA-CB	-5.28	100.75	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	84	ALA	N-CA-C	5.28	116.72	111.07
8	H	46	LEU	N-CA-C	-5.27	106.62	113.16
8	H	103	LEU	N-CA-C	-5.26	105.44	111.07
4	D	363	VAL	N-CA-C	5.24	116.31	111.81
7	G	600	GLU	CB-CA-C	-5.23	102.96	111.06
6	F	412	LEU	N-CA-C	-5.22	105.76	111.82
8	H	146	MET	N-CA-C	-5.22	105.48	111.07
8	H	305	ILE	N-CA-C	-5.21	106.06	111.58
1	A	79	ILE	N-CA-C	-5.21	104.39	111.89
4	D	391	VAL	N-CA-C	5.18	113.84	109.02
7	G	713	ALA	N-CA-C	-5.18	105.53	111.07
22	r	107	SER	N-CA-C	-5.18	102.19	109.96
22	r	25	GLN	N-CA-C	5.17	118.85	112.54
3	C	156	VAL	N-CA-C	-5.17	104.04	111.17
7	G	277	MET	N-CA-CB	-5.17	101.76	109.71
3	C	109	SER	N-CA-C	5.15	118.21	109.76
13	S	85	ASP	N-CA-C	5.15	117.79	111.82
7	G	569	GLN	CB-CA-C	-5.14	104.23	112.05
8	H	277	TYR	N-CA-C	5.14	117.96	110.10
6	F	271	SER	N-CA-C	-5.14	99.92	108.34
20	b	82	LYS	N-CA-C	-5.13	103.75	110.53
3	C	164	TRP	N-CA-C	5.13	116.95	111.36
9	I	95	PRO	N-CA-C	5.13	121.25	113.81
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	-5.12	103.08	111.68
7	G	172	ILE	N-CA-C	-5.11	98.71	109.34
22	r	111	PRO	CA-N-CD	5.10	119.14	112.00
1	A	66	ASP	N-CA-C	-5.09	105.64	111.14
1	A	48	ARG	N-CA-C	-5.08	106.64	114.16
10	P	204	SER	CA-C-O	-5.08	115.14	121.50
7	G	393	GLY	N-CA-C	-5.07	107.75	115.66
1	A	2	ASN	CA-C-N	-5.06	113.10	120.29
1	A	2	ASN	C-N-CA	-5.06	113.10	120.29
5	E	181	ASN	N-CA-C	-5.06	99.55	108.20
7	G	280	ASP	N-CA-CB	-5.06	102.69	110.12
6	F	293	SER	CB-CA-C	-5.05	104.43	111.80
1	A	69	ILE	N-CA-C	-5.04	105.06	110.36
10	P	376	ASN	CB-CA-C	-5.04	102.28	110.85
17	X	112	LEU	N-CA-CB	5.04	117.38	110.07
5	E	137	THR	N-CA-C	5.04	120.94	109.81
14	T	140	CYS	N-CA-C	5.04	116.69	109.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	140	CYS	CB-CA-C	-5.03	104.11	109.85
21	q	13	GLN	N-CA-C	-5.03	105.68	111.07
7	G	203	ASP	CA-C-O	5.03	127.16	121.32
9	I	160	GLU	CB-CA-C	5.03	119.19	110.84
3	C	221	GLU	N-CA-C	-5.02	102.43	108.25
21	q	89	TRP	N-CA-CB	5.02	117.34	110.07
16	W	112	GLU	N-CA-C	5.02	116.83	111.36
3	C	208	GLU	CA-C-O	-5.01	115.74	121.40
22	r	4	ALA	N-CA-C	-5.01	105.92	112.23
4	D	224	ALA	N-CA-C	5.00	117.11	111.11
9	I	90	LYS	N-CA-C	5.00	117.64	109.59

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	901	0	947	158	0
2	B	1247	0	1256	172	0
3	C	1641	0	1596	115	0
4	D	3088	0	3059	315	0
5	E	1635	0	1626	174	0
6	F	3273	0	3231	309	0
7	G	5287	0	5323	530	0
8	H	2531	0	2619	352	0
9	I	1389	0	1352	136	0
10	P	2720	0	2740	225	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	77	0
16	W	970	0	991	74	0
17	X	1153	0	1141	98	0
18	Z	1152	0	1148	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	a	548	0	562	59	0
20	b	620	0	617	75	0
21	q	1020	0	976	92	0
22	r	418	0	434	49	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	21	0	20	31	0
25	H	35	0	43	17	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	97	0	151	19	0
30	P	48	0	26	5	0
31	R	1	0	0	0	0
32	W	32	0	0	7	0
33	q	57	0	58	22	0
All	All	34090	0	34085	2922	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 43.

All (2922) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PHE:CD2	4:D:96:ARG:HD2	1.45	1.52
2:B:121:PHE:CD1	25:B:302:UQ9:H10A	1.46	1.49
1:A:33:LYS:HG2	8:H:61:MET:CE	1.55	1.36
1:A:41:PHE:CE2	4:D:96:ARG:HD2	1.62	1.32
2:B:121:PHE:CE1	25:B:302:UQ9:H10A	1.67	1.28
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
1:A:41:PHE:CE2	4:D:96:ARG:CD	2.25	1.19
15:V:44:TYR:CE1	15:V:48:THR:HG21	1.77	1.18
1:A:62:PHE:HA	8:H:290:TRP:HH2	1.07	1.17
16:W:42:TRP:CH2	32:W:201:EHZ:O1	1.97	1.16
1:A:65:PHE:CZ	1:A:102:LEU:HB2	1.80	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:MET:HG2	25:B:302:UQ9:H7A	1.30	1.13
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.22	1.12
12:R:38:TYR:CE2	21:q:127:TYR:HB2	1.85	1.12
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.47	1.11
12:R:38:TYR:HE2	21:q:127:TYR:HB2	1.04	1.11
9:I:53:ALA:HB1	20:b:14:ALA:HB2	1.27	1.10
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.34	1.09
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.12	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	1.08
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.08
1:A:33:LYS:HG2	8:H:61:MET:HE1	1.13	1.07
2:B:104:MET:HE2	2:B:121:PHE:CE2	1.88	1.07
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
2:B:121:PHE:CD1	25:B:302:UQ9:C10	2.36	1.07
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.34	1.06
13:S:23:LEU:HD12	13:S:23:LEU:O	1.54	1.06
14:T:138:LEU:HD12	14:T:138:LEU:O	1.55	1.06
6:F:270:ASN:OD1	6:F:270:ASN:O	1.70	1.06
1:A:62:PHE:HA	8:H:290:TRP:CH2	1.90	1.05
2:B:121:PHE:CG	25:B:302:UQ9:C10	2.39	1.05
9:I:54:THR:HG22	20:b:13:TRP:HE1	1.02	1.05
1:A:41:PHE:CD2	4:D:96:ARG:CD	2.38	1.05
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	1.05
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.70	1.05
1:A:62:PHE:CE1	8:H:144:VAL:CG2	2.40	1.04
2:B:149:TYR:HA	2:B:152:MET:HE2	1.36	1.04
1:A:65:PHE:HZ	1:A:102:LEU:HB2	0.92	1.03
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.03
2:B:121:PHE:CG	25:B:302:UQ9:H10A	1.93	1.03
9:I:53:ALA:CB	20:b:14:ALA:HB2	1.88	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.57	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.76	1.02
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.95	1.02
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	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	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:66:THR:HG22	21:q:74:PHE:HB2	1.39	1.00
2:B:104:MET:HE2	2:B:121:PHE:CZ	1.97	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	1.00
5:E:134:CYS:HG	27:E:301:FES:FE1	0.77	0.99
5:E:203:ILE:HG23	5:E:213:PRO:HG2	1.43	0.99
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.99
15:V:44:TYR:CZ	15:V:48:THR:HG21	1.97	0.99
17:X:90:ASP:OD2	19:a:62:VAL:HG11	1.59	0.99
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.98
2:B:82:ILE:HG23	8:H:57:MET:SD	2.03	0.97
1:A:33:LYS:HG2	8:H:61:MET:HE3	1.41	0.97
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.47	0.97
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.97
6:F:379:CYS:SG	24:F:502:SF4:FE1	1.56	0.97
9:I:54:THR:CG2	20:b:13:TRP:HE1	1.77	0.97
16:W:55:LEU:HB3	16:W:107:MET:CE	1.94	0.97
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.96
6:F:382:CYS:HG	24:F:502:SF4:FE2	0.78	0.96
10:P:376:ASN:OD1	10:P:377:TYR:N	1.98	0.96
2:B:121:PHE:CE1	25:B:302:UQ9:C10	2.48	0.96
2:B:121:PHE:CE2	25:B:302:UQ9:H10	2.01	0.96
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.96
6:F:63:TYR:HB3	6:F:256:ARG:HE	1.29	0.96
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.96
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.95
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.95
9:I:54:THR:HG22	20:b:13:TRP:NE1	1.80	0.95
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.95
2:B:108:ALA:HB1	25:B:302:UQ9:H12	1.46	0.95
1:A:33:LYS:CG	8:H:61:MET:HE1	1.97	0.95
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.95
1:A:62:PHE:CD1	8:H:144:VAL:HG21	2.02	0.94
5:E:189:ASP:CG	6:F:163:TYR:HB3	1.92	0.94
13:S:16:LEU:HD11	13:S:51:LEU:HD11	1.46	0.94
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.47	0.94
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.94
3:C:85:ILE:CD1	3:C:140:ILE:HD11	1.98	0.94
7:G:78:CYS:SG	27:G:803:FES:FE2	1.59	0.94
7:G:64:CYS:HG	27:G:803:FES:FE1	0.71	0.94
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
9:I:162:CYS:SG	24:I:303:SF4:FE4	1.60	0.93
1:A:33:LYS:HG3	2:B:150:ASP:O	1.69	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	0.93
7:G:176:CYS:SG	24:G:802:SF4:FE4	1.59	0.92
18:Z:90:ASN:O	18:Z:94:GLU:HB2	1.69	0.92
1:A:62:PHE:CD1	8:H:144:VAL:CG2	2.53	0.92
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.35	0.92
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.51	0.91
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.91
16:W:55:LEU:HB3	16:W:107:MET:HE1	1.52	0.90
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.90
9:I:80:GLU:HG3	19:a:1:MET:SD	2.11	0.90
5:E:179:CYS:SG	27:E:301:FES:FE2	1.63	0.90
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.06	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
3:C:63:TYR:HH	3:C:102:HIS:HE2	1.19	0.90
7:G:362:ASP:HB2	13:S:71:PHE:CE1	2.06	0.90
2:B:105:MET:HG2	25:B:302:UQ9:C7	2.02	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
5:E:39:VAL:HG22	7:G:205:GLN:HE22	1.34	0.89
21:q:76:ASP:OD1	21:q:76:ASP:O	1.90	0.89
13:S:16:LEU:HD22	13:S:19:ILE:HD11	1.53	0.89
7:G:431:LEU:HD22	7:G:438:LEU:HD11	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
3:C:102:HIS:HE1	15:V:48:THR:HG22	1.35	0.89
9:I:67:ILE:HG23	26:I:301:PC1:H381	1.53	0.89
14:T:79:ILE:HB	14:T:145:VAL:HG13	1.55	0.89
6:F:41:ILE:HG21	6:F:250:VAL:HG12	1.54	0.88
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.88
16:W:32:LYS:NZ	32:W:201:EHZ:C19	2.37	0.88
4:D:270:ASN:HB3	8:H:284:GLN:NE2	1.87	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
6:F:55:GLY:HA2	6:F:58:ARG:HD2	1.54	0.88
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.88
6:F:379:CYS:HG	24:F:502:SF4:FE1	0.89	0.87
10:P:221:ARG:HD3	10:P:286:ARG:CD	2.05	0.87
10:P:122:HIS:HB2	12:R:46:VAL:HG12	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:CYS:HB3	4:D:141:TYR:CD2	2.10	0.87
1:A:62:PHE:HE1	8:H:144:VAL:CG2	1.84	0.87
12:R:32:THR:HG22	12:R:36:GLN:H	1.40	0.87
12:R:51:ARG:HH21	21:q:125:VAL:HG12	1.38	0.87
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.56	0.86
22:r:2:ALA:N	22:r:26:LEU:CD1	2.37	0.86
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.03	0.86
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.86
3:C:217:ARG:HH12	16:W:112:GLU:HB2	1.38	0.86
7:G:617:ARG:NH1	16:W:129:HIS:HA	1.90	0.86
26:B:303:PC1:H322	26:B:303:PC1:H232	1.55	0.86
2:B:121:PHE:CD2	25:B:302:UQ9:C10	2.58	0.86
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.55	0.86
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.54	0.86
3:C:217:ARG:NH1	16:W:112:GLU:HB2	1.90	0.86
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.56	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
1:A:69:ILE:HD11	8:H:144:VAL:HG13	1.58	0.85
6:F:425:CYS:HG	24:F:502:SF4:FE4	0.58	0.85
2:B:116:ARG:HA	8:H:37:PRO:HA	1.56	0.85
13:S:16:LEU:HD12	13:S:16:LEU:O	1.76	0.85
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.07	0.85
5:E:147:ILE:HG23	5:E:200:ILE:HG12	1.57	0.85
2:B:82:ILE:HG12	8:H:57:MET:CE	2.07	0.85
17:X:50:GLU:HG2	17:X:138:PRO:HG3	1.59	0.85
15:V:56:LEU:HD12	15:V:57:ASP:N	1.92	0.85
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.06	0.85
26:B:303:PC1:H142	8:H:39:ILE:HD11	1.55	0.84
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.42	0.84
3:C:114:THR:HG22	4:D:421:ARG:NH1	1.93	0.84
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.77	0.84
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.95	0.84
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.84
4:D:137:ASP:OD1	4:D:148:GLU:CD	2.20	0.84
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.84
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.84
2:B:152:MET:HB3	2:B:153:PRO:HD2	1.57	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.84
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:55:LEU:HD22	16:W:107:MET:HE2	1.58	0.84
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
20:b:67:PRO:HD3	20:b:74:LEU:HB2	1.60	0.83
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.61	0.83
2:B:105:MET:HE2	25:B:302:UQ9:C5	2.09	0.83
13:S:48:HIS:CE1	13:S:95:LEU:HD22	2.13	0.83
15:V:75:GLY:HA2	22:r:103:ARG:HD2	1.59	0.83
4:D:254:ARG:HH11	22:r:25:GLN:HB2	1.44	0.83
10:P:94:LEU:HA	10:P:97:MET:HE2	1.59	0.83
16:W:42:TRP:CZ3	32:W:201:EHZ:O1	2.31	0.83
21:q:85:GLU:HG2	21:q:98:PRO:HB3	1.59	0.83
1:A:19:LEU:HD11	1:A:23:TRP:HD1	1.40	0.83
7:G:674:LEU:HD11	13:S:46:LYS:HE2	1.60	0.83
1:A:62:PHE:HD1	8:H:144:VAL:HG21	1.37	0.83
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.83
7:G:176:CYS:HG	24:G:802:SF4:FE4	0.54	0.83
10:P:122:HIS:CB	12:R:46:VAL:HG12	2.08	0.82
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.82
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.82
3:C:85:ILE:HG13	3:C:140:ILE:HD11	1.60	0.82
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
1:A:41:PHE:CG	4:D:96:ARG:HD2	2.15	0.82
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.62	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.10	0.82
6:F:278:ILE:HD11	6:F:299:LEU:HD21	1.61	0.82
7:G:64:CYS:SG	27:G:803:FES:FE1	1.72	0.82
13:S:36:PHE:HZ	13:S:44:LEU:HD11	1.45	0.82
22:r:4:ALA:HB1	22:r:9:GLN:HB2	1.60	0.82
16:W:55:LEU:CD2	16:W:107:MET:HE2	2.09	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.62	0.81
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.81
5:E:174:GLU:OE2	6:F:373:PHE:CD1	2.33	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
21:q:71:LYS:O	21:q:72:ASN:OD1	1.99	0.81
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.60	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
8:H:97:ASN:HD22	19:a:38:VAL:HG13	1.46	0.81
14:T:93:ILE:HG21	14:T:110:LEU:HD22	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:162:CYS:HG	24:I:303:SF4:FE4	0.50	0.80
2:B:99:CYS:HB3	4:D:141:TYR:CE2	2.16	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.12	0.80
7:G:432:ILE:HG23	7:G:451:ILE:HD11	1.63	0.80
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.46	0.80
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.63	0.80
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.80
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.80
8:H:187:ILE:HD12	29:H:403:3PE:H242	1.62	0.80
3:C:85:ILE:CG1	3:C:140:ILE:HD11	2.12	0.80
7:G:334:GLU:OE1	13:S:71:PHE:HE1	1.64	0.80
10:P:163:ARG:HD2	10:P:253:THR:HA	1.62	0.80
9:I:113:CYS:HG	24:I:303:SF4:FE3	0.49	0.80
2:B:122:ARG:HD2	25:H:401:UQ9:H10A	1.64	0.79
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.95	0.79
1:A:44:THR:HG22	16:W:99:VAL:HG11	1.64	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
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.64	0.79
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.79
2:B:121:PHE:CZ	25:B:302:UQ9:C10	2.65	0.79
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.97	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
10:P:208:GLY:H	10:P:211:ASP:HB3	1.48	0.79
2:B:82:ILE:HA	8:H:57:MET:HE1	1.65	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.31	0.79
7:G:272:ARG:HD2	7:G:274:LEU:HD23	1.63	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.78
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	1.97	0.78
4:D:254:ARG:HE	22:r:25:GLN:NE2	1.81	0.78
17:X:9:THR:HG22	17:X:12:GLU:HB2	1.65	0.78
1:A:65:PHE:HZ	1:A:102:LEU:CB	1.87	0.78
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.61	0.78
8:H:17:MET:SD	8:H:229:THR:OG1	2.40	0.78
13:S:20:ARG:HG3	13:S:54:LEU:HB2	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	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:87:LEU:HD21	14:T:104:PHE:HZ	1.47	0.78
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.65	0.78
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.78
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.65	0.78
17:X:20:VAL:HG22	17:X:24:VAL:HG21	1.65	0.77
17:X:86:TRP:CZ2	19:a:64:LYS:HB3	2.18	0.77
8:H:116:ILE:HG13	8:H:117:LEU:N	1.99	0.77
19:a:3:PHE:HE2	33:q:201:CDL:HA4	1.47	0.77
2:B:112:TYR:OH	9:I:91:GLY:CA	2.31	0.77
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.77
1:A:62:PHE:CE1	8:H:144:VAL:HG23	2.19	0.77
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.50	0.77
1:A:41:PHE:CE2	4:D:96:ARG:CG	2.67	0.77
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.77
17:X:8:PRO:HG2	18:Z:84:LEU:HD13	1.66	0.77
2:B:104:MET:HE2	2:B:121:PHE:HE2	1.48	0.77
14:T:83:VAL:CG2	14:T:126:PHE:HZ	1.97	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.77
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.49	0.77
18:Z:144:THR:HA	19:a:45:TRP:HZ3	1.50	0.77
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.65	0.77
6:F:424:ILE:HD11	7:G:73:GLY:O	1.84	0.76
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.76
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.76
7:G:664:TYR:OH	13:S:23:LEU:HD11	1.84	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
4:D:271:ARG:HD2	8:H:279:ARG:O	1.85	0.76
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	1.83	0.76
7:G:454:ASP:HA	7:G:459:ARG:HH21	1.48	0.76
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.49	0.76
7:G:355:LYS:HA	7:G:366:LEU:HD11	1.65	0.76
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.76
1:A:62:PHE:CE1	8:H:144:VAL:HG22	2.19	0.76
9:I:64:THR:HG22	26:I:301:PC1:H231	1.68	0.76
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.76
2:B:105:MET:CG	25:B:302:UQ9:H7A	2.11	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:143:ASP:HA	10:P:147:ASN:HB2	1.67	0.76
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.76
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
14:T:93:ILE:HG23	14:T:110:LEU:HD13	1.66	0.76
18:Z:89:GLU:O	18:Z:93:GLU:HG2	1.84	0.76
7:G:655:ARG:NH1	13:S:59:SER:HB3	2.01	0.76
16:W:55:LEU:HB3	16:W:107:MET:HE2	1.66	0.76
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.75
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.75
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.00	0.75
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.67	0.75
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	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
16:W:32:LYS:HZ3	32:W:201:EHZ:C19	1.98	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.75
10:P:170:LEU:HA	10:P:202:ARG:HB3	1.68	0.75
4:D:270:ASN:HB3	8:H:284:GLN:HE22	1.51	0.75
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	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
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.75
8:H:85:LEU:HD21	8:H:108:THR:HB	1.68	0.75
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.68	0.75
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
14:T:117:GLU:HA	14:T:120:MET:HE3	1.68	0.74
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.69	0.74
20:b:35:ILE:HD12	20:b:35:ILE:O	1.88	0.74
2:B:121:PHE:CE2	25:B:302:UQ9:C10	2.68	0.74
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.74
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.03	0.74
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.66	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.74
14:T:88:LYS:HG3	14:T:98:LEU:HD22	1.70	0.74
1:A:38:GLU:HB3	1:A:41:PHE:O	1.87	0.74
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.18	0.74
2:B:147:LYS:HE3	2:B:151:GLN:HE21	1.51	0.74
10:P:235:THR:OG1	10:P:273:LEU:HB3	1.87	0.74
16:W:32:LYS:HZ2	32:W:201:EHZ:C19	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:213:ILE:HG23	6:F:235:VAL:HA	1.68	0.74
18:Z:93:GLU:O	18:Z:97:ILE:HG13	1.88	0.74
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.88	0.73
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.70	0.73
2:B:92:PRO:HD3	2:B:119:VAL:HG13	1.70	0.73
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.68	0.73
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.69	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
21:q:68:MET:SD	21:q:81:MET:HB3	2.28	0.73
11:Q:167:ASN:O	11:Q:168:LYS:HD2	1.88	0.73
14:T:94:ASP:HB3	14:T:98:LEU:HB2	1.68	0.73
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.73
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.73
8:H:21:THR:HG21	25:H:401:UQ9:H15A	1.69	0.73
14:T:103:HIS:CG	14:T:106:LYS:HD2	2.23	0.73
17:X:29:ALA:HB2	18:Z:71:LEU:HD11	1.69	0.73
1:A:62:PHE:CA	8:H:290:TRP:CH2	2.72	0.73
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.73
1:A:62:PHE:HE1	8:H:144:VAL:HG23	1.52	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
21:q:56:PHE:HA	21:q:59:HIS:CD2	2.24	0.73
2:B:121:PHE:CZ	25:B:302:UQ9:H10	2.24	0.73
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.69	0.73
2:B:98:ALA:H	2:B:135:GLY:HA3	1.54	0.73
4:D:383:LYS:HD3	7:G:140:GLN:NE2	2.03	0.73
5:E:128:LYS:HB3	5:E:167:LEU:HA	1.72	0.72
6:F:42:PHE:HA	6:F:137:LYS:NZ	2.04	0.72
10:P:317:ASP:HB3	10:P:321:ARG:NH2	2.04	0.72
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.72
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.72
2:B:121:PHE:CD2	25:B:302:UQ9:H10	2.23	0.72
6:F:127:ASP:HB3	6:F:245:VAL:HG21	1.69	0.72
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.72
18:Z:65:LEU:O	18:Z:69:ILE:HG12	1.90	0.72
1:A:37:TYR:CZ	1:A:39:CYS:HA	2.25	0.72
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.72
9:I:93:LEU:O	21:q:93:MET:HG2	1.89	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	1.69	0.72
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:166:HIS:HB3	10:P:200:ILE:HD13	1.72	0.72
17:X:44:MET:HE3	17:X:48:TRP:HE1	1.53	0.72
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.72
4:D:206:GLU:OE1	22:r:25:GLN:NE2	2.22	0.72
5:E:151:LEU:HD12	5:E:204:ILE:HD11	1.72	0.72
8:H:307:LEU:HA	8:H:310:PHE:CE2	2.25	0.72
5:E:174:GLU:HG2	6:F:369:ARG:NH1	1.96	0.71
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.72	0.71
8:H:175:LEU:HD21	26:I:301:PC1:H2C2	1.71	0.71
6:F:278:ILE:HD11	6:F:299:LEU:CD2	2.19	0.71
18:Z:90:ASN:O	18:Z:94:GLU:CB	2.39	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.71
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.71
20:b:31:ILE:HA	20:b:34:MET:HE2	1.71	0.71
2:B:123:ALA:CB	4:D:89:PRO:HG3	2.20	0.71
6:F:37:ASP:HA	6:F:40:ARG:HD2	1.72	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
21:q:56:PHE:HD1	21:q:59:HIS:HE2	1.35	0.71
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	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
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.71
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	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
17:X:52:ASP:HB3	18:Z:116:TRP:CB	2.20	0.71
17:X:53:PRO:O	17:X:57:LEU:HG	1.90	0.71
6:F:327:ILE:HG23	6:F:332:CYS:SG	2.29	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
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.26	0.71
25:H:401:UQ9:H16A	25:H:401:UQ9:H20	1.71	0.71
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.71
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
4:D:137:ASP:OD1	4:D:148:GLU:CG	2.39	0.71
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.56	0.71
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.71	0.71
5:E:179:CYS:HG	27:E:301:FES:FE2	0.48	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.70
8:H:33:LEU:CD2	22:r:25:GLN:HG2	2.21	0.70
7:G:117:MET:HE3	7:G:143:SER:HA	1.73	0.70
15:V:56:LEU:HD12	15:V:56:LEU:C	2.16	0.70
8:H:104:PHE:CE2	29:H:402:3PE:H362	2.27	0.70
10:P:172:ALA:O	10:P:185:ALA:HB2	1.91	0.70
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.70
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.55	0.70
17:X:124:GLN:O	20:b:70:PRO:HB2	1.91	0.70
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.72	0.70
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.70
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.70
1:A:44:THR:HG22	16:W:99:VAL:CG1	2.22	0.70
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.56	0.70
4:D:254:ARG:NH1	22:r:25:GLN:HB2	2.06	0.70
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.71	0.70
7:G:362:ASP:HB2	13:S:71:PHE:CD1	2.27	0.70
7:G:78:CYS:HG	27:G:803:FES:FE2	0.46	0.70
7:G:463:CYS:O	7:G:467:LYS:HG2	1.92	0.70
8:H:25:ARG:HG2	25:H:401:UQ9:H4MA	1.74	0.70
9:I:62:MET:HE2	9:I:62:MET:HA	1.72	0.70
4:D:141:TYR:O	4:D:144:MET:SD	2.49	0.70
5:E:222:PHE:H	5:E:225:GLU:HG2	1.55	0.70
17:X:18:VAL:HG21	18:Z:74:LEU:HD11	1.74	0.70
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
12:R:67:GLN:HG2	12:R:109:LEU:CD2	2.21	0.69
6:F:41:ILE:HD11	6:F:262:PHE:HE1	1.56	0.69
10:P:55:VAL:HG12	10:P:123:SER:HA	1.74	0.69
2:B:131:MET:HE3	2:B:152:MET:CE	2.23	0.69
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.41	0.69
8:H:93:HIS:HB3	19:a:27:HIS:ND1	2.06	0.69
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.74	0.69
14:T:138:LEU:HD13	14:T:144:ILE:CG1	2.22	0.69
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.69
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.28	0.69
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.69
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.69
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:63:TYR:HB3	6:F:256:ARG:NE	2.04	0.69
7:G:43:VAL:HG12	7:G:55:LYS:HD3	1.75	0.69
8:H:92:PRO:HD3	8:H:255:TYR:CD2	2.27	0.69
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.69
13:S:51:LEU:HD13	13:S:95:LEU:HD12	1.75	0.69
16:W:42:TRP:CZ2	32:W:201:EHZ:O1	2.45	0.69
3:C:85:ILE:CD1	3:C:140:ILE:CD1	2.71	0.69
6:F:41:ILE:HD11	6:F:262:PHE:CE1	2.28	0.69
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.69
10:P:320:GLU:O	10:P:324:ILE:HG12	1.93	0.69
2:B:99:CYS:HB2	4:D:141:TYR:CG	2.28	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
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.75	0.69
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.58	0.68
4:D:254:ARG:HH11	22:r:25:GLN:CB	2.06	0.68
14:T:100:VAL:HB	14:T:142:GLN:HB2	1.74	0.68
3:C:141:ARG:NH1	4:D:410:TYR:HE1	1.90	0.68
7:G:341:ILE:HG13	7:G:545:LEU:HD11	1.74	0.68
8:H:23:VAL:HG11	19:a:9:LEU:HD21	1.72	0.68
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.28	0.68
8:H:116:ILE:HA	8:H:211:PHE:CE1	2.27	0.68
2:B:105:MET:HE2	25:B:302:UQ9:C6	2.23	0.68
2:B:105:MET:HG3	25:B:302:UQ9:H1MA	1.73	0.68
5:E:39:VAL:HG22	7:G:205:GLN:NE2	2.09	0.68
14:T:87:LEU:HD22	14:T:104:PHE:HE1	1.58	0.68
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.68
4:D:279:THR:HG23	15:V:13:GLY:CA	2.19	0.68
4:D:279:THR:HA	15:V:12:VAL:HG13	1.75	0.68
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.68
17:X:44:MET:HE3	17:X:48:TRP:NE1	2.08	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
7:G:651:PRO:HG3	13:S:57:GLU:H	1.58	0.68
8:H:90:PRO:HD3	8:H:162:LEU:HD23	1.75	0.68
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.74	0.68
9:I:78:PHE:HB3	22:r:8:ILE:HG22	1.76	0.68
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.08	0.68
4:D:279:THR:HA	15:V:12:VAL:CG1	2.24	0.68
7:G:335:GLY:HA2	7:G:362:ASP:O	1.93	0.68
10:P:317:ASP:HB3	10:P:321:ARG:HH22	1.58	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.75	0.68
6:F:39:ASP:HB3	6:F:265:PHE:CZ	2.29	0.68
2:B:110:PRO:HB3	8:H:33:LEU:O	1.93	0.68
22:r:20:LEU:C	22:r:20:LEU:HD12	2.18	0.68
6:F:296:LEU:HD23	6:F:332:CYS:HB3	1.75	0.68
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
8:H:33:LEU:HD21	22:r:25:GLN:HG2	1.74	0.68
10:P:185:ALA:O	10:P:188:GLU:HG2	1.94	0.68
17:X:132:LYS:HB3	20:b:59:ASP:HB3	1.77	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
4:D:375:MET:HE1	7:G:126:LEU:HA	1.75	0.67
16:W:121:PHE:HA	16:W:124:LYS:HE2	1.75	0.67
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.58	0.67
8:H:54:LYS:HG3	8:H:55:LEU:N	2.07	0.67
13:S:16:LEU:HB3	13:S:69:TYR:HD1	1.58	0.67
15:V:116:ILE:HG23	15:V:116:ILE:O	1.92	0.67
2:B:92:PRO:CD	2:B:119:VAL:HG13	2.25	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.27	0.67
8:H:30:TYR:CE1	19:a:1:MET:O	2.47	0.67
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.25	0.67
12:R:48:PHE:CD2	21:q:125:VAL:HG21	2.29	0.67
14:T:87:LEU:CD2	14:T:104:PHE:CZ	2.78	0.67
3:C:85:ILE:HD11	3:C:140:ILE:HD11	1.76	0.67
5:E:206:GLU:HB2	5:E:213:PRO:HG3	1.76	0.67
6:F:225:LEU:H	11:Q:160:TYR:HE2	1.42	0.67
7:G:304:GLU:OE2	10:P:41:ILE:HG12	1.94	0.67
7:G:382:ARG:HD2	13:S:56:ARG:CD	2.25	0.67
8:H:92:PRO:HD3	8:H:255:TYR:HD2	1.58	0.67
17:X:56:CYS:HA	17:X:135:ARG:HH12	1.60	0.67
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.77	0.67
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.76	0.67
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.76	0.67
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.67
9:I:68:ARG:HH22	18:Z:26:PRO:HD2	1.60	0.67
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.58	0.66
9:I:92:PRO:HA	21:q:91:HIS:O	1.95	0.66
21:q:13:GLN:HE22	33:q:201:CDL:HA31	1.60	0.66
1:A:61:THR:O	1:A:62:PHE:C	2.35	0.66
2:B:98:ALA:HB2	2:B:136:THR:H	1.61	0.66
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.56	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:MET:SD	2:B:121:PHE:CE1	2.89	0.66
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.66
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.66
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.72	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
7:G:655:ARG:NH1	13:S:59:SER:CB	2.58	0.66
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.66
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.77	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
13:S:24:CYS:SG	13:S:61:VAL:O	2.53	0.66
10:P:263:PHE:HD1	10:P:333:PRO:HB2	1.60	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:O	15:V:72:LEU:CD1	2.42	0.66
6:F:42:PHE:HA	6:F:137:LYS:HZ2	1.58	0.66
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.28	0.66
7:G:617:ARG:HH12	16:W:129:HIS:N	1.93	0.66
14:T:118:ILE:HG23	14:T:122:MET:HE3	1.77	0.66
1:A:3:LEU:HD23	29:H:402:3PE:H251	1.77	0.66
1:A:19:LEU:CD1	1:A:23:TRP:HD1	2.09	0.66
5:E:43:THR:OG1	5:E:44:PRO:HD2	1.96	0.66
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.31	0.66
1:A:41:PHE:CD2	4:D:86:PRO:HD3	2.31	0.66
5:E:138:PRO:HD2	27:E:301:FES:S2	2.36	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
10:P:288:PHE:CZ	10:P:290:PRO:HB3	2.30	0.66
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.66
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.77	0.66
16:W:65:LYS:HE2	16:W:110:PHE:HA	1.78	0.66
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.78	0.65
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.31	0.65
4:D:260:GLU:HG3	18:Z:25:LEU:HD22	1.78	0.65
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.65
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.65
2:B:104:MET:CE	2:B:121:PHE:CE2	2.74	0.65
3:C:102:HIS:CE1	15:V:48:THR:HG22	2.27	0.65
9:I:200:GLU:OE2	21:q:93:MET:SD	2.54	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:135:GLU:HB2	10:P:140:ASP:HA	1.78	0.65
10:P:141:PHE:CD2	10:P:179:LYS:HD2	2.28	0.65
2:B:121:PHE:CG	25:B:302:UQ9:H10B	2.30	0.65
13:S:16:LEU:HB3	13:S:69:TYR:CD1	2.32	0.65
14:T:130:ILE:HG23	14:T:131:PRO:HD2	1.77	0.65
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.65
7:G:126:LEU:CD1	12:R:89:PRO:HB3	2.25	0.65
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.65
13:S:58:CYS:HB2	13:S:61:VAL:HG12	1.78	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
5:E:79:LEU:HB2	5:E:80:PRO:HD3	1.78	0.65
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.65
8:H:90:PRO:HG2	8:H:240:ILE:HG21	1.77	0.65
12:R:32:THR:HG22	12:R:36:GLN:N	2.10	0.65
3:C:73:GLN:NE2	15:V:112:TRP:HE1	1.95	0.65
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.65
8:H:138:GLN:HG3	8:H:139:THR:N	2.11	0.65
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.65
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.32	0.65
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.78	0.65
10:P:166:HIS:HB3	10:P:200:ILE:CD1	2.27	0.65
12:R:42:ASP:HB3	12:R:44:ARG:HH11	1.61	0.65
12:R:52:GLN:HE21	21:q:122:GLU:C	2.04	0.65
13:S:48:HIS:CE1	13:S:95:LEU:CD2	2.80	0.65
2:B:98:ALA:CB	2:B:136:THR:H	2.10	0.64
5:E:147:ILE:HD11	5:E:183:PRO:HB3	1.77	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	0.64
5:E:136:THR:HG22	5:E:137:THR:H	1.62	0.64
6:F:110:PRO:HB3	6:F:152:ARG:HH12	1.62	0.64
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.64
8:H:90:PRO:HD3	8:H:162:LEU:CD2	2.27	0.64
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.64
14:T:120:MET:HG2	16:W:44:ARG:HH11	1.61	0.64
17:X:65:GLY:HA2	17:X:68:LEU:HD12	1.78	0.64
4:D:101:LEU:HD11	4:D:106:VAL:HG22	1.78	0.64
6:F:152:ARG:NH2	23:s:60:PRO:HG3	2.13	0.64
11:Q:163:ASN:OD1	11:Q:164:PHE:N	2.31	0.64
13:S:15:GLY:HA3	13:S:17:ARG:HH22	1.62	0.64
15:V:44:TYR:CE1	15:V:48:THR:HG23	2.30	0.64
1:A:41:PHE:HD2	4:D:86:PRO:HD3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:386:LEU:HD21	7:G:523:VAL:CG1	2.28	0.64
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.59	0.64
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.79	0.64
20:b:48:ALA:O	20:b:49:THR:C	2.40	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.38	0.64
2:B:70:ARG:HG3	2:B:73:TYR:H	1.63	0.64
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.28	0.64
2:B:92:PRO:HG3	2:B:119:VAL:HG13	1.80	0.64
4:D:97:LEU:O	4:D:99:LEU:HG	1.98	0.64
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.80	0.64
2:B:99:CYS:CB	4:D:141:TYR:CG	2.80	0.64
3:C:206:TYR:C	3:C:223:VAL:HG23	2.23	0.64
14:T:83:VAL:HG23	14:T:126:PHE:HZ	1.63	0.64
14:T:93:ILE:CG2	14:T:110:LEU:HD13	2.28	0.64
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.64
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.79	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.63
13:S:16:LEU:HD12	13:S:16:LEU:C	2.22	0.63
14:T:87:LEU:HD21	14:T:104:PHE:CZ	2.32	0.63
1:A:42:ASP:OD2	16:W:102:GLN:NE2	2.30	0.63
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.63
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.63
10:P:88:VAL:HG12	10:P:92:MET:HE2	1.80	0.63
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.63
6:F:278:ILE:HG22	6:F:282:VAL:HG21	1.80	0.63
8:H:145:THR:HG22	8:H:289:LEU:HD11	1.79	0.63
10:P:169:HIS:H	10:P:184:LYS:HE3	1.63	0.63
18:Z:65:LEU:O	18:Z:68:ARG:HG2	1.98	0.63
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.77	0.63
6:F:388:GLY:HA3	6:F:419:ILE:HD11	1.80	0.63
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.63
33:q:201:CDL:H1	22:r:3:SER:HB2	1.80	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.63
10:P:284:THR:HG23	10:P:356:HIS:HB2	1.79	0.63
17:X:37:ASP:OD1	17:X:38:LYS:N	2.31	0.63
1:A:19:LEU:HD11	1:A:23:TRP:CD1	2.30	0.63
2:B:99:CYS:CB	4:D:141:TYR:CD2	2.82	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:117:MET:HE3	7:G:143:SER:CA	2.28	0.63
10:P:172:ALA:H	10:P:202:ARG:HH21	1.45	0.63
14:T:138:LEU:HD12	14:T:138:LEU:C	2.24	0.63
17:X:52:ASP:HA	18:Z:116:TRP:CD1	2.34	0.63
20:b:66:VAL:HG22	20:b:75:GLY:HA3	1.80	0.63
1:A:62:PHE:HE1	8:H:144:VAL:HG22	1.61	0.63
4:D:148:GLU:OE2	4:D:225:ALA:HA	1.98	0.63
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.63
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.80	0.63
10:P:163:ARG:CD	10:P:253:THR:HA	2.27	0.63
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.63	0.63
14:T:138:LEU:O	14:T:138:LEU:CD1	2.40	0.63
18:Z:70:ALA:O	18:Z:73:PRO:HD2	1.99	0.63
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.63
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	0.63
8:H:51:ASP:HA	8:H:54:LYS:HG2	1.80	0.63
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.34	0.63
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	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
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.63	0.63
12:R:51:ARG:NH2	21:q:125:VAL:HG12	2.13	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
5:E:140:MET:HE1	6:F:366:ALA:HA	1.81	0.62
8:H:248:TYR:HB3	8:H:250:ASN:OD1	1.99	0.62
13:S:16:LEU:HA	13:S:69:TYR:HA	1.79	0.62
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.34	0.62
1:A:62:PHE:HB2	8:H:290:TRP:CZ2	2.34	0.62
4:D:348:LEU:O	18:Z:11:PRO:HB3	1.98	0.62
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.62	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
7:G:445:LEU:HD21	7:G:462:PHE:HB2	1.81	0.62
26:I:301:PC1:H361	26:I:301:PC1:H322	1.79	0.62
10:P:165:ILE:HA	10:P:199:ILE:O	1.99	0.62
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.81	0.62
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.62
16:W:55:LEU:CB	16:W:107:MET:HE2	2.30	0.62
5:E:48:PRO:HA	5:E:95:SER:HB2	1.81	0.62
5:E:245:GLN:HB2	6:F:257:ARG:C	2.23	0.62
7:G:127:ASP:HA	12:R:106:TYR:OH	1.99	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
22:r:109:ASP:O	22:r:110:GLN:HG2	1.99	0.62
2:B:99:CYS:HB2	4:D:141:TYR:CD1	2.35	0.62
4:D:142:VAL:HG13	4:D:207:ARG:NH1	2.14	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.62
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.81	0.62
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.62
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.62
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.34	0.62
2:B:121:PHE:CZ	25:B:302:UQ9:H10A	2.25	0.62
4:D:253:LEU:HD22	22:r:23:LYS:HB2	1.81	0.62
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.82	0.62
17:X:25:LEU:HD11	19:a:50:ARG:NH2	2.13	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.78	0.62
18:Z:28:ARG:HG3	18:Z:28:ARG:O	1.99	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
17:X:69:ASN:O	17:X:73:GLN:HG3	2.00	0.62
22:r:20:LEU:HD12	22:r:21:GLN:N	2.14	0.62
2:B:108:ALA:CB	25:B:302:UQ9:H12	2.23	0.62
5:E:131:ILE:HD11	5:E:168:PHE:HD2	1.65	0.62
6:F:35:LEU:HD11	6:F:39:ASP:O	1.99	0.62
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.82	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
7:G:339:ALA:C	7:G:545:LEU:HD12	2.25	0.62
12:R:98:GLU:CD	12:R:98:GLU:H	2.07	0.62
20:b:67:PRO:HD2	20:b:72:ASP:HB2	1.82	0.62
2:B:154:GLU:HB3	2:B:155:PRO:HD3	1.81	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
8:H:289:LEU:O	8:H:289:LEU:HD23	1.99	0.62
17:X:129:THR:HG23	20:b:68:SER:HA	1.81	0.62
17:X:130:LYS:NZ	20:b:63:MET:HB2	2.14	0.62
4:D:94:VAL:O	4:D:94:VAL:HG23	1.99	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.62
7:G:334:GLU:OE1	13:S:71:PHE:CE1	2.51	0.62
8:H:289:LEU:HD23	8:H:289:LEU:C	2.25	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.64	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.61
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:222:PHE:N	5:E:225:GLU:HG2	2.15	0.61
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.61
7:G:311:LYS:HE3	7:G:313:LEU:HD13	1.82	0.61
16:W:55:LEU:CB	16:W:107:MET:CE	2.75	0.61
21:q:34:ARG:NE	21:q:58:ARG:NH2	2.48	0.61
6:F:71:LYS:HE2	6:F:71:LYS:HA	1.82	0.61
1:A:33:LYS:CG	8:H:61:MET:CE	2.52	0.61
1:A:65:PHE:O	1:A:69:ILE:HG13	2.00	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61
4:D:109:CYS:O	4:D:111:PRO:HD3	1.99	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
1:A:58:VAL:HG22	1:A:111:LEU:HB2	1.83	0.61
2:B:142:ALA:HB3	2:B:143:PRO:HD3	1.82	0.61
6:F:266:GLY:HA3	6:F:271:SER:HA	1.82	0.61
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.61
17:X:52:ASP:HB3	18:Z:116:TRP:HB3	1.81	0.61
20:b:11:ASN:O	20:b:15:LYS:N	2.31	0.61
1:A:33:LYS:CG	2:B:150:ASP:O	2.46	0.61
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.58	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
7:G:395:GLU:HA	7:G:421:SER:OG	2.00	0.61
8:H:14:LEU:HB3	25:H:401:UQ9:H27	1.82	0.61
8:H:87:VAL:HG13	8:H:95:LEU:HD23	1.83	0.61
8:H:116:ILE:HD12	8:H:135:ALA:CB	2.30	0.61
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.81	0.61
13:S:48:HIS:HE1	13:S:95:LEU:HD22	1.63	0.61
4:D:202:TRP:CZ3	4:D:261:MET:HG3	2.36	0.61
5:E:193:GLU:HB2	5:E:217:PRO:HG3	1.81	0.61
5:E:222:PHE:CE1	6:F:48:ARG:HG3	2.36	0.61
8:H:81:LEU:HD22	8:H:108:THR:HG23	1.82	0.61
8:H:301:CYS:O	8:H:305:ILE:HG13	2.00	0.61
5:E:204:ILE:HG22	5:E:208:LYS:HG3	1.82	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.61
8:H:127:TYR:CD2	8:H:207:LEU:HG	2.36	0.61
14:T:103:HIS:ND1	14:T:140:CYS:SG	2.73	0.61
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.61
4:D:304:LYS:HE2	9:I:35:THR:N	2.16	0.61
7:G:35:PHE:O	7:G:101:ASN:HA	2.01	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
17:X:50:GLU:CG	17:X:138:PRO:HG3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
7:G:343:GLY:HA3	7:G:550:ALA:HA	1.82	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	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
12:R:32:THR:HA	12:R:55:VAL:HG23	1.83	0.61
14:T:79:ILE:CB	14:T:145:VAL:HG13	2.28	0.61
21:q:71:LYS:O	21:q:72:ASN:CG	2.43	0.61
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.83	0.60
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.60
2:B:98:ALA:O	24:B:301:SF4:S3	2.59	0.60
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.60
8:H:195:ARG:O	8:H:199:ASP:HB2	2.02	0.60
10:P:55:VAL:CG1	10:P:123:SER:HA	2.31	0.60
17:X:127:LYS:HD3	20:b:66:VAL:HG21	1.83	0.60
21:q:10:GLY:HA2	33:q:201:CDL:OA6	2.00	0.60
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.28	0.60
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.60
9:I:64:THR:HG21	26:I:301:PC1:H121	1.83	0.60
18:Z:143:TYR:O	18:Z:144:THR:C	2.45	0.60
21:q:74:PHE:CD2	21:q:75:TRP:CD1	2.89	0.60
3:C:73:GLN:HE21	15:V:112:TRP:HE1	1.47	0.60
4:D:80:MET:O	4:D:100:GLU:HA	2.02	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
7:G:126:LEU:HD11	12:R:89:PRO:HB3	1.82	0.60
22:r:12:ARG:HB3	22:r:20:LEU:HD21	1.84	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
13:S:23:LEU:O	13:S:23:LEU:CD1	2.41	0.60
17:X:7:LEU:HD11	18:Z:88:ARG:HE	1.66	0.60
6:F:158:ILE:CD1	6:F:166:ALA:HB2	2.31	0.60
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.67	0.60
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.32	0.60
2:B:141:MET:HE2	4:D:115:LEU:HD23	1.84	0.60
3:C:102:HIS:HE1	15:V:48:THR:CG2	2.12	0.60
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.37	0.60
5:E:182:ALA:O	5:E:183:PRO:C	2.43	0.60
13:S:16:LEU:CB	13:S:69:TYR:HD1	2.15	0.60
3:C:84:GLU:OE2	3:C:141:ARG:NH1	2.35	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.02	0.60
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.83	0.60
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:306:MET:HG2	7:G:316:TYR:HA	1.84	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.84	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.60
1:A:39:CYS:SG	4:D:87:GLN:O	2.60	0.60
1:A:62:PHE:HB2	8:H:290:TRP:HZ2	1.66	0.60
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.60
6:F:191:TYR:HE2	6:F:193:PHE:HD2	1.50	0.60
10:P:136:THR:CG2	10:P:139:PHE:HB2	2.31	0.60
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.60
16:W:64:ASP:O	16:W:68:GLU:HG3	2.02	0.60
17:X:20:VAL:HG12	17:X:25:LEU:HD21	1.84	0.60
17:X:37:ASP:HA	17:X:40:ASN:HB2	1.84	0.60
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.02	0.60
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.59
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.59
6:F:90:GLY:O	6:F:350:GLY:HA2	2.01	0.59
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.59
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.59
4:D:253:LEU:HB2	22:r:23:LYS:CD	2.31	0.59
5:E:175:CYS:SG	6:F:122:PRO:HA	2.42	0.59
6:F:44:ASN:OD1	6:F:49:HIS:HB2	2.02	0.59
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.59
7:G:391:ILE:HG22	7:G:417:ARG:HE	1.66	0.59
10:P:180:SER:O	10:P:184:LYS:HG3	2.03	0.59
10:P:229:VAL:HB	10:P:323:HIS:CD2	2.37	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
12:R:40:GLU:HA	12:R:45:ARG:CZ	2.33	0.59
14:T:83:VAL:CG2	14:T:126:PHE:CZ	2.83	0.59
4:D:202:TRP:CH2	4:D:261:MET:HG3	2.36	0.59
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.59
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.32	0.59
8:H:116:ILE:HD12	8:H:135:ALA:HB1	1.85	0.59
10:P:146:VAL:HG23	10:P:187:GLY:HA2	1.84	0.59
10:P:328:MET:HG3	10:P:330:THR:H	1.67	0.59
20:b:8:PHE:HA	20:b:11:ASN:ND2	2.17	0.59
1:A:7:ILE:HD12	29:H:402:3PE:H392	1.85	0.59
5:E:225:GLU:HG3	5:E:226:PRO:O	2.02	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	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
11:Q:167:ASN:HB3	23:s:64:ARG:HE	1.67	0.59
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.59
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.33	0.59
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.68	0.59
21:q:96:ASP:OD1	21:q:97:PRO:CD	2.50	0.59
21:q:137:TRP:CZ2	21:q:140:PRO:HD3	2.38	0.59
2:B:115:ASP:HA	2:B:119:VAL:O	2.03	0.59
2:B:123:ALA:O	2:B:124:SER:C	2.44	0.59
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.59
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.59
8:H:183:MET:HE2	26:I:301:PC1:H291	1.85	0.59
10:P:318:LYS:O	10:P:322:ILE:HG13	2.02	0.59
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.85	0.59
16:W:104:THR:O	16:W:108:ARG:HG3	2.02	0.59
17:X:7:LEU:HD11	18:Z:88:ARG:NE	2.18	0.59
19:a:3:PHE:CE2	33:q:201:CDL:HA4	2.35	0.59
21:q:51:ASP:O	21:q:59:HIS:HB2	2.02	0.59
3:C:186:ILE:HG13	3:C:187:LEU:N	2.18	0.59
4:D:388:GLY:HA3	4:D:417:SER:OG	2.03	0.59
7:G:337:ALA:O	7:G:543:LYS:N	2.36	0.59
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
20:b:6:SER:O	20:b:9:LEU:HB3	2.03	0.59
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.61	0.59
10:P:357:ARG:HD3	10:P:361:TRP:O	2.03	0.59
17:X:52:ASP:HB3	18:Z:116:TRP:HB2	1.85	0.59
17:X:78:CYS:SG	17:X:110:CYS:HB3	2.42	0.59
18:Z:98:MET:HB2	18:Z:104:TRP:NE1	2.18	0.59
21:q:98:PRO:O	21:q:99:THR:C	2.46	0.59
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.36	0.58
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
8:H:104:PHE:HE2	29:H:402:3PE:H362	1.67	0.58
14:T:90:TYR:CE2	14:T:92:LYS:HB3	2.38	0.58
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.58
33:q:201:CDL:H722	33:q:201:CDL:H512	1.84	0.58
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
12:R:42:ASP:HB3	12:R:44:ARG:NH1	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:122:GLY:O	18:Z:126:GLY:N	2.34	0.58
18:Z:144:THR:HA	19:a:45:TRP:CZ3	2.35	0.58
1:A:68:GLU:CB	1:A:98:LEU:HG	2.32	0.58
2:B:98:ALA:HB3	2:B:135:GLY:HA2	1.85	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
25:H:401:UQ9:H25	25:H:401:UQ9:H21A	1.85	0.58
11:Q:166:TRP:HE3	23:s:67:PRO:HG3	1.67	0.58
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.85	0.58
17:X:127:LYS:HD3	20:b:66:VAL:CG2	2.34	0.58
1:A:41:PHE:CE2	4:D:96:ARG:HG3	2.37	0.58
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.19	0.58
5:E:150:THR:O	5:E:154:LYS:HG2	2.02	0.58
6:F:410:ASP:OD1	6:F:411:SER:N	2.36	0.58
7:G:49:VAL:HB	7:G:91:ALA:HA	1.86	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
11:Q:166:TRP:CE3	23:s:67:PRO:HG3	2.38	0.58
1:A:52:SER:O	4:D:103:GLY:HA2	2.04	0.58
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.58
1:A:73:LEU:N	1:A:74:PRO:HD2	2.18	0.58
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.69	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.58
14:T:103:HIS:HB2	14:T:106:LYS:HB2	1.83	0.58
18:Z:86:ILE:HG23	18:Z:128:ARG:NE	2.15	0.58
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	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
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.58
8:H:288:LEU:HA	8:H:292:ASN:HB2	1.86	0.58
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.86	0.58
14:T:90:TYR:CE2	14:T:92:LYS:CB	2.86	0.58
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.58
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.04	0.58
4:D:375:MET:HE1	7:G:126:LEU:CA	2.34	0.58
6:F:109:ARG:NH2	6:F:232:ASP:O	2.36	0.58
6:F:116:ASN:OD1	6:F:244:ASN:HA	2.03	0.58
8:H:224:PHE:CD2	25:H:401:UQ9:H16A	2.38	0.58
13:S:47:ALA:O	13:S:49:PRO:HD3	2.03	0.58
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.04	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)
5:E:135:THR:OG1	5:E:172:GLU:CG	2.52	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.58
2:B:112:TYR:CZ	9:I:84:ILE:HD11	2.37	0.58
13:S:16:LEU:HD11	13:S:51:LEU:CD1	2.29	0.58
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.85	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
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.86	0.57
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.57
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	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
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.57
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
10:P:56:ALA:HA	10:P:125:VAL:O	2.03	0.57
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.04	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.85	0.57
18:Z:120:LEU:HB2	18:Z:123:GLU:HG3	1.87	0.57
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.34	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.57
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.17	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.57
7:G:387:LEU:HD21	7:G:516:LEU:HB3	1.85	0.57
11:Q:167:ASN:O	11:Q:168:LYS:HG2	2.05	0.57
17:X:20:VAL:C	19:a:54:ILE:HD13	2.29	0.57
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.87	0.57
3:C:104:ASN:O	22:r:97:PRO:HD3	2.04	0.57
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.70	0.57
7:G:73:GLY:HA2	27:G:803:FES:S1	2.45	0.57
8:H:90:PRO:HA	8:H:94:PRO:HB3	1.86	0.57
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.57
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.57
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.29	0.57
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.86	0.57
18:Z:129:THR:HB	18:Z:132:GLU:HG3	1.86	0.57
4:D:84:PHE:CE2	4:D:91:ALA:HB2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.87	0.57
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	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: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
2:B:108:ALA:HB1	25:B:302:UQ9:C12	2.27	0.57
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.19	0.57
7:G:41:VAL:HG21	7:G:56:VAL:HB	1.86	0.57
4:D:137:ASP:OD1	4:D:148:GLU:HG3	2.04	0.57
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.57
5:E:151:LEU:CD2	5:E:170:LEU:HD13	2.35	0.57
6:F:76:ILE:HG23	6:F:255:CYS:SG	2.45	0.57
7:G:102:ILE:H	7:G:102:ILE:HD12	1.70	0.57
7:G:171:THR:HB	7:G:173:MET:HG3	1.87	0.57
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.57
8:H:19:PHE:CE1	19:a:11:ILE:HD12	2.40	0.57
14:T:130:ILE:HD11	14:T:148:ILE:HD11	1.86	0.57
18:Z:7:LYS:HB2	18:Z:7:LYS:NZ	2.20	0.57
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
25:B:302:UQ9:C8	25:B:302:UQ9:H1MB	2.35	0.56
6:F:39:ASP:HB3	6:F:265:PHE:HZ	1.69	0.56
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.86	0.56
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.56
21:q:65:THR:HG22	21:q:66:THR:N	2.20	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
12:R:37:VAL:O	12:R:38:TYR:C	2.44	0.56
14:T:134:ASP:OD1	14:T:134:ASP:O	2.23	0.56
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.87	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.56
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.37	0.56
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.22	0.56
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.40	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
10:P:168:SER:HA	10:P:184:LYS:HE3	1.87	0.56
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.56
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.56
18:Z:105:LYS:O	18:Z:106:VAL:C	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:129:THR:O	21:q:129:THR:HG22	2.03	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
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.56
6:F:171:VAL:HA	6:F:174:ARG:HH12	1.70	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:190:LEU:HD21	8:H:270:PHE:CD1	2.40	0.56
10:P:145:PHE:O	10:P:149:PRO:HG2	2.05	0.56
21:q:14:VAL:HG13	21:q:23:LEU:CD2	2.35	0.56
5:E:180:VAL:HG21	6:F:286:CYS:HA	1.87	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
9:I:80:GLU:HB3	22:r:26:LEU:HD11	1.88	0.56
10:P:211:ASP:OD1	10:P:214:LEU:HB3	2.04	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
2:B:92:PRO:CG	2:B:119:VAL:HG13	2.35	0.56
4:D:128:THR:H	4:D:131:GLN:NE2	2.01	0.56
5:E:84:LEU:HD12	23:s:46:LEU:HD13	1.88	0.56
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.56
8:H:113:VAL:O	8:H:116:ILE:HG12	2.05	0.56
9:I:35:THR:CG2	22:r:107:SER:HA	2.36	0.56
11:Q:166:TRP:CE3	23:s:67:PRO:CG	2.88	0.56
12:R:59:PHE:O	12:R:63:LEU:HG	2.06	0.56
12:R:62:ASP:O	12:R:66:GLN:HG3	2.06	0.56
2:B:121:PHE:CD1	25:B:302:UQ9:H12A	2.41	0.56
26:B:303:PC1:H143	21:q:29:ARG:O	2.05	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.05	0.56
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.88	0.56
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.56
17:X:9:THR:HA	18:Z:88:ARG:HH22	1.71	0.56
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.56
1:A:41:PHE:CZ	4:D:96:ARG:CD	2.87	0.56
4:D:145:MET:O	4:D:148:GLU:N	2.39	0.56
4:D:359:ASP:O	7:G:150:ARG:NH2	2.38	0.56
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.56
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.56
8:H:142:TYR:HE1	8:H:285:LEU:CD2	2.19	0.56
8:H:318:MET:HE3	18:Z:57:ARG:HH21	1.71	0.56
14:T:87:LEU:HD22	14:T:104:PHE:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:217:ARG:HH12	16:W:112:GLU:CB	2.13	0.56
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.56
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.21	0.56
10:P:311:GLU:O	10:P:312:PRO:C	2.49	0.56
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.56
1:A:30:TYR:CZ	1:A:33:LYS:HD3	2.41	0.55
1:A:96:THR:O	1:A:100:LEU:HG	2.06	0.55
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55
8:H:90:PRO:CG	8:H:162:LEU:HB3	2.31	0.55
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.41	0.55
10:P:251:ASN:OD1	10:P:254:LYS:HE3	2.06	0.55
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.49	0.55
17:X:39:THR:HG23	17:X:40:ASN:N	2.20	0.55
17:X:124:GLN:C	17:X:125:LEU:HD12	2.31	0.55
18:Z:91:LEU:O	18:Z:94:GLU:HB3	2.06	0.55
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.88	0.55
2:B:114:MET:SD	2:B:121:PHE:HE1	2.28	0.55
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.55
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.55
7:G:666:GLN:NE2	13:S:38:VAL:HG13	2.21	0.55
10:P:206:ILE:HG13	30:P:401:NDP:H42N	1.88	0.55
10:P:265:PHE:CZ	10:P:338:LEU:HD12	2.41	0.55
14:T:90:TYR:HE2	14:T:92:LYS:CB	2.19	0.55
3:C:85:ILE:HD11	3:C:140:ILE:CD1	2.35	0.55
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.42	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:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
8:H:11:VAL:O	8:H:12:PRO:C	2.50	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
12:R:36:GLN:HG2	21:q:127:TYR:CD2	2.40	0.55
20:b:8:PHE:CG	20:b:9:LEU:N	2.74	0.55
4:D:254:ARG:HH11	22:r:25:GLN:CA	2.19	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.55
7:G:126:LEU:CD1	12:R:89:PRO:HB2	2.37	0.55
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.55
10:P:219:ASN:ND2	10:P:313:TRP:HE1	2.04	0.55
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:CG	8:H:61:MET:HE3	2.27	0.55
1:A:72:LEU:O	1:A:75:LEU:HG	2.06	0.55
2:B:105:MET:CG	25:B:302:UQ9:H1MA	2.36	0.55
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.55
7:G:94:MET:CE	7:G:100:TRP:HH2	2.20	0.55
13:S:30:SER:O	13:S:31:GLN:C	2.49	0.55
21:q:64:TYR:CE2	21:q:82:VAL:HG13	2.42	0.55
1:A:68:GLU:HG3	1:A:69:ILE:N	2.21	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.72	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
8:H:51:ASP:CA	8:H:54:LYS:HG2	2.37	0.55
12:R:38:TYR:HE2	21:q:127:TYR:CB	1.97	0.55
14:T:128:PHE:CE2	14:T:130:ILE:HG13	2.42	0.55
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.89	0.55
10:P:64:PHE:HE1	10:P:209:ARG:O	1.90	0.55
19:a:1:MET:HG3	33:q:201:CDL:HB21	1.87	0.55
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.55
1:A:72:LEU:C	1:A:74:PRO:HD2	2.32	0.55
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.37	0.55
7:G:356:ASP:O	7:G:360:LYS:HG3	2.06	0.55
7:G:456:ALA:O	7:G:499:LYS:HE2	2.06	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
10:P:208:GLY:H	10:P:211:ASP:CB	2.18	0.55
14:T:103:HIS:HD1	14:T:140:CYS:HG	1.50	0.55
18:Z:89:GLU:CD	18:Z:128:ARG:HH22	2.15	0.55
21:q:68:MET:HE1	21:q:81:MET:O	2.06	0.55
2:B:96:GLY:HA3	25:B:302:UQ9:H3MB	1.89	0.55
4:D:232:VAL:HG23	4:D:356:ILE:HD13	1.88	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.55
8:H:26:LYS:O	8:H:30:TYR:HD2	1.89	0.55
8:H:212:ASN:HB3	8:H:215:TYR:HB2	1.89	0.55
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.21	0.55
15:V:50:GLN:HE22	22:r:94:ALA:H	1.54	0.55
1:A:103:ALA:O	1:A:107:THR:HG23	2.06	0.55
2:B:170:TYR:CB	9:I:153:ILE:HG21	2.36	0.55
4:D:97:LEU:HG	4:D:99:LEU:HD21	1.89	0.55
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.55
4:D:202:TRP:CH2	9:I:72:MET:HG2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.55
10:P:258:ALA:HA	10:P:263:PHE:HZ	1.71	0.55
19:a:31:ASN:HD21	19:a:36:LYS:HB2	1.71	0.55
20:b:8:PHE:O	20:b:9:LEU:C	2.50	0.55
1:A:38:GLU:HG3	4:D:83:ASN:OD1	2.08	0.54
2:B:210:ARG:HD3	21:q:76:ASP:HB2	1.88	0.54
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.42	0.54
4:D:81:THR:HG22	4:D:100:GLU:HG2	1.88	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.07	0.54
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.89	0.54
10:P:195:PHE:HD1	10:P:198:ALA:HB2	1.72	0.54
10:P:196:PRO:O	10:P:197:GLU:HB2	2.07	0.54
10:P:235:THR:OG1	10:P:273:LEU:CB	2.54	0.54
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.06	0.54
18:Z:56:GLU:HA	18:Z:59:ARG:HH11	1.71	0.54
1:A:42:ASP:OD2	16:W:102:GLN:HG3	2.08	0.54
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.89	0.54
5:E:40:HIS:HB2	7:G:209:TYR:CZ	2.41	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.54
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.54
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.54
11:Q:165:SER:HB3	11:Q:168:LYS:O	2.06	0.54
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.89	0.54
1:A:25:PRO:HG3	8:H:56:PHE:O	2.06	0.54
1:A:105:GLU:CG	1:A:111:LEU:HB3	2.37	0.54
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.54
6:F:275:LEU:HA	6:F:289:GLU:HA	1.90	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
10:P:315:THR:O	10:P:316:LYS:C	2.49	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
3:C:73:GLN:NE2	15:V:107:PRO:HB3	2.22	0.54
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
7:G:617:ARG:HH12	16:W:128:GLY:C	2.14	0.54
9:I:53:ALA:CA	20:b:14:ALA:HB2	2.36	0.54
10:P:199:ILE:HD13	10:P:258:ALA:HB1	1.90	0.54
10:P:208:GLY:O	10:P:209:ARG:C	2.48	0.54
10:P:300:TRP:O	10:P:304:LEU:HG	2.08	0.54
17:X:7:LEU:HD12	17:X:8:PRO:O	2.07	0.54
4:D:210:MET:O	4:D:211:PHE:C	2.51	0.54
5:E:135:THR:OG1	5:E:135:THR:O	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:152:ARG:HD3	23:s:57:LEU:HD11	1.87	0.54
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.54
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.88	0.54
10:P:315:THR:HG22	10:P:316:LYS:N	2.21	0.54
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.90	0.54
19:a:58:ASN:HB2	19:a:61:TYR:CD2	2.43	0.54
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.41	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
7:G:617:ARG:NH1	16:W:128:GLY:C	2.66	0.54
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
10:P:213:PHE:CE2	10:P:239:PRO:HB3	2.42	0.54
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.54
16:W:88:LYS:O	16:W:92:GLU:HG2	2.08	0.54
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.54
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.23	0.54
6:F:270:ASN:OD1	6:F:270:ASN:C	2.48	0.54
6:F:297:LYS:O	6:F:301:GLU:HG2	2.08	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
7:G:50:LEU:O	7:G:54:GLU:HG2	2.07	0.54
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.54
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.89	0.54
10:P:142:GLU:HA	10:P:146:VAL:HG12	1.90	0.54
10:P:209:ARG:N	10:P:352:VAL:HG22	2.23	0.54
11:Q:160:TYR:CZ	11:Q:164:PHE:HZ	2.26	0.54
14:T:83:VAL:HG22	14:T:126:PHE:HZ	1.66	0.54
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.54
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.73	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
8:H:303:TRP:CZ3	20:b:28:LEU:HG	2.43	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.54
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.43	0.54
2:B:141:MET:CE	4:D:115:LEU:HD23	2.37	0.54
6:F:152:ARG:CZ	23:s:60:PRO:HG3	2.38	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
8:H:69:SER:O	8:H:72:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:52:LEU:HG	16:W:21:LYS:HG2	1.90	0.54
16:W:67:ARG:HD2	16:W:71:MET:HE2	1.89	0.54
21:q:95:ASP:OD1	21:q:96:ASP:N	2.41	0.54
1:A:41:PHE:HB2	4:D:83:ASN:HD22	1.73	0.54
1:A:65:PHE:O	1:A:68:GLU:HG2	2.08	0.54
1:A:77:TRP:CD1	8:H:317:TYR:CE1	2.96	0.54
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.43	0.54
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.54
6:F:276:PHE:HD1	6:F:352:ALA:HB1	1.72	0.54
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.54
7:G:355:LYS:HG3	7:G:366:LEU:CD1	2.38	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	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
13:S:16:LEU:O	13:S:16:LEU:CD1	2.51	0.54
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.54
21:q:68:MET:SD	21:q:81:MET:CB	2.95	0.54
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.38	0.53
1:A:61:THR:O	1:A:64:LEU:N	2.41	0.53
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.53
6:F:67:GLU:O	6:F:71:LYS:HG2	2.07	0.53
6:F:109:ARG:HE	6:F:239:PRO:HD3	1.73	0.53
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.53
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.53
10:P:376:ASN:OD1	10:P:376:ASN:C	2.50	0.53
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.53
17:X:120:PRO:HG3	20:b:71:GLN:HE21	1.73	0.53
21:q:56:PHE:HD1	21:q:59:HIS:NE2	2.06	0.53
21:q:125:VAL:HG23	21:q:125:VAL:O	2.08	0.53
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.23	0.53
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.53
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.53
6:F:171:VAL:HA	6:F:174:ARG:NH1	2.24	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
16:W:53:MET:HB2	16:W:55:LEU:HG	1.89	0.53
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.53
6:F:127:ASP:HB3	6:F:245:VAL:CG2	2.38	0.53
7:G:382:ARG:HD2	13:S:56:ARG:HD3	1.90	0.53
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.53
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.53
10:P:122:HIS:CB	12:R:46:VAL:CG1	2.85	0.53
17:X:64:ASN:O	17:X:68:LEU:HG	2.07	0.53
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.90	0.53
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.43	0.53
5:E:39:VAL:CG2	7:G:205:GLN:HE22	2.16	0.53
6:F:235:VAL:HG12	6:F:240:THR:OG1	2.09	0.53
6:F:388:GLY:CA	6:F:419:ILE:HD11	2.37	0.53
7:G:94:MET:HE2	7:G:100:TRP:HH2	1.74	0.53
9:I:78:PHE:CG	22:r:8:ILE:HG23	2.44	0.53
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.53
21:q:132:LYS:HD3	21:q:135:HIS:ND1	2.23	0.53
1:A:41:PHE:HE2	4:D:96:ARG:HG3	1.73	0.53
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.89	0.53
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.53
7:G:360:LYS:HB2	7:G:632:ILE:CD1	2.28	0.53
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	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
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.53
3:C:224:GLU:OE1	10:P:48:ARG:O	2.26	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:129:TYR:CZ	5:E:207:LEU:HB3	2.43	0.53
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.53
8:H:172:MET:HE1	18:Z:46:GLY:HA3	1.91	0.53
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.53
1:A:37:TYR:HD1	2:B:151:GLN:OE1	1.92	0.53
1:A:52:SER:O	4:D:103:GLY:CA	2.57	0.53
6:F:270:ASN:ND2	6:F:338:ASP:HB2	2.23	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
10:P:164:PHE:HB3	10:P:198:ALA:CB	2.38	0.53
13:S:16:LEU:HD13	13:S:19:ILE:CD1	2.38	0.53
2:B:114:MET:SD	2:B:119:VAL:HG12	2.48	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:36:VAL:CG1	7:G:56:VAL:HG11	2.34	0.53
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.09	0.53
7:G:163:LYS:HE2	12:R:97:LYS:NZ	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
9:I:153:ILE:HD12	9:I:153:ILE:O	2.09	0.53
10:P:370:LYS:HG3	10:P:370:LYS:O	2.08	0.53
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.53
17:X:25:LEU:HD11	19:a:50:ARG:CZ	2.39	0.53
17:X:80:GLU:HB3	17:X:81:PRO:HD3	1.91	0.53
17:X:130:LYS:HZ2	20:b:63:MET:HB2	1.74	0.53
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.53
2:B:135:GLY:O	2:B:165:ALA:HB2	2.08	0.53
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.53
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.53
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.91	0.53
7:G:347:ASP:N	7:G:347:ASP:OD1	2.41	0.53
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.90	0.53
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
12:R:69:VAL:HG12	12:R:112:LYS:N	2.24	0.53
21:q:3:LEU:HD13	33:q:201:CDL:OB6	2.09	0.53
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.53
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.53
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.44	0.53
5:E:77:ALA:C	5:E:80:PRO:HD2	2.33	0.53
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.53
7:G:30:ASN:O	7:G:45:PRO:HD3	2.09	0.53
4:D:80:MET:SD	8:H:126:LYS:HD3	2.49	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
10:P:283:MET:HE2	10:P:366:ILE:HG22	1.92	0.52
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.52
14:T:114:ASP:OD1	16:W:67:ARG:NH1	2.42	0.52
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.91	0.52
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.91	0.52
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.52
8:H:51:ASP:OD1	8:H:51:ASP:C	2.52	0.52
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.52
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.52
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.52
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.35	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HD23	1:A:49:LEU:H	1.72	0.52
1:A:53:MET:HE3	1:A:55:PHE:CE1	2.45	0.52
2:B:173:TYR:O	3:C:203:LEU:HD22	2.09	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.52
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.52
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.52
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.74	0.52
1:A:77:TRP:HD1	8:H:317:TYR:CE1	2.27	0.52
2:B:141:MET:HE1	4:D:86:PRO:HB2	1.90	0.52
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.22	0.52
7:G:140:GLN:HG3	7:G:141:ASP:OD1	2.10	0.52
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
10:P:94:LEU:O	10:P:97:MET:HG2	2.09	0.52
10:P:239:PRO:HG2	10:P:345:LEU:CD1	2.40	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:CD1	2.44	0.52
1:A:37:TYR:OH	1:A:39:CYS:HA	2.09	0.52
1:A:87:MET:HE1	8:H:309:ILE:HD11	1.92	0.52
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.92	0.52
7:G:30:ASN:O	7:G:44:GLU:HA	2.09	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.52
8:H:23:VAL:HG11	19:a:9:LEU:CD2	2.39	0.52
12:R:98:GLU:HA	12:R:113:GLN:CD	2.34	0.52
19:a:3:PHE:HE2	33:q:201:CDL:H112	1.74	0.52
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.52
21:q:13:GLN:HE22	33:q:201:CDL:CA3	2.22	0.52
1:A:36:PRO:CG	1:A:43:PRO:HG2	2.40	0.52
1:A:68:GLU:HB3	1:A:98:LEU:HG	1.92	0.52
2:B:95:PHE:CE2	2:B:97:LEU:HD21	2.45	0.52
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.45	0.52
5:E:178:ALA:HA	6:F:125:CYS:SG	2.49	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
7:G:634:LEU:HD13	7:G:636:TYR:CZ	2.43	0.52
8:H:102:ILE:CD1	8:H:154:LEU:HD21	2.39	0.52
21:q:6:VAL:HG11	33:q:201:CDL:HB4	1.91	0.52
21:q:66:THR:HG22	21:q:74:PHE:CB	2.28	0.52
2:B:103:GLU:O	2:B:106:HIS:HB2	2.10	0.52
4:D:280:ALA:CB	15:V:11:LEU:CG	2.81	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.52
4:D:368:ARG:HA	4:D:371:MET:HG2	1.90	0.52
5:E:188:ASN:O	5:E:189:ASP:HB3	2.10	0.52
5:E:192:TYR:CE2	5:E:213:PRO:HB2	2.45	0.52
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.52
8:H:223:PHE:O	8:H:224:PHE:C	2.52	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
16:W:73:ASN:O	16:W:76:VAL:HG12	2.10	0.52
17:X:6:GLU:HG3	17:X:6:GLU:O	2.08	0.52
22:r:28:TYR:O	22:r:29:GLN:C	2.53	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.10	0.52
1:A:36:PRO:HG2	1:A:43:PRO:HG2	1.92	0.52
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.52
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.33	0.52
5:E:240:PRO:HG3	6:F:60:GLY:HA2	1.91	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
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
8:H:85:LEU:CD2	8:H:108:THR:HB	2.38	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
10:P:353:LEU:HA	10:P:356:HIS:HD2	1.74	0.52
17:X:54:ARG:HH21	18:Z:116:TRP:HB2	1.74	0.52
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.42	0.52
1:A:104:TYR:O	1:A:105:GLU:C	2.51	0.52
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.52
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.39	0.52
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
7:G:47:THR:O	7:G:96:VAL:HG12	2.10	0.52
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.52
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.52
21:q:65:THR:CG2	21:q:66:THR:N	2.72	0.52
1:A:19:LEU:O	1:A:20:VAL:C	2.50	0.52
3:C:114:THR:CG2	4:D:421:ARG:HH12	2.17	0.52
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.15	0.52
7:G:64:CYS:HG	7:G:75:CYS:HG	1.56	0.52
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.10	0.52
7:G:401:LEU:HD21	7:G:466:LEU:HD21	1.92	0.52
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:317:TYR:O	8:H:318:MET:C	2.52	0.52
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.45	0.52
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.52
17:X:129:THR:CG2	20:b:68:SER:HA	2.39	0.52
4:D:106:VAL:HG21	4:D:447:VAL:CG2	2.41	0.51
4:D:259:GLU:C	4:D:261:MET:H	2.18	0.51
6:F:63:TYR:H	6:F:256:ARG:HH21	1.57	0.51
6:F:217:GLU:CD	11:Q:166:TRP:HE1	2.18	0.51
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.51
7:G:386:LEU:HD21	7:G:523:VAL:HG13	1.91	0.51
7:G:671:LEU:CD1	13:S:42:VAL:HG12	2.41	0.51
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.51
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.41	0.51
7:G:367:CYS:HB3	7:G:533:GLY:O	2.10	0.51
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.51
10:P:195:PHE:CD1	10:P:198:ALA:HB2	2.45	0.51
14:T:79:ILE:CG2	14:T:145:VAL:HG13	2.40	0.51
14:T:140:CYS:HB2	14:T:143:GLU:CG	2.40	0.51
17:X:77:HIS:HD2	17:X:115:LEU:HD21	1.75	0.51
18:Z:65:LEU:HB2	20:b:50:PRO:HG2	1.91	0.51
4:D:218:SER:CB	4:D:224:ALA:HB1	2.41	0.51
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.74	0.51
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.45	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
8:H:33:LEU:HD23	22:r:25:GLN:HG2	1.92	0.51
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	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
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51
7:G:75:CYS:SG	7:G:76:ARG:N	2.84	0.51
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.51
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
7:G:614:GLY:O	16:W:129:HIS:NE2	2.41	0.51
8:H:51:ASP:O	8:H:54:LYS:HG2	2.10	0.51
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.51
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.91	0.51
10:P:207:PHE:O	10:P:241:TYR:HA	2.10	0.51
17:X:56:CYS:HA	17:X:135:ARG:NH1	2.25	0.51
20:b:36:SER:HB3	20:b:39:THR:OG1	2.10	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.51
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.51
5:E:129:TYR:CE2	5:E:207:LEU:HB3	2.46	0.51
5:E:180:VAL:HG22	5:E:221:ARG:HH12	1.75	0.51
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.51
7:G:253:VAL:O	7:G:253:VAL:HG12	2.11	0.51
7:G:355:LYS:HA	7:G:366:LEU:CD1	2.37	0.51
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	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	2.45	0.51
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.51
17:X:7:LEU:HD12	17:X:7:LEU:C	2.36	0.51
19:a:1:MET:HG3	33:q:201:CDL:CB2	2.40	0.51
21:q:29:ARG:HD3	21:q:74:PHE:CE1	2.44	0.51
21:q:89:TRP:HB2	21:q:98:PRO:HD3	1.92	0.51
7:G:41:VAL:HG21	7:G:56:VAL:CB	2.41	0.51
7:G:275:PRO:HB2	11:Q:86:ASN:ND2	2.25	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.98	0.51
9:I:38:TYR:HB3	9:I:41:LYS:HB2	1.93	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	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	2.29	0.51
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.10	0.51
6:F:42:PHE:CE1	6:F:130:ILE:HD12	2.46	0.51
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:142:TYR:CE1	8:H:285:LEU:HD21	2.46	0.51
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.51
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
5:E:43:THR:HG23	5:E:46:ASN:H	1.75	0.51
6:F:122:PRO:HG3	6:F:373:PHE:CZ	2.46	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.51
1:A:68:GLU:O	1:A:69:ILE:C	2.53	0.51
4:D:145:MET:O	4:D:146:CYS:C	2.54	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
7:G:358:LEU:HD12	7:G:366:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
8:H:74:ALA:HB3	8:H:75:PRO:HD3	1.93	0.51
8:H:142:TYR:CE1	8:H:285:LEU:CD2	2.94	0.51
17:X:8:PRO:O	18:Z:88:ARG:NH1	2.43	0.51
4:D:166:ARG:CZ	18:Z:8:GLN:HG2	2.41	0.51
9:I:71:GLY:HA2	26:I:301:PC1:H351	1.93	0.51
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.51
10:P:367:GLU:HG2	10:P:368:GLU:N	2.26	0.51
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.51
14:T:105:MET:HB2	14:T:139:MET:SD	2.51	0.51
17:X:38:LYS:O	17:X:42:GLU:HG3	2.11	0.51
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.51
2:B:123:ALA:O	2:B:125:PRO:N	2.43	0.50
25:B:302:UQ9:H1MB	25:B:302:UQ9:H8	1.92	0.50
8:H:90:PRO:CG	8:H:240:ILE:HG21	2.39	0.50
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	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
14:T:87:LEU:HD23	14:T:122:MET:CE	2.41	0.50
20:b:11:ASN:OD1	20:b:12:ALA:N	2.44	0.50
4:D:83:ASN:O	4:D:84:PHE:C	2.55	0.50
4:D:266:ARG:HD3	29:H:403:3PE:O12	2.11	0.50
6:F:113:LEU:HB3	6:F:154:ALA:HB2	1.92	0.50
7:G:304:GLU:HB2	7:G:316:TYR:HD2	1.75	0.50
7:G:401:LEU:HD21	7:G:462:PHE:CE2	2.46	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.50
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.50
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.50
17:X:9:THR:CG2	17:X:12:GLU:HB2	2.38	0.50
19:a:3:PHE:CE2	33:q:201:CDL:H112	2.47	0.50
20:b:66:VAL:HG22	20:b:75:GLY:CA	2.40	0.50
22:r:6:ARG:HG2	22:r:6:ARG:O	2.11	0.50
1:A:37:TYR:CE1	2:B:125:PRO:HG2	2.47	0.50
1:A:73:LEU:N	1:A:74:PRO:CD	2.74	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
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
8:H:30:TYR:OH	19:a:4:GLU:HB2	2.11	0.50
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.93	0.50
12:R:32:THR:CG2	12:R:36:GLN:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:44:TYR:CD1	15:V:48:THR:HG23	2.46	0.50
18:Z:88:ARG:HD3	18:Z:91:LEU:HB3	1.92	0.50
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.50
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.92	0.50
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.93	0.50
8:H:42:PRO:HB3	21:q:27:PHE:HE2	1.76	0.50
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.50
11:Q:167:ASN:C	11:Q:168:LYS:HG2	2.36	0.50
19:a:42:GLN:O	19:a:43:TYR:C	2.50	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.50
4:D:84:PHE:HB2	4:D:97:LEU:HB3	1.93	0.50
4:D:137:ASP:OD1	4:D:148:GLU:OE2	2.28	0.50
5:E:136:THR:HG22	5:E:137:THR:N	2.26	0.50
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
8:H:52:ALA:HB2	25:H:401:UQ9:H22A	1.93	0.50
8:H:103:LEU:HG	8:H:160:TYR:CD1	2.46	0.50
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.50
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.92	0.50
16:W:95:GLU:HB3	16:W:101:LYS:HG3	1.94	0.50
17:X:25:LEU:O	17:X:29:ALA:N	2.44	0.50
19:a:4:GLU:O	19:a:7:PRO:HD2	2.11	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
4:D:207:ARG:O	4:D:208:GLU:C	2.54	0.50
4:D:253:LEU:HB2	22:r:23:LYS:HD3	1.92	0.50
6:F:238:CYS:O	6:F:239:PRO:C	2.54	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
7:G:382:ARG:O	7:G:386:LEU:HD12	2.10	0.50
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.11	0.50
12:R:55:VAL:HG22	12:R:56:ASN:H	1.77	0.50
15:V:56:LEU:HA	15:V:59:VAL:HB	1.94	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
5:E:152:GLN:HE21	5:E:159:VAL:HB	1.76	0.50
6:F:174:ARG:O	6:F:178:GLU:HG3	2.11	0.50
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.50
10:P:150:ARG:O	10:P:151:ALA:C	2.55	0.50
10:P:208:GLY:N	10:P:211:ASP:HB3	2.20	0.50
10:P:374:THR:HG23	10:P:374:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:167:ASN:HA	23:s:64:ARG:HD3	1.94	0.50
21:q:6:VAL:HG12	33:q:201:CDL:OA9	2.11	0.50
1:A:33:LYS:HE2	8:H:61:MET:HE1	1.94	0.50
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.50
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.51	0.50
5:E:227:ALA:HB3	6:F:284:HIS:ND1	2.27	0.50
6:F:295:PRO:HD2	6:F:298:GLU:OE2	2.11	0.50
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.94	0.50
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.50
8:H:26:LYS:O	8:H:30:TYR:CD2	2.65	0.50
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50
26:B:303:PC1:H232	26:B:303:PC1:C32	2.37	0.50
5:E:130:HIS:O	5:E:132:GLN:HG3	2.12	0.50
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.50
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.50
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.46	0.50
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.50
4:D:105:MET:SD	4:D:441:GLY:HA2	2.53	0.49
4:D:250:ASN:O	4:D:251:PHE:C	2.54	0.49
4:D:289:SER:N	4:D:293:LEU:HG	2.27	0.49
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.12	0.49
7:G:298:LYS:O	21:q:134:ILE:HA	2.12	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
8:H:12:PRO:O	19:a:15:CYS:HB3	2.12	0.49
8:H:17:MET:CE	8:H:225:MET:HB3	2.41	0.49
10:P:166:HIS:CE1	10:P:168:SER:HB2	2.45	0.49
10:P:246:SER:O	10:P:247:LYS:C	2.55	0.49
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.49
15:V:56:LEU:C	15:V:56:LEU:CD1	2.85	0.49
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.93	0.49
18:Z:140:PHE:O	18:Z:141:THR:C	2.55	0.49
1:A:40:GLY:O	1:A:41:PHE:C	2.54	0.49
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.42	0.49
7:G:344:GLY:O	7:G:345:LEU:HB2	2.12	0.49
7:G:617:ARG:NH1	16:W:129:HIS:N	2.57	0.49
8:H:202:GLU:OE2	8:H:211:PHE:HB3	2.12	0.49
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.49
18:Z:129:THR:HG22	18:Z:131:GLU:H	1.77	0.49
3:C:216:LYS:HG3	10:P:209:ARG:HH11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:460:GLU:O	4:D:463:ARG:HG2	2.12	0.49
8:H:63:PRO:O	8:H:66:THR:HG22	2.12	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.94	0.49
10:P:157:LYS:O	10:P:158:GLU:C	2.54	0.49
14:T:140:CYS:O	14:T:144:ILE:HG13	2.12	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.95	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:HG3	1.93	0.49
7:G:304:GLU:HB2	7:G:316:TYR:CD2	2.46	0.49
8:H:172:MET:SD	18:Z:46:GLY:HA2	2.51	0.49
17:X:115:LEU:HD13	17:X:117:TRP:CZ3	2.48	0.49
1:A:65:PHE:CZ	1:A:102:LEU:CB	2.74	0.49
2:B:91:TRP:N	2:B:91:TRP:CD1	2.80	0.49
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.77	0.49
25:B:302:UQ9:C8	25:B:302:UQ9:C1M	2.90	0.49
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.49
5:E:235:GLU:HB2	6:F:37:ASP:CB	2.42	0.49
6:F:36:LYS:HB3	6:F:38:GLU:HG2	1.93	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.47	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
7:G:117:MET:HE3	7:G:143:SER:N	2.27	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
10:P:178:SER:O	10:P:179:LYS:C	2.55	0.49
13:S:36:PHE:CZ	13:S:44:LEU:HD11	2.36	0.49
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.38	0.49
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	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
5:E:233:LEU:HD13	6:F:48:ARG:HH22	1.76	0.49
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.35	0.49
14:T:104:PHE:CZ	14:T:118:ILE:HG21	2.48	0.49
14:T:138:LEU:HD13	14:T:144:ILE:CD1	2.42	0.49
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.94	0.49
17:X:112:LEU:HD13	17:X:118:VAL:HG22	1.94	0.49
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.94	0.49
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.93	0.49
1:A:97:ILE:HG13	1:A:98:LEU:HD22	1.93	0.49
3:C:100:ARG:HH12	15:V:86:LYS:NZ	2.11	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:227:ALA:H	6:F:284:HIS:HB3	1.76	0.49
6:F:146:GLY:O	6:F:150:GLY:N	2.46	0.49
6:F:171:VAL:O	6:F:175:GLU:HG2	2.12	0.49
7:G:43:VAL:CG1	7:G:55:LYS:HD3	2.41	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
10:P:168:SER:O	10:P:202:ARG:HA	2.13	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
1:A:78:ALA:C	1:A:80:GLN:N	2.68	0.49
2:B:104:MET:HE2	2:B:121:PHE:HZ	1.67	0.49
2:B:194:CYS:HB2	9:I:153:ILE:O	2.12	0.49
5:E:244:VAL:HG23	6:F:256:ARG:CG	2.42	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.49
8:H:93:HIS:O	19:a:23:THR:HG22	2.13	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
18:Z:66:GLU:HA	18:Z:69:ILE:HG12	1.93	0.49
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.49
1:A:105:GLU:HG3	1:A:111:LEU:HD22	1.95	0.49
3:C:124:ARG:HD2	11:Q:140:LYS:HZ2	1.78	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.49
5:E:134:CYS:SG	5:E:139:CYS:SG	3.11	0.49
5:E:135:THR:O	6:F:369:ARG:NE	2.41	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
8:H:116:ILE:CG1	8:H:117:LEU:N	2.74	0.49
10:P:354:ARG:NH2	16:W:56:ASP:OD1	2.45	0.49
13:S:24:CYS:N	13:S:58:CYS:SG	2.85	0.49
13:S:42:VAL:O	13:S:46:LYS:HG3	2.12	0.49
14:T:88:LYS:NZ	14:T:96:GLU:H	2.11	0.49
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.49
16:W:103:ARG:O	16:W:104:THR:C	2.55	0.49
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
4:D:339:GLN:HE21	9:I:37:LYS:NZ	2.11	0.49
7:G:386:LEU:HD21	7:G:523:VAL:HG11	1.95	0.49
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
8:H:70:LEU:HD22	8:H:121:TRP:CZ3	2.48	0.49
10:P:211:ASP:O	10:P:215:ASN:HB2	2.12	0.49
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:67:GLN:HG2	12:R:109:LEU:HD21	1.94	0.49
17:X:4:ILE:HD12	18:Z:107:GLY:O	2.13	0.49
19:a:37:ARG:CB	19:a:48:MET:HE2	2.42	0.49
22:r:12:ARG:HE	22:r:20:LEU:HD21	1.78	0.49
1:A:89:ILE:O	1:A:93:ILE:HG12	2.13	0.48
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.48
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.38	0.48
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.48	0.48
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.94	0.48
6:F:225:LEU:HB2	11:Q:160:TYR:CD2	2.45	0.48
6:F:288:VAL:O	6:F:289:GLU:HB3	2.13	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
7:G:357:LEU:HD13	7:G:627:SER:OG	2.12	0.48
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.48
8:H:179:TRP:CZ3	9:I:62:MET:HE1	2.48	0.48
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.48
6:F:35:LEU:HB2	6:F:291:GLU:HB2	1.94	0.48
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.48
29:H:403:3PE:H241	29:H:403:3PE:H272	1.55	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.95	0.48
17:X:69:ASN:O	17:X:70:PHE:C	2.56	0.48
23:s:64:ARG:HD2	23:s:64:ARG:N	2.29	0.48
1:A:41:PHE:CE2	4:D:96:ARG:HD3	2.36	0.48
2:B:115:ASP:O	2:B:116:ARG:C	2.54	0.48
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.48
5:E:201:GLU:HA	5:E:204:ILE:HD12	1.95	0.48
6:F:224:ARG:HD2	11:Q:164:PHE:CE1	2.48	0.48
8:H:116:ILE:HG13	8:H:117:LEU:H	1.76	0.48
9:I:80:GLU:CB	22:r:26:LEU:HD11	2.43	0.48
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.48
16:W:46:VAL:N	16:W:47:PRO:HD2	2.29	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.78	0.48
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.77	0.48
6:F:116:ASN:O	6:F:245:VAL:HG13	2.13	0.48
6:F:274:LYS:HZ2	6:F:352:ALA:HB3	1.77	0.48
6:F:289:GLU:O	6:F:289:GLU:CD	2.56	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:222:LEU:O	8:H:223:PHE:C	2.50	0.48
29:H:403:3PE:HN3	20:b:18:VAL:HG23	1.78	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:122:HIS:HB3	12:R:46:VAL:CG1	2.43	0.48
10:P:197:GLU:HA	10:P:260:GLY:HA2	1.96	0.48
2:B:210:ARG:CD	21:q:76:ASP:HB2	2.44	0.48
3:C:134:LEU:H	3:C:134:LEU:HD12	1.79	0.48
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.48
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.48
8:H:116:ILE:HA	8:H:211:PHE:HE1	1.75	0.48
10:P:235:THR:HB	10:P:273:LEU:HB2	1.95	0.48
10:P:265:PHE:HZ	10:P:338:LEU:HD12	1.78	0.48
16:W:120:ASP:OD1	16:W:121:PHE:N	2.46	0.48
1:A:4:TYR:CE1	29:H:402:3PE:H282	2.48	0.48
1:A:41:PHE:CZ	4:D:96:ARG:HD2	2.36	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48
26:B:303:PC1:H132	21:q:29:ARG:HA	1.96	0.48
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.48
6:F:227:PRO:HG3	7:G:94:MET:SD	2.54	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
10:P:328:MET:O	10:P:330:THR:HG23	2.12	0.48
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.48
1:A:30:TYR:CZ	1:A:33:LYS:HB2	2.49	0.48
1:A:57:LEU:HD12	1:A:110:GLY:O	2.14	0.48
2:B:92:PRO:HG3	2:B:119:VAL:CG1	2.42	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.13	0.48
7:G:66:HIS:HB3	7:G:69:LEU:HB2	1.96	0.48
7:G:662:THR:HB	13:S:25:GLN:NE2	2.28	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.44	0.48
8:H:51:ASP:OD1	25:H:401:UQ9:H17	2.13	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
17:X:80:GLU:O	17:X:81:PRO:C	2.56	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
8:H:127:TYR:HD2	8:H:207:LEU:HG	1.78	0.48
10:P:294:PRO:HB3	10:P:296:PHE:HD1	1.79	0.48
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.48
12:R:36:GLN:HG2	21:q:127:TYR:HD2	1.78	0.48
14:T:117:GLU:HG2	16:W:43:TYR:CZ	2.49	0.48
21:q:23:LEU:HD11	21:q:33:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HD23	1:A:94:LEU:HD23	1.96	0.48
1:A:106:TRP:CZ2	8:H:291:LYS:HA	2.49	0.48
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.48
4:D:260:GLU:HG3	18:Z:25:LEU:CD2	2.44	0.48
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.48
5:E:221:ARG:HH22	6:F:285:PRO:HB2	1.79	0.48
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.48
7:G:53:CYS:O	7:G:56:VAL:HG12	2.13	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
8:H:130:PHE:O	8:H:134:ARG:HG3	2.14	0.48
29:H:403:3PE:H3E1	29:H:403:3PE:H3I2	1.95	0.48
16:W:46:VAL:O	16:W:50:VAL:HG23	2.14	0.48
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.44	0.48
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.96	0.48
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.78	0.48
4:D:259:GLU:C	4:D:261:MET:N	2.68	0.48
7:G:32:ILE:N	7:G:43:VAL:O	2.46	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	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
8:H:85:LEU:HB3	8:H:233:LEU:CD2	2.42	0.48
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.48	0.48
10:P:360:ARG:HD3	10:P:360:ARG:O	2.14	0.48
13:S:58:CYS:HB2	13:S:61:VAL:CG1	2.43	0.48
2:B:91:TRP:CE3	2:B:122:ARG:HG3	2.49	0.47
2:B:131:MET:HE3	2:B:152:MET:HE2	1.95	0.47
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.49	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
6:F:102:MET:HE3	6:F:102:MET:HB2	1.73	0.47
6:F:146:GLY:HA3	6:F:193:PHE:CE2	2.48	0.47
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.49	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.47
14:T:117:GLU:HA	14:T:120:MET:CE	2.41	0.47
17:X:20:VAL:CG2	17:X:24:VAL:HG21	2.40	0.47
21:q:68:MET:SD	21:q:81:MET:HG2	2.54	0.47
2:B:141:MET:HE1	4:D:86:PRO:CB	2.44	0.47
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.67	0.47
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.96	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.50	0.47
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:30:TYR:HE1	19:a:1:MET:O	1.96	0.47
8:H:96:ILE:HG12	18:Z:143:TYR:OH	2.14	0.47
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.48	0.47
12:R:79:CYS:O	12:R:88:HIS:CE1	2.67	0.47
17:X:52:ASP:HB2	17:X:54:ARG:HD3	1.96	0.47
1:A:84:THR:HG23	20:b:46:ASN:HD21	1.78	0.47
4:D:260:GLU:CG	18:Z:25:LEU:HD22	2.43	0.47
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.47
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.30	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
8:H:91:MET:O	8:H:92:PRO:C	2.54	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
10:P:44:GLY:HA2	11:Q:107:TRP:CE3	2.49	0.47
10:P:157:LYS:HD3	10:P:194:VAL:O	2.14	0.47
14:T:133:ILE:O	14:T:136:GLU:N	2.46	0.47
1:A:30:TYR:CE1	1:A:33:LYS:HD3	2.49	0.47
1:A:33:LYS:CE	8:H:61:MET:HE1	2.44	0.47
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.47
7:G:557:ARG:CG	7:G:579:MET:HE3	2.33	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
8:H:210:GLY:HA2	8:H:213:VAL:CG2	2.44	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
10:P:97:MET:O	10:P:103:LEU:HD11	2.15	0.47
10:P:221:ARG:HD2	10:P:286:ARG:HD3	1.92	0.47
13:S:50:ASN:O	13:S:51:LEU:C	2.57	0.47
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.47
2:B:104:MET:CE	2:B:121:PHE:CZ	2.85	0.47
3:C:149:LEU:CD1	16:W:80:ARG:HH21	2.23	0.47
6:F:57:LEU:HD23	6:F:61:ASP:OD1	2.13	0.47
6:F:230:PRO:HA	6:F:233:VAL:O	2.15	0.47
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.48	0.47
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.47
8:H:20:LEU:HA	19:a:12:MET:SD	2.53	0.47
8:H:200:LEU:CD2	8:H:285:LEU:HD13	2.44	0.47
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.97	0.47
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.14	0.47
23:s:49:ASN:HA	23:s:52:LEU:HD12	1.97	0.47
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.47
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.47
6:F:209:GLU:OE2	6:F:230:PRO:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:210:GLU:HG3	10:P:210:GLU:O	2.15	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.47
22:r:12:ARG:HB3	22:r:20:LEU:CD2	2.44	0.47
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.47
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.47
4:D:198:THR:HG23	8:H:275:ALA:O	2.14	0.47
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.30	0.47
5:E:43:THR:OG1	5:E:44:PRO:CD	2.61	0.47
5:E:45:GLU:HB3	5:E:91:TRP:HH2	1.78	0.47
5:E:47:ASN:H	5:E:50:THR:HG23	1.79	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:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.47
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.43	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
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.95	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
7:G:651:PRO:CD	13:S:56:ARG:HB3	2.45	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.47	0.47
10:P:85:ARG:HE	30:P:401:NDP:C2A	2.27	0.47
10:P:209:ARG:O	10:P:210:GLU:HB3	2.15	0.47
14:T:119:ILE:HG13	14:T:135:ALA:HB1	1.95	0.47
19:a:22:SER:O	19:a:23:THR:C	2.57	0.47
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.96	0.47
5:E:141:LEU:HD22	6:F:281:HIS:NE2	2.30	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.47
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.47
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.47
8:H:1:MET:HE3	19:a:29:PHE:CE1	2.50	0.47
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.96	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
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.48	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.50	0.47
1:A:75:LEU:N	1:A:76:PRO:CD	2.77	0.47
2:B:123:ALA:HB1	4:D:89:PRO:HG3	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.47
4:D:254:ARG:NH1	22:r:25:GLN:N	2.62	0.47
5:E:226:PRO:HD2	5:E:230:LEU:HB3	1.97	0.47
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.96	0.47
6:F:382:CYS:HA	7:G:74:ASN:O	2.15	0.47
8:H:18:ALA:HB2	25:H:401:UQ9:C25	2.44	0.47
17:X:39:THR:CG2	17:X:40:ASN:N	2.77	0.47
2:B:138:THR:HG21	4:D:116:LEU:HA	1.97	0.47
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.47
7:G:382:ARG:NH1	7:G:386:LEU:HD11	2.30	0.47
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.47
14:T:87:LEU:CD2	14:T:104:PHE:CE1	2.94	0.47
15:V:56:LEU:HD12	15:V:57:ASP:CA	2.44	0.47
17:X:115:LEU:HD13	17:X:117:TRP:CZ2	2.50	0.47
18:Z:72:MET:N	18:Z:73:PRO:CD	2.78	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	0.46
6:F:168:ASN:ND2	23:s:40:TYR:HE2	2.13	0.46
7:G:140:GLN:HG3	7:G:141:ASP:N	2.30	0.46
15:V:22:GLU:O	15:V:26:ILE:HG12	2.16	0.46
16:W:32:LYS:O	16:W:36:ARG:HG3	2.15	0.46
16:W:50:VAL:HA	16:W:55:LEU:HD12	1.97	0.46
17:X:129:THR:HG23	20:b:68:SER:CA	2.44	0.46
1:A:41:PHE:CD2	4:D:96:ARG:CG	2.96	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.46
6:F:46:TYR:O	6:F:48:ARG:HG3	2.15	0.46
11:Q:166:TRP:CZ3	23:s:67:PRO:HG2	2.50	0.46
20:b:41:TYR:HD1	20:b:80:TRP:CZ3	2.33	0.46
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.46
2:B:121:PHE:CE1	25:B:302:UQ9:H12A	2.51	0.46
2:B:154:GLU:O	10:P:89:TYR:OH	2.33	0.46
4:D:235:ASP:OD2	18:Z:8:GLN:NE2	2.41	0.46
6:F:41:ILE:O	6:F:137:LYS:NZ	2.47	0.46
6:F:292:MET:HG2	6:F:293:SER:H	1.80	0.46
9:I:105:ARG:NH2	12:R:56:ASN:ND2	2.63	0.46
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.46
17:X:41:LYS:O	17:X:42:GLU:C	2.59	0.46
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.44	0.46
2:B:104:MET:HE3	2:B:132:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
5:E:45:GLU:CD	5:E:45:GLU:H	2.23	0.46
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.46
12:R:38:TYR:CD1	12:R:44:ARG:HB2	2.51	0.46
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.46
15:V:56:LEU:HD13	15:V:60:LYS:HE2	1.98	0.46
16:W:45:GLU:O	16:W:46:VAL:C	2.58	0.46
17:X:4:ILE:HG23	18:Z:107:GLY:O	2.15	0.46
17:X:35:GLN:HG3	17:X:70:PHE:HE1	1.80	0.46
22:r:109:ASP:O	22:r:110:GLN:OE1	2.32	0.46
4:D:142:VAL:HG21	4:D:185:MET:HG2	1.98	0.46
6:F:270:ASN:C	6:F:292:MET:HE3	2.40	0.46
6:F:278:ILE:CG2	6:F:282:VAL:HG21	2.46	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.46
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.46
8:H:306:SER:OG	20:b:33:PRO:HG3	2.15	0.46
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.80	0.46
9:I:48:VAL:O	20:b:10:LYS:NZ	2.49	0.46
12:R:39:ASP:CG	12:R:40:GLU:N	2.74	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.59	0.46
19:a:49:GLU:CD	19:a:52:ARG:HH11	2.22	0.46
33:q:201:CDL:OB7	22:r:8:ILE:HD11	2.16	0.46
3:C:141:ARG:NH1	4:D:410:TYR:CE1	2.77	0.46
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.37	0.46
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.46
5:E:154:LYS:HE3	5:E:201:GLU:HB2	1.97	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.31	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
7:G:401:LEU:HD12	7:G:474:VAL:HG22	1.96	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
10:P:328:MET:HB2	10:P:329:PRO:HD2	1.98	0.46
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.46
17:X:120:PRO:CB	17:X:125:LEU:CD1	2.91	0.46
18:Z:85:GLN:O	18:Z:89:GLU:HG3	2.15	0.46
18:Z:88:ARG:O	18:Z:91:LEU:HB3	2.15	0.46
20:b:38:TYR:O	20:b:39:THR:C	2.59	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46
4:D:238:LEU:HA	18:Z:9:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:381:HIS:HE1	9:I:161:ALA:O	1.99	0.46
5:E:238:LYS:HE2	5:E:242:PHE:CZ	2.51	0.46
6:F:111:LYS:HG2	6:F:239:PRO:HB2	1.97	0.46
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.46
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.46
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.81	0.46
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.46
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.46
9:I:89:GLU:HG3	21:q:61:TRP:HB3	1.97	0.46
10:P:163:ARG:HH11	10:P:199:ILE:HD11	1.81	0.46
10:P:276:LEU:O	10:P:280:ILE:HG13	2.14	0.46
12:R:39:ASP:H	12:R:42:ASP:CG	2.21	0.46
20:b:28:LEU:O	20:b:32:MET:HG2	2.15	0.46
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.16	0.46
2:B:164:CYS:SG	24:B:301:SF4:S4	3.14	0.46
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.46
5:E:141:LEU:O	5:E:142:ARG:HB2	2.15	0.46
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.98	0.46
7:G:308:ARG:HH11	7:G:580:ALA:H	1.64	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
8:H:249:ILE:HG13	19:a:35:GLU:OE2	2.15	0.46
8:H:293:PHE:CE1	29:H:403:3PE:H32	2.51	0.46
10:P:206:ILE:HB	30:P:401:NDP:N7N	2.30	0.46
12:R:32:THR:HA	12:R:55:VAL:CG2	2.45	0.46
17:X:122:LEU:HD21	20:b:81:LEU:HD23	1.98	0.46
19:a:58:ASN:HB2	19:a:61:TYR:CE2	2.50	0.46
4:D:198:THR:HA	8:H:32:GLN:HG2	1.98	0.46
5:E:134:CYS:SG	5:E:175:CYS:HA	2.56	0.46
6:F:86:ARG:HB2	6:F:88:ARG:HH12	1.81	0.46
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	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
21:q:86:TRP:HA	21:q:98:PRO:HG2	1.98	0.46
22:r:109:ASP:O	22:r:110:GLN:CG	2.64	0.46
1:A:109:LYS:HG2	1:A:112:GLU:HB2	1.98	0.46
2:B:71:ALA:O	2:B:75:VAL:N	2.47	0.46
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
5:E:204:ILE:O	5:E:208:LYS:HG3	2.16	0.46
6:F:146:GLY:HA3	6:F:193:PHE:HE2	1.81	0.46
6:F:168:ASN:HD21	23:s:40:TYR:HE2	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.46
9:I:80:GLU:N	19:a:1:MET:HE1	2.31	0.46
10:P:207:PHE:CZ	10:P:345:LEU:HA	2.51	0.46
10:P:285:HIS:CE1	10:P:364:SER:HB3	2.51	0.46
10:P:334:GLY:O	10:P:337:ASP:HB3	2.16	0.46
12:R:33:HIS:HE1	12:R:56:ASN:HD22	1.64	0.46
14:T:87:LEU:CD2	14:T:122:MET:HE1	2.46	0.46
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.46
15:V:116:ILE:O	15:V:116:ILE:CG2	2.62	0.46
21:q:76:ASP:OD1	21:q:76:ASP:C	2.57	0.46
4:D:142:VAL:HG13	4:D:207:ARG:HH12	1.78	0.45
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.45
6:F:179:ALA:HB3	6:F:181:LEU:HG	1.98	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.45
10:P:170:LEU:HD13	10:P:264:ALA:HB1	1.97	0.45
21:q:10:GLY:HA2	33:q:201:CDL:CA5	2.45	0.45
23:s:48:LEU:O	23:s:52:LEU:HG	2.15	0.45
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.45
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.26	0.45
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.97	0.45
7:G:83:GLU:HB2	7:G:101:ASN:HB3	1.98	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
8:H:248:TYR:CD1	8:H:254:LEU:HD23	2.51	0.45
8:H:311:THR:O	8:H:312:ALA:C	2.56	0.45
14:T:133:ILE:HG23	14:T:134:ASP:N	2.32	0.45
21:q:6:VAL:HG13	33:q:201:CDL:CA2	2.47	0.45
1:A:56:PHE:O	1:A:57:LEU:C	2.58	0.45
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.45
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.45
5:E:87:ARG:HD2	23:s:42:THR:HB	1.98	0.45
6:F:69:LEU:HD22	6:F:147:ARG:HB2	1.98	0.45
10:P:55:VAL:HA	10:P:79:GLN:O	2.16	0.45
10:P:95:ARG:HG2	10:P:105:PHE:CE2	2.51	0.45
10:P:169:HIS:ND1	30:P:401:NDP:H5N	2.31	0.45
10:P:264:ALA:O	10:P:266:THR:HG23	2.17	0.45
21:q:14:VAL:HA	21:q:23:LEU:HD22	1.97	0.45
2:B:126:ARG:HG3	8:H:214:GLU:HA	1.99	0.45
5:E:128:LYS:CB	5:E:167:LEU:HA	2.42	0.45
6:F:41:ILE:CD1	6:F:262:PHE:HE1	2.24	0.45
6:F:110:PRO:CB	6:F:152:ARG:HH22	2.30	0.45
7:G:36:VAL:O	7:G:39:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.30	0.45
10:P:208:GLY:N	10:P:211:ASP:OD2	2.49	0.45
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.45
2:B:170:TYR:HB2	9:I:153:ILE:CG2	2.39	0.45
3:C:243:ALA:C	7:G:105:ASN:ND2	2.75	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
5:E:184:MET:HG3	5:E:192:TYR:O	2.16	0.45
6:F:154:ALA:HB2	6:F:193:PHE:HZ	1.82	0.45
6:F:213:ILE:HG23	6:F:235:VAL:CA	2.41	0.45
7:G:360:LYS:CE	7:G:632:ILE:HB	2.41	0.45
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.45
8:H:200:LEU:HD22	8:H:282:TYR:HD1	1.82	0.45
10:P:287:THR:HG23	10:P:289:ILE:HD11	1.97	0.45
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.45
15:V:56:LEU:HD11	15:V:57:ASP:OD1	2.17	0.45
21:q:97:PRO:C	21:q:99:THR:N	2.70	0.45
2:B:95:PHE:CE2	2:B:145:LEU:HD13	2.51	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.45
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.45
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.98	0.45
6:F:81:LYS:HE3	6:F:96:GLY:C	2.41	0.45
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.45
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.45
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.45
8:H:212:ASN:O	8:H:213:VAL:C	2.60	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
18:Z:66:GLU:HA	18:Z:69:ILE:CG1	2.47	0.45
1:A:51:PHE:CD2	8:H:133:LEU:HD13	2.51	0.45
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.45
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.52	0.45
5:E:147:ILE:CG2	5:E:200:ILE:HG12	2.37	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: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:447:ASP:O	7:G:447:ASP:CG	2.59	0.45
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:135:ALA:HB2	8:H:201:THR:HG22	1.98	0.45
8:H:140:ILE:HG13	8:H:141:SER:N	2.32	0.45
8:H:225:MET:HG2	25:H:401:UQ9:H21	1.99	0.45
8:H:240:ILE:HD11	8:H:259:PHE:CD1	2.51	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
13:S:19:ILE:HD12	13:S:94:VAL:CG1	2.44	0.45
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.45
1:A:60:ILE:O	1:A:61:THR:C	2.57	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
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:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD21	1.99	0.45
7:G:401:LEU:HD11	7:G:466:LEU:CD2	2.47	0.45
7:G:432:ILE:HG12	7:G:451:ILE:HD11	1.99	0.45
7:G:454:ASP:OD1	7:G:459:ARG:NH2	2.50	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
10:P:68:TYR:CZ	10:P:242:VAL:HG11	2.51	0.45
10:P:310:PHE:O	10:P:311:GLU:C	2.60	0.45
11:Q:166:TRP:CE3	23:s:67:PRO:HG2	2.51	0.45
14:T:90:TYR:HE2	14:T:92:LYS:HB3	1.78	0.45
1:A:4:TYR:CE2	29:H:402:3PE:H231	2.52	0.45
5:E:180:VAL:HG11	5:E:224:CYS:CB	2.47	0.45
6:F:158:ILE:HD13	6:F:166:ALA:HB2	1.98	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.45
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.45
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.43	0.45
9:I:56:ASN:O	9:I:60:ILE:HG13	2.16	0.45
9:I:59:ARG:HA	9:I:64:THR:HG23	1.99	0.45
10:P:192:ARG:HH11	10:P:197:GLU:HA	1.81	0.45
11:Q:51:GLN:HB3	16:W:26:ARG:HH22	1.82	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
18:Z:98:MET:HB2	18:Z:104:TRP:CE2	2.52	0.45
21:q:71:LYS:HB2	21:q:73:THR:HG23	1.98	0.45
1:A:30:TYR:CE2	1:A:33:LYS:HB2	2.52	0.45
2:B:77:LYS:HD3	2:B:77:LYS:HA	1.64	0.45
2:B:122:ARG:NH2	2:B:127:GLN:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:83:ASN:C	4:D:85:GLY:N	2.69	0.45
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.45
5:E:94:ILE:O	5:E:98:ASN:ND2	2.50	0.45
5:E:131:ILE:HD11	5:E:168:PHE:CD2	2.49	0.45
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.99	0.45
7:G:381:LEU:HD23	13:S:55:ILE:HG13	1.98	0.45
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.45
8:H:250:ASN:OD1	8:H:250:ASN:N	2.50	0.45
29:H:403:3PE:H331	9:I:63:TRP:CZ2	2.51	0.45
10:P:169:HIS:N	10:P:184:LYS:HE3	2.29	0.45
10:P:227:PRO:HA	10:P:291:TYR:O	2.16	0.45
14:T:82:ARG:NH2	14:T:126:PHE:HD1	2.15	0.45
16:W:83:ASP:O	16:W:87:ILE:HG12	2.17	0.45
17:X:40:ASN:O	17:X:41:LYS:C	2.58	0.45
18:Z:68:ARG:O	18:Z:69:ILE:C	2.60	0.45
21:q:74:PHE:HD2	21:q:75:TRP:CD1	2.33	0.45
1:A:53:MET:HE3	1:A:55:PHE:CD1	2.52	0.44
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.44
6:F:209:GLU:CD	6:F:230:PRO:HG2	2.42	0.44
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.44
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.44
10:P:315:THR:CG2	10:P:316:LYS:N	2.80	0.44
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.44
18:Z:91:LEU:O	18:Z:95:ALA:N	2.50	0.44
19:a:2:TRP:HZ2	33:q:201:CDL:OB7	2.00	0.44
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.44
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.44
5:E:180:VAL:CG2	6:F:286:CYS:HA	2.46	0.44
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.44
6:F:168:ASN:ND2	23:s:40:TYR:CE2	2.85	0.44
6:F:234:GLY:HA3	6:F:240:THR:HB	1.98	0.44
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.44
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.44
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.44
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.44
10:P:182:ARG:O	10:P:186:VAL:HG23	2.18	0.44
14:T:90:TYR:O	14:T:91:ASP:HB2	2.17	0.44
14:T:113:LEU:O	14:T:116:VAL:HB	2.17	0.44
33:q:201:CDL:OB7	33:q:201:CDL:HB62	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:CD1	1:A:23:TRP:CD1	2.96	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:244:ILE:HG22	4:D:244:ILE:O	2.18	0.44
5:E:49:ASP:O	5:E:50:THR:C	2.60	0.44
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:50:ASP:OD2	6:F:52:ARG:HB2	2.17	0.44
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.99	0.44
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.99	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.44
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
10:P:178:SER:O	10:P:182:ARG:HG3	2.17	0.44
10:P:323:HIS:O	10:P:323:HIS:CG	2.71	0.44
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.98	0.44
14:T:92:LYS:O	14:T:92:LYS:HG2	2.16	0.44
14:T:119:ILE:CD1	14:T:138:LEU:HD11	2.43	0.44
19:a:37:ARG:HB2	19:a:48:MET:HE2	1.99	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	1.99	0.44
4:D:201:PHE:HB2	8:H:32:GLN:HB3	2.00	0.44
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.44
4:D:258:VAL:O	4:D:261:MET:HB2	2.17	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
5:E:128:LYS:HD3	5:E:167:LEU:HG	2.00	0.44
6:F:98:LYS:HA	6:F:101:PHE:CE2	2.53	0.44
6:F:226:LYS:O	6:F:227:PRO:C	2.60	0.44
6:F:283:ASN:ND2	6:F:306:GLY:H	2.16	0.44
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.98	0.44
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.44
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.43	0.44
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.99	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
14:T:130:ILE:CG2	14:T:131:PRO:CD	2.95	0.44
18:Z:10:MET:HE2	18:Z:10:MET:HB3	1.72	0.44
18:Z:66:GLU:HG3	20:b:50:PRO:HG3	1.98	0.44
1:A:53:MET:HE2	1:A:56:PHE:N	2.32	0.44
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:200:LEU:HD21	8:H:285:LEU:HD13	1.99	0.44
8:H:224:PHE:CD2	25:H:401:UQ9:H20	2.53	0.44
8:H:305:ILE:O	8:H:308:PRO:HD2	2.17	0.44
29:H:402:3PE:H2I2	29:H:402:3PE:H2E1	2.00	0.44
13:S:48:HIS:HE1	13:S:95:LEU:CD2	2.25	0.44
18:Z:92:GLU:O	18:Z:96:ILE:HG13	2.17	0.44
22:r:5:THR:HG22	22:r:5:THR:O	2.18	0.44
1:A:41:PHE:CZ	4:D:96:ARG:HD3	2.53	0.44
1:A:109:LYS:HG2	1:A:109:LYS:O	2.17	0.44
2:B:104:MET:CE	2:B:121:PHE:HE2	2.23	0.44
5:E:235:GLU:HB2	6:F:37:ASP:HB2	2.00	0.44
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.99	0.44
7:G:306:MET:HA	7:G:316:TYR:HA	1.99	0.44
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.44
8:H:288:LEU:O	8:H:293:PHE:N	2.50	0.44
8:H:289:LEU:O	8:H:294:LEU:HB2	2.18	0.44
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.80	0.44
10:P:126:VAL:HG23	10:P:161:VAL:HG11	1.99	0.44
16:W:86:VAL:O	16:W:90:LYS:HG3	2.18	0.44
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.52	0.44
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.52	0.44
1:A:39:CYS:O	4:D:86:PRO:HD2	2.18	0.44
2:B:105:MET:HG2	25:B:302:UQ9:C8	2.46	0.44
6:F:47:GLY:C	6:F:49:HIS:H	2.24	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:259:SER:HA	7:G:281:ILE:HD13	1.98	0.44
7:G:346:VAL:O	7:G:521:SER:HB3	2.17	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
10:P:165:ILE:HG12	10:P:199:ILE:HB	1.98	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44
13:S:42:VAL:HB	13:S:46:LYS:HE3	1.98	0.44
17:X:11:GLU:OE1	17:X:11:GLU:HA	2.17	0.44
17:X:46:CYS:SG	17:X:135:ARG:NH1	2.91	0.44
2:B:114:MET:SD	2:B:119:VAL:CG1	3.06	0.44
4:D:88:HIS:HE1	8:H:205:SER:O	2.01	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
6:F:93:PHE:O	6:F:94:PRO:C	2.59	0.44
6:F:147:ARG:HD2	6:F:191:TYR:CD1	2.53	0.44
7:G:43:VAL:HG12	7:G:55:LYS:CD	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:16:ALA:HB2	19:a:15:CYS:HB2	1.99	0.44
10:P:55:VAL:HG11	10:P:122:HIS:O	2.18	0.44
10:P:211:ASP:CG	10:P:214:LEU:HB3	2.43	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
12:R:32:THR:HG21	21:q:129:THR:HG23	2.00	0.44
21:q:85:GLU:CG	21:q:98:PRO:HB3	2.39	0.44
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.48	0.44
1:A:51:PHE:HZ	8:H:130:PHE:CE1	2.36	0.44
1:A:67:LEU:O	1:A:70:ALA:HB3	2.18	0.44
3:C:85:ILE:HD12	3:C:140:ILE:CD1	2.48	0.44
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.35	0.44
4:D:201:PHE:CB	8:H:32:GLN:HB3	2.48	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:196:THR:O	5:E:197:PRO:C	2.61	0.44
5:E:246:ALA:O	5:E:247:GLY:C	2.60	0.44
6:F:109:ARG:NE	6:F:239:PRO:HD3	2.33	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	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
7:G:607:LYS:HG2	11:Q:78:ARG:HH11	1.82	0.44
8:H:17:MET:HE1	8:H:225:MET:HE3	2.00	0.44
8:H:18:ALA:HB2	25:H:401:UQ9:H25B	1.99	0.44
10:P:96:LEU:C	10:P:96:LEU:HD12	2.43	0.44
10:P:163:ARG:NE	10:P:253:THR:HA	2.33	0.44
10:P:212:ARG:O	10:P:213:PHE:C	2.61	0.44
10:P:321:ARG:CZ	10:P:321:ARG:HB2	2.48	0.44
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.44
12:R:44:ARG:C	12:R:46:VAL:N	2.73	0.44
12:R:47:ARG:HG3	12:R:48:PHE:N	2.32	0.44
16:W:87:ILE:O	16:W:91:MET:HG3	2.18	0.44
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.83	0.43
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.43
7:G:114:GLU:HG3	7:G:148:SER:HB3	2.00	0.43
7:G:303:THR:HB	7:G:614:GLY:HA3	1.98	0.43
7:G:355:LYS:HG2	7:G:359:ASN:ND2	2.33	0.43
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.43
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.99	0.43
10:P:246:SER:O	10:P:249:ILE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.43
13:S:51:LEU:CD1	13:S:95:LEU:HD12	2.46	0.43
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.43
13:S:85:ASP:O	13:S:89:ARG:N	2.41	0.43
1:A:39:CYS:HB3	4:D:85:GLY:HA3	2.00	0.43
1:A:81:THR:O	20:b:46:ASN:ND2	2.51	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:93:ILE:HD11	3:C:153:ASP:HB3	1.99	0.43
6:F:62:TRP:CH2	6:F:140:GLU:HA	2.53	0.43
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:306:MET:HG2	7:G:316:TYR:CA	2.46	0.43
7:G:338:VAL:HA	7:G:544:MET:O	2.17	0.43
8:H:116:ILE:HD12	8:H:135:ALA:HB3	1.99	0.43
10:P:376:ASN:O	10:P:377:TYR:C	2.61	0.43
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.43
15:V:56:LEU:CD1	15:V:57:ASP:OD1	2.67	0.43
16:W:20:VAL:HG21	16:W:80:ARG:CZ	2.48	0.43
16:W:42:TRP:O	16:W:46:VAL:HG23	2.17	0.43
17:X:134:ASP:O	17:X:135:ARG:C	2.58	0.43
1:A:98:LEU:HD13	1:A:98:LEU:HA	1.90	0.43
1:A:105:GLU:HG2	1:A:111:LEU:HB3	1.99	0.43
2:B:114:MET:HE1	2:B:121:PHE:CE1	2.53	0.43
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
5:E:81:VAL:HB	5:E:104:LEU:HD11	2.00	0.43
5:E:81:VAL:O	5:E:82:LEU:C	2.60	0.43
5:E:87:ARG:NH2	6:F:163:TYR:CD1	2.87	0.43
5:E:180:VAL:HG22	5:E:221:ARG:NH1	2.33	0.43
7:G:279:GLU:HG3	11:Q:154:LYS:HG3	2.00	0.43
7:G:467:LYS:HA	7:G:467:LYS:HD3	1.83	0.43
7:G:651:PRO:HB3	13:S:57:GLU:O	2.18	0.43
8:H:21:THR:HG21	25:H:401:UQ9:C15	2.45	0.43
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.43
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.43
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
4:D:378:LEU:HD23	7:G:126:LEU:HB2	2.00	0.43
5:E:183:PRO:HB2	5:E:195:LEU:N	2.33	0.43
7:G:336:ASN:HB3	7:G:540:ASN:ND2	2.33	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
7:G:666:GLN:HE22	13:S:38:VAL:HG13	1.83	0.43
8:H:39:ILE:HG13	21:q:31:ASN:ND2	2.33	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
10:P:73:LEU:HD23	10:P:73:LEU:HA	1.89	0.43
10:P:156:SER:HB2	10:P:161:VAL:CG2	2.47	0.43
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.43
13:S:24:CYS:SG	13:S:61:VAL:HG12	2.58	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
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.43
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.43
6:F:88:ARG:HH21	6:F:262:PHE:HZ	1.66	0.43
6:F:226:LYS:N	6:F:227:PRO:CD	2.82	0.43
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.43
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.43
13:S:23:LEU:HB3	13:S:33:VAL:HG12	2.01	0.43
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.43
20:b:82:LYS:HB3	20:b:82:LYS:HE2	1.81	0.43
2:B:131:MET:HE1	2:B:149:TYR:HB2	2.00	0.43
2:B:192:PRO:HD3	9:I:176:SER:HA	1.98	0.43
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.43
4:D:232:VAL:CG2	4:D:356:ILE:HB	2.48	0.43
4:D:261:MET:HE3	4:D:261:MET:HB3	1.90	0.43
5:E:63:GLU:O	5:E:64:ALA:C	2.62	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
5:E:179:CYS:SG	6:F:123:GLY:HA2	2.58	0.43
7:G:126:LEU:HD13	12:R:89:PRO:HB3	2.01	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.43
8:H:77:LEU:O	8:H:81:LEU:HG	2.19	0.43
10:P:172:ALA:N	10:P:202:ARG:HH21	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.83	0.43
21:q:129:THR:O	21:q:129:THR:CG2	2.67	0.43
1:A:38:GLU:HB2	1:A:43:PRO:HD3	2.00	0.43
1:A:81:THR:O	1:A:82:ILE:C	2.62	0.43
2:B:111:ARG:CZ	4:D:208:GLU:HG2	2.49	0.43
2:B:125:PRO:O	2:B:126:ARG:C	2.60	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
4:D:299:GLN:HB3	22:r:104:TRP:CE3	2.53	0.43
5:E:126:VAL:HG21	5:E:130:HIS:CG	2.53	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
5:E:233:LEU:CD2	6:F:40:ARG:HD3	2.48	0.43
6:F:268:GLU:CG	6:F:269:ARG:H	2.30	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
6:F:412:LEU:CD2	6:F:435:VAL:HG13	2.48	0.43
7:G:662:THR:HB	13:S:25:GLN:HE21	1.84	0.43
8:H:186:PHE:CE2	29:H:403:3PE:H2B1	2.54	0.43
10:P:203:PRO:HG2	30:P:401:NDP:C5N	2.48	0.43
10:P:235:THR:O	10:P:273:LEU:N	2.52	0.43
10:P:354:ARG:HG3	10:P:362:LEU:CD2	2.48	0.43
18:Z:129:THR:HG22	18:Z:131:GLU:N	2.33	0.43
19:a:55:SER:O	19:a:56:GLY:C	2.61	0.43
2:B:95:PHE:CE2	2:B:97:LEU:HD11	2.54	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
7:G:347:ASP:O	7:G:351:LEU:HG	2.18	0.43
7:G:355:LYS:HG3	7:G:366:LEU:HD12	2.00	0.43
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.43
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.00	0.43
13:S:30:SER:HB3	13:S:63:PRO:HG3	2.00	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.43
18:Z:28:ARG:O	18:Z:28:ARG:CG	2.64	0.43
1:A:105:GLU:O	1:A:110:GLY:N	2.52	0.43
4:D:92:HIS:HD2	4:D:456:ILE:O	2.02	0.43
4:D:104:GLU:CG	8:H:130:PHE:HZ	2.32	0.43
7:G:163:LYS:HE2	12:R:97:LYS:HZ3	1.84	0.43
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.43
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
8:H:14:LEU:HD23	8:H:14:LEU:HA	1.86	0.43
8:H:140:ILE:O	8:H:143:GLU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.43
10:P:313:TRP:CE3	10:P:314:THR:HB	2.54	0.43
14:T:87:LEU:HD11	14:T:141:PRO:HB3	2.01	0.43
19:a:2:TRP:NE1	33:q:201:CDL:OB4	2.51	0.43
1:A:18:ILE:O	1:A:21:ALA:HB3	2.19	0.43
1:A:29:LEU:HD12	1:A:29:LEU:N	2.34	0.43
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.43
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.19	0.43
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.81	0.43
4:D:197:MET:HG3	8:H:32:GLN:NE2	2.33	0.43
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.43
4:D:379:ILE:HG23	7:G:140:GLN:HB2	2.01	0.43
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.43
6:F:128:ARG:HD2	6:F:162:PHE:CE1	2.54	0.43
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.83	0.43
8:H:200:LEU:CD2	8:H:282:TYR:HA	2.49	0.43
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.43
16:W:65:LYS:O	16:W:69:MET:HG2	2.18	0.43
18:Z:108:GLU:O	18:Z:109:SER:C	2.61	0.43
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.43
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.43
20:b:67:PRO:O	20:b:68:SER:C	2.61	0.43
1:A:25:PRO:HB3	8:H:57:MET:O	2.18	0.42
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.43	0.42
4:D:245:TYR:O	4:D:246:GLU:C	2.59	0.42
6:F:64:LYS:O	6:F:68:ILE:HG13	2.19	0.42
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.42
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.42
9:I:188:GLU:OE2	12:R:56:ASN:HB2	2.19	0.42
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.42
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.42
17:X:38:LYS:NZ	20:b:68:SER:OG	2.52	0.42
22:r:113:LEU:HD12	22:r:113:LEU:HA	1.76	0.42
2:B:163:SER:HB2	9:I:150:THR:O	2.18	0.42
3:C:240:ALA:O	3:C:241:PHE:C	2.62	0.42
4:D:90:ALA:O	4:D:91:ALA:C	2.61	0.42
6:F:65:THR:HA	6:F:68:ILE:HD12	2.01	0.42
6:F:295:PRO:O	6:F:296:LEU:C	2.60	0.42
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.42
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.42
7:G:381:LEU:HD23	13:S:55:ILE:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:613:PRO:O	7:G:616:ALA:HB3	2.20	0.42
8:H:54:LYS:CG	8:H:55:LEU:N	2.78	0.42
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
10:P:169:HIS:H	10:P:184:LYS:CE	2.30	0.42
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.62	0.42
17:X:75:LYS:O	17:X:79:ALA:HB2	2.19	0.42
1:A:38:GLU:O	1:A:39:CYS:CB	2.67	0.42
1:A:44:THR:CG2	16:W:99:VAL:HG11	2.40	0.42
1:A:65:PHE:CZ	1:A:102:LEU:HD13	2.55	0.42
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.33	0.42
4:D:162:GLN:HB2	4:D:163:PRO:HD2	2.01	0.42
4:D:318:VAL:HG21	22:r:104:TRP:CZ3	2.54	0.42
5:E:62:ILE:HD12	5:E:81:VAL:HG13	2.00	0.42
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.42
5:E:233:LEU:HB2	6:F:48:ARG:HH12	1.84	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
7:G:388:ASN:O	7:G:511:LYS:HE2	2.19	0.42
9:I:50:MET:O	9:I:54:THR:HG23	2.19	0.42
9:I:153:ILE:CD1	9:I:155:CYS:HB3	2.39	0.42
10:P:216:HIS:CD2	10:P:318:LYS:HE3	2.54	0.42
12:R:31:ILE:HG22	12:R:55:VAL:HG21	2.01	0.42
12:R:45:ARG:HA	12:R:48:PHE:HE1	1.83	0.42
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.42
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.42
19:a:28:LYS:HE3	19:a:35:GLU:HG2	2.01	0.42
20:b:15:LYS:O	20:b:15:LYS:HG3	2.19	0.42
22:r:18:GLN:OE1	22:r:18:GLN:N	2.52	0.42
2:B:154:GLU:CB	8:H:59:GLU:HB2	2.49	0.42
5:E:109:MET:HE1	7:G:198:THR:CG2	2.50	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
8:H:89:LEU:HG	8:H:90:PRO:HD2	2.00	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
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.42
13:S:16:LEU:HD13	13:S:19:ILE:HD11	2.02	0.42
17:X:139:GLU:O	17:X:140:ASN:C	2.62	0.42
18:Z:74:LEU:O	18:Z:78:GLU:HG3	2.19	0.42
19:a:49:GLU:OE2	19:a:49:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
1:A:106:TRP:N	1:A:106:TRP:CD1	2.85	0.42
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.42
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.42
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	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	2.46	0.42
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.20	0.42
6:F:166:ALA:O	6:F:167:SER:C	2.63	0.42
6:F:272:GLY:O	6:F:292:MET:HB2	2.19	0.42
8:H:7:LEU:HD13	8:H:7:LEU:HA	1.75	0.42
10:P:134:TRP:CD1	10:P:134:TRP:O	2.72	0.42
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.42
14:T:80:LYS:O	14:T:84:LEU:HG	2.20	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.54	0.42
1:A:51:PHE:CZ	8:H:130:PHE:CE1	3.07	0.42
1:A:68:GLU:HB2	1:A:98:LEU:HG	2.01	0.42
1:A:72:LEU:HB3	8:H:151:LEU:HD21	2.02	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.19	0.42
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
5:E:230:LEU:HD13	5:E:232:SER:O	2.19	0.42
6:F:81:LYS:HE2	6:F:97:LEU:CD2	2.47	0.42
6:F:410:ASP:OD1	6:F:410:ASP:C	2.62	0.42
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.42
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.42
8:H:203:GLY:O	8:H:205:SER:N	2.49	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.02	0.42
17:X:26:LYS:HD3	17:X:95:GLN:OE1	2.19	0.42
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.88	0.42
4:D:106:VAL:N	4:D:442:HIS:O	2.41	0.42
4:D:144:MET:HG2	4:D:223:HIS:H	1.85	0.42
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.42
4:D:339:GLN:HE22	9:I:37:LYS:HZ1	1.61	0.42
5:E:180:VAL:HG11	5:E:224:CYS:HB2	2.02	0.42
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.52	0.42
8:H:157:ASN:ND2	8:H:164:THR:OG1	2.49	0.42
8:H:287:HIS:O	8:H:291:LYS:N	2.51	0.42
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.01	0.42
10:P:223:PHE:O	10:P:224:LEU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:247:LYS:NZ	10:P:340:VAL:HG23	2.35	0.42
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.42
14:T:87:LEU:CD2	14:T:122:MET:CE	2.98	0.42
14:T:90:TYR:CD2	14:T:92:LYS:HB3	2.54	0.42
16:W:58:THR:O	16:W:61:GLN:HB3	2.20	0.42
16:W:61:GLN:O	16:W:64:ASP:HB2	2.19	0.42
17:X:20:VAL:O	19:a:54:ILE:CD1	2.67	0.42
2:B:126:ARG:HG3	8:H:213:VAL:O	2.19	0.42
3:C:236:SER:OG	7:G:145:MET:HE1	2.19	0.42
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.42
6:F:110:PRO:O	6:F:238:CYS:HB3	2.20	0.42
6:F:170:GLN:HG2	23:s:52:LEU:HD11	2.02	0.42
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.42
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.42
9:I:93:LEU:O	21:q:93:MET:CG	2.65	0.42
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.42
10:P:300:TRP:NE1	10:P:304:LEU:HD21	2.35	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
19:a:17:VAL:O	19:a:18:ILE:C	2.62	0.42
1:A:94:LEU:O	1:A:97:ILE:HG12	2.19	0.42
1:A:104:TYR:HA	1:A:107:THR:OG1	2.20	0.42
2:B:84:TRP:HA	2:B:87:ARG:HG2	2.02	0.42
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.42
4:D:345:GLU:HB2	18:Z:19:ILE:HD12	2.02	0.42
4:D:375:MET:HE2	4:D:375:MET:HB2	1.66	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
6:F:120:GLY:O	6:F:121:GLU:C	2.61	0.42
6:F:153:ALA:HB1	6:F:194:ASP:O	2.19	0.42
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.19	0.42
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.42
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.42
8:H:224:PHE:HD2	25:H:401:UQ9:H20	1.84	0.42
12:R:60:ALA:O	12:R:61:ILE:C	2.63	0.42
13:S:19:ILE:O	13:S:53:ILE:HD12	2.20	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:O	1:A:58:VAL:C	2.62	0.42
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.01	0.42
4:D:259:GLU:O	4:D:261:MET:N	2.53	0.42
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.42
5:E:62:ILE:HG21	5:E:103:VAL:HG11	2.01	0.42
5:E:179:CYS:SG	6:F:123:GLY:CA	3.08	0.42
6:F:53:LEU:O	6:F:57:LEU:HG	2.20	0.42
6:F:315:LEU:HD23	6:F:315:LEU:O	2.20	0.42
7:G:64:CYS:SG	7:G:75:CYS:SG	3.14	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
8:H:42:PRO:HG3	21:q:28:PHE:HE1	1.85	0.42
9:I:54:THR:HA	20:b:13:TRP:NE1	2.35	0.42
10:P:207:PHE:HB3	10:P:213:PHE:HD2	1.85	0.42
11:Q:167:ASN:C	11:Q:168:LYS:CG	2.93	0.42
21:q:74:PHE:HE2	21:q:75:TRP:HE1	1.68	0.42
1:A:46:SER:O	1:A:47:ALA:HB3	2.20	0.41
3:C:121:ARG:NH2	15:V:114:TRP:HA	2.35	0.41
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.41
6:F:38:GLU:HG3	6:F:39:ASP:OD1	2.20	0.41
6:F:115:VAL:HG22	6:F:248:VAL:HG21	2.02	0.41
6:F:208:GLU:OE1	6:F:210:THR:N	2.52	0.41
7:G:41:VAL:HG21	7:G:56:VAL:CA	2.50	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	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
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.41
8:H:288:LEU:HD23	8:H:288:LEU:C	2.45	0.41
10:P:208:GLY:O	10:P:211:ASP:N	2.53	0.41
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.41
10:P:293:LEU:HD12	10:P:294:PRO:HD2	2.01	0.41
12:R:54:GLU:HB2	21:q:124:TYR:HD1	1.84	0.41
13:S:20:ARG:HD2	13:S:22:HIS:NE2	2.35	0.41
18:Z:102:PRO:O	18:Z:103:ASN:C	2.62	0.41
20:b:31:ILE:HG23	20:b:32:MET:N	2.33	0.41
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
1:A:61:THR:OG1	1:A:62:PHE:N	2.52	0.41
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.41
3:C:243:ALA:C	7:G:105:ASN:HD21	2.28	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:213:PRO:O	5:E:215:PRO:HD3	2.20	0.41
7:G:283:GLU:O	7:G:283:GLU:CG	2.50	0.41
7:G:365:ASN:HB3	7:G:537:ILE:HD11	2.02	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.54	0.41
8:H:19:PHE:CB	19:a:12:MET:HG3	2.49	0.41
9:I:80:GLU:CG	19:a:1:MET:SD	2.98	0.41
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.35	0.41
15:V:98:LYS:HG2	15:V:100:TRP:CZ2	2.55	0.41
17:X:23:ALA:HB2	17:X:95:GLN:HE22	1.82	0.41
20:b:11:ASN:O	20:b:15:LYS:HG2	2.20	0.41
20:b:15:LYS:O	20:b:16:GLU:HB2	2.20	0.41
20:b:16:GLU:N	20:b:17:PRO:HD3	2.35	0.41
20:b:35:ILE:O	20:b:35:ILE:CG1	2.67	0.41
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.55	0.41
1:A:61:THR:C	1:A:63:LEU:N	2.75	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.03	0.41
5:E:47:ASN:CG	5:E:49:ASP:HB3	2.45	0.41
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.44	0.41
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.54	0.41
6:F:270:ASN:CG	6:F:338:ASP:HB2	2.46	0.41
6:F:280:GLY:O	6:F:281:HIS:C	2.63	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
8:H:196:ALA:C	8:H:198:PHE:N	2.77	0.41
9:I:78:PHE:HD1	19:a:2:TRP:CD1	2.37	0.41
9:I:162:CYS:SG	24:I:303:SF4:S3	3.18	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	2.01	0.41
12:R:55:VAL:HG22	12:R:56:ASN:N	2.35	0.41
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.84	0.41
14:T:93:ILE:HD11	14:T:118:ILE:HD11	2.01	0.41
14:T:100:VAL:O	14:T:141:PRO:HD2	2.20	0.41
14:T:115:GLN:O	14:T:116:VAL:C	2.63	0.41
17:X:37:ASP:OD1	17:X:37:ASP:C	2.62	0.41
17:X:70:PHE:CE1	17:X:117:TRP:CZ3	3.08	0.41
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.41
20:b:41:TYR:CD1	20:b:80:TRP:CZ3	3.08	0.41
21:q:50:GLU:HA	21:q:59:HIS:O	2.20	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
1:A:49:LEU:HD23	1:A:49:LEU:N	2.34	0.41
2:B:114:MET:CE	2:B:121:PHE:CE1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:TYR:CE2	4:D:135:TYR:CD1	3.09	0.41
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.48	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
6:F:113:LEU:HB3	6:F:154:ALA:CB	2.49	0.41
6:F:363:ILE:O	6:F:364:VAL:C	2.64	0.41
8:H:87:VAL:O	8:H:95:LEU:HB3	2.21	0.41
8:H:96:ILE:HG23	18:Z:143:TYR:CE1	2.55	0.41
16:W:53:MET:SD	16:W:106:VAL:HG21	2.60	0.41
16:W:120:ASP:OD1	16:W:120:ASP:C	2.61	0.41
20:b:25:VAL:O	20:b:26:TRP:C	2.64	0.41
20:b:31:ILE:O	20:b:32:MET:C	2.63	0.41
2:B:93:MET:HG2	4:D:87:GLN:NE2	2.34	0.41
3:C:70:LYS:O	15:V:103:LEU:HA	2.21	0.41
3:C:75:VAL:HG13	3:C:83:LEU:HD11	2.02	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
6:F:76:ILE:O	6:F:79:GLU:HB2	2.20	0.41
6:F:210:THR:HG23	6:F:226:LYS:HE3	2.01	0.41
6:F:225:LEU:HB2	11:Q:160:TYR:HE2	1.75	0.41
7:G:253:VAL:O	7:G:253:VAL:CG1	2.68	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.02	0.41
7:G:649:VAL:HA	13:S:20:ARG:NH1	2.36	0.41
8:H:8:THR:O	8:H:9:LEU:CB	2.67	0.41
8:H:110:SER:O	8:H:113:VAL:HG12	2.19	0.41
8:H:283:ASP:OD1	8:H:284:GLN:N	2.53	0.41
16:W:78:ASP:HB3	16:W:81:VAL:HG23	2.03	0.41
16:W:101:LYS:HB3	16:W:101:LYS:NZ	2.34	0.41
20:b:53:TYR:CE2	20:b:55:VAL:HA	2.55	0.41
1:A:78:ALA:HA	1:A:81:THR:HG23	2.03	0.41
1:A:111:LEU:HD23	1:A:112:GLU:H	1.86	0.41
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.19	0.41
4:D:301:ASP:N	22:r:104:TRP:HH2	2.18	0.41
6:F:62:TRP:CE2	6:F:181:LEU:HD13	2.56	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:48:THR:O	7:G:49:VAL:C	2.63	0.41
7:G:277:MET:HE1	11:Q:153:PRO:HD3	2.03	0.41
7:G:567:VAL:HG23	7:G:567:VAL:O	2.20	0.41
8:H:224:PHE:CE2	25:H:401:UQ9:C14	3.03	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
29:H:403:3PE:H122	9:I:60:ILE:HG21	2.02	0.41
11:Q:166:TRP:O	11:Q:167:ASN:C	2.64	0.41
17:X:70:PHE:O	17:X:74:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:q:201:CDL:H112	33:q:201:CDL:H312	2.02	0.41
22:r:12:ARG:HH21	22:r:20:LEU:CD1	2.33	0.41
2:B:194:CYS:O	24:B:301:SF4:S2	2.78	0.41
2:B:224:ARG:HG3	10:P:85:ARG:HH22	1.85	0.41
3:C:72:VAL:O	3:C:72:VAL:HG23	2.20	0.41
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.41
5:E:190:ASN:HD22	5:E:192:TYR:HE1	1.69	0.41
6:F:225:LEU:N	11:Q:160:TYR:HE2	2.16	0.41
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.51	0.41
8:H:136:VAL:HG13	8:H:137:ALA:N	2.35	0.41
13:S:22:HIS:CD2	13:S:66:TRP:HD1	2.39	0.41
14:T:87:LEU:CD2	14:T:104:PHE:HZ	2.12	0.41
16:W:42:TRP:CZ3	32:W:201:EHZ:C5	3.03	0.41
21:q:132:LYS:HE2	21:q:135:HIS:HA	2.01	0.41
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.41
4:D:140:ASP:O	4:D:147:ASN:ND2	2.53	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.03	0.41
5:E:71:GLU:HB3	23:s:60:PRO:O	2.21	0.41
6:F:297:LYS:HG3	6:F:301:GLU:CG	2.51	0.41
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.35	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.49	0.41
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.41
8:H:306:SER:O	8:H:307:LEU:C	2.63	0.41
9:I:36:TYR:CZ	22:r:106:LEU:HD23	2.56	0.41
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.41
10:P:146:VAL:HG13	10:P:147:ASN:OD1	2.21	0.41
13:S:16:LEU:CB	13:S:69:TYR:CD1	2.97	0.41
4:D:119:GLY:O	4:D:123:LEU:HD23	2.21	0.41
4:D:269:ARG:O	4:D:273:VAL:HG23	2.21	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
6:F:81:LYS:HD3	6:F:96:GLY:HA3	2.03	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
6:F:274:LYS:HB3	6:F:276:PHE:CZ	2.56	0.41
6:F:296:LEU:HB2	6:F:337:MET:HE3	2.03	0.41
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:102:ILE:HD12	7:G:102:ILE:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:309:ASN:CG	7:G:310:GLU:H	2.29	0.41
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.41
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.86	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.41
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.86	0.41
8:H:130:PHE:CZ	8:H:134:ARG:HD3	2.56	0.41
8:H:187:ILE:CD1	29:H:403:3PE:H242	2.42	0.41
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.41
10:P:93:HIS:O	10:P:96:LEU:HG	2.21	0.41
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.41
10:P:170:LEU:O	10:P:171:ASN:C	2.62	0.41
10:P:355:ARG:HH11	10:P:356:HIS:HE1	1.66	0.41
11:Q:85:ASN:C	11:Q:87:MET:N	2.76	0.41
12:R:48:PHE:CD2	12:R:53:LYS:HB2	2.56	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
22:r:24:LEU:HD23	22:r:24:LEU:HA	1.85	0.41
1:A:38:GLU:HG3	1:A:38:GLU:O	2.21	0.41
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.41
4:D:181:LEU:HD21	4:D:210:MET:CB	2.51	0.41
4:D:213:PHE:O	4:D:214:TYR:C	2.64	0.41
4:D:375:MET:HG2	7:G:121:LEU:HD22	2.02	0.41
5:E:68:ASN:OD1	23:s:56:ARG:NH1	2.54	0.41
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:651:PRO:HG3	13:S:57:GLU:N	2.29	0.41
8:H:95:LEU:HG	8:H:96:ILE:HG13	2.03	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
9:I:201:ILE:O	9:I:205:ILE:HG12	2.21	0.41
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.41
13:S:21:VAL:HG22	13:S:91:MET:HE1	2.03	0.41
21:q:3:LEU:HD13	33:q:201:CDL:C51	2.51	0.41
1:A:1:MET:O	1:A:2:ASN:C	2.64	0.40
1:A:16:THR:O	1:A:20:VAL:HG23	2.21	0.40
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.54	0.40
4:D:198:THR:N	4:D:199:PRO:CD	2.83	0.40
6:F:47:GLY:O	6:F:48:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:102:MET:O	6:F:102:MET:HG3	2.20	0.40
6:F:127:ASP:O	6:F:128:ARG:C	2.65	0.40
6:F:185:ASN:HA	6:F:189:SER:O	2.21	0.40
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.40
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
8:H:204:GLU:HA	8:H:204:GLU:OE1	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
10:P:201:ILE:HD13	10:P:265:PHE:CZ	2.55	0.40
11:Q:57:GLU:O	11:Q:58:LYS:C	2.65	0.40
20:b:11:ASN:CG	20:b:15:LYS:HE3	2.46	0.40
2:B:78:LEU:HD23	2:B:78:LEU:HA	1.90	0.40
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.56	0.40
3:C:70:LYS:HD3	3:C:71:TYR:CZ	2.56	0.40
4:D:104:GLU:HG3	8:H:130:PHE:CZ	2.56	0.40
5:E:139:CYS:HB3	5:E:144:SER:HB3	2.03	0.40
6:F:226:LYS:HA	6:F:226:LYS:HD3	1.86	0.40
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.40
7:G:404:GLY:HA2	7:G:684:LEU:HD11	2.00	0.40
25:H:401:UQ9:H7	25:H:401:UQ9:H1MB	1.94	0.40
10:P:61:ALA:HA	10:P:66:GLY:HA3	2.02	0.40
10:P:105:PHE:C	10:P:106:LEU:HD12	2.46	0.40
10:P:163:ARG:NH1	10:P:199:ILE:HD11	2.36	0.40
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.40
16:W:117:ARG:HA	16:W:118:PRO:HD3	1.95	0.40
4:D:90:ALA:HB2	8:H:205:SER:O	2.21	0.40
4:D:235:ASP:OD2	18:Z:8:GLN:HG3	2.21	0.40
5:E:81:VAL:HG21	5:E:104:LEU:HD21	2.03	0.40
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.56	0.40
7:G:47:THR:HG23	7:G:51:GLN:HB2	2.03	0.40
7:G:169:VAL:HG12	7:G:231:LEU:HB2	2.03	0.40
7:G:334:GLU:HA	7:G:361:VAL:HG22	2.03	0.40
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.40
26:I:301:PC1:H112	18:Z:29:GLY:HA3	2.02	0.40
13:S:59:SER:O	13:S:60:GLU:C	2.63	0.40
16:W:27:ASP:O	16:W:28:LEU:C	2.64	0.40
1:A:49:LEU:H	1:A:49:LEU:CD2	2.34	0.40
1:A:75:LEU:CB	8:H:155:LEU:HD21	2.52	0.40
1:A:88:MET:HG3	1:A:92:PHE:CE2	2.56	0.40
4:D:116:LEU:O	4:D:118:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:128:THR:HG22	4:D:131:GLN:CG	2.52	0.40
5:E:48:PRO:CA	5:E:95:SER:HB2	2.50	0.40
6:F:171:VAL:HG13	6:F:174:ARG:HH22	1.86	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.54	0.40
7:G:160:VAL:CG1	7:G:161:GLU:N	2.83	0.40
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.40
7:G:272:ARG:NH2	11:Q:87:MET:HE3	2.36	0.40
7:G:388:ASN:N	7:G:514:ASN:CB	2.83	0.40
7:G:462:PHE:HD2	7:G:466:LEU:HG	1.86	0.40
7:G:598:ASN:ND2	7:G:600:GLU:OE2	2.51	0.40
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.40
8:H:200:LEU:HD22	8:H:282:TYR:HA	2.03	0.40
8:H:293:PHE:O	8:H:294:LEU:C	2.63	0.40
29:H:403:3PE:N	20:b:18:VAL:HG23	2.36	0.40
29: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
13:S:45:LYS:O	13:S:46:LYS:C	2.64	0.40
17:X:130:LYS:NZ	20:b:63:MET:O	2.53	0.40
4:D:158:LEU:O	4:D:392:PRO:HG2	2.22	0.40
4:D:448:VAL:HG21	8:H:206:GLU:HA	2.03	0.40
6:F:76:ILE:O	6:F:80:MET:HG2	2.21	0.40
6:F:176:ALA:HB3	6:F:182:ILE:HD11	2.03	0.40
7:G:36:VAL:O	7:G:37:ASP:HB2	2.22	0.40
7:G:177:ILE:HG12	7:G:228:VAL:CG2	2.51	0.40
8:H:137:ALA:HB3	8:H:282:TYR:OH	2.22	0.40
8:H:153:VAL:O	8:H:154:LEU:C	2.65	0.40
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.56	0.40
8:H:210:GLY:CA	8:H:213:VAL:HG23	2.50	0.40
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.40
10:P:54:VAL:O	10:P:78:SER:HB3	2.21	0.40
10:P:198:ALA:O	10:P:199:ILE:C	2.61	0.40
10:P:360:ARG:C	10:P:362:LEU:N	2.78	0.40
14:T:87:LEU:HD11	14:T:141:PRO:HG3	2.03	0.40
14:T:123:GLU:HG2	14:T:130:ILE:HD12	2.02	0.40
17:X:4:ILE:HD13	18:Z:108:GLU:OE1	2.22	0.40
18:Z:90:ASN:O	18:Z:94:GLU:N	2.54	0.40
20:b:69:HIS:CD2	20:b:71:GLN:H	2.39	0.40
23:s:44:THR:O	23:s:48:LEU:HG	2.21	0.40
23:s:66:SER:O	23:s:67:PRO:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	110/115 (96%)	105 (96%)	5 (4%)	0	100	100
2	B	154/224 (69%)	141 (92%)	12 (8%)	1 (1%)	21	52
3	C	196/263 (74%)	186 (95%)	10 (5%)	0	100	100
4	D	383/463 (83%)	357 (93%)	26 (7%)	0	100	100
5	E	208/248 (84%)	193 (93%)	15 (7%)	0	100	100
6	F	422/464 (91%)	402 (95%)	20 (5%)	0	100	100
7	G	685/727 (94%)	631 (92%)	54 (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
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	139/172 (81%)	131 (94%)	8 (6%)	0	100	100
18	Z	137/144 (95%)	131 (96%)	6 (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	4160/5036 (83%)	3926 (94%)	233 (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 ⓘ

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	101/104 (97%)	100 (99%)	1 (1%)	68	76
2	B	132/185 (71%)	132 (100%)	0	100	100
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
6	F	340/370 (92%)	340 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	88
8	H	279/280 (100%)	278 (100%)	1 (0%)	84	84
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	76
12	R	70/96 (73%)	69 (99%)	1 (1%)	59	73
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	73
14	T	69/135 (51%)	68 (99%)	1 (1%)	59	73
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	128/154 (83%)	128 (100%)	0	100	100
18	Z	120/123 (98%)	118 (98%)	2 (2%)	53	71
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	s	28/95 (30%)	28 (100%)	0	100	100
All	All	3651/4292 (85%)	3642 (100%)	9 (0%)	85	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
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
18	Z	91	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	26	GLN
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

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Mol	Chain	Res	Type
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
6	F	393	ASN
6	F	436	GLN
7	G	59	GLN
7	G	74	ASN
7	G	105	ASN
7	G	164	ASN
7	G	205	GLN
7	G	260	ASN
7	G	278	HIS
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
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	138	GLN
8	H	163	GLN
8	H	169	GLN
8	H	258	ASN
8	H	284	GLN
8	H	292	ASN
10	P	71	ASN
10	P	154	GLN
10	P	166	HIS
10	P	171	ASN

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Mol	Chain	Res	Type
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
13	S	48	HIS
15	V	41	HIS
15	V	50	GLN
16	W	54	GLN
17	X	30	HIS
17	X	77	HIS
19	a	31	ASN
20	b	69	HIS
20	b	71	GLN
20	b	83	ASN
21	q	31	ASN
21	q	52	ASN
21	q	54	GLN
21	q	87	HIS
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
24	SF4	F	502	6	0,12,12	-	-	-		
28	FMN	F	501	-	33,33,33	1.37	5 (15%)	48,50,50	1.23	7 (14%)
25	UQ9	H	401	-	35,35,58	0.81	2 (5%)	42,45,73	0.50	0
27	FES	G	803	7	0,4,4	-	-	-		
24	SF4	I	303	9	0,12,12	-	-	-		
26	PC1	I	301	-	42,42,53	1.03	2 (4%)	48,50,61	1.03	3 (6%)
25	UQ9	B	302	-	21,21,58	1.10	3 (14%)	25,28,73	0.70	0
33	CDL	q	201	-	56,56,99	1.21	4 (7%)	62,68,111	1.20	5 (8%)
29	3PE	H	403	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	2 (3%)
24	SF4	I	302	9	0,12,12	-	-	-		
29	3PE	H	402	-	45,45,50	0.97	2 (4%)	48,50,55	0.97	2 (4%)
32	EHZ	W	201	-	27,31,37	1.90	7 (25%)	37,41,47	1.86	11 (29%)
24	SF4	G	802	7	0,12,12	-	-	-		
27	FES	E	301	5	0,4,4	-	-	-		
24	SF4	G	801	7	0,12,12	-	-	-		
30	NDP	P	401	-	49,52,52	1.21	5 (10%)	66,80,80	1.67	11 (16%)
26	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.16	4 (10%)
24	SF4	B	301	2	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
28	FMN	F	501	-	-	1/18/18/18	0/3/3/3
24	SF4	F	502	6	-	-	0/6/5/5
25	UQ9	H	401	-	-	11/30/54/81	0/1/1/1
27	FES	G	803	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PC1	I	301	-	-	9/46/46/57	-
24	SF4	I	303	9	-	-	0/6/5/5
25	UQ9	B	302	-	-	6/13/37/81	0/1/1/1
33	CDL	q	201	-	-	20/67/67/110	-
29	3PE	H	403	-	-	11/54/54/54	-
29	3PE	H	402	-	-	13/49/49/54	-
32	EHZ	W	201	-	-	21/39/39/45	-
24	SF4	I	302	9	-	-	0/6/5/5
24	SF4	G	802	7	-	-	0/6/5/5
30	NDP	P	401	-	-	4/34/77/77	0/5/5/5
24	SF4	G	801	7	-	-	0/6/5/5
27	FES	E	301	5	-	-	0/1/1/1
26	PC1	B	303	-	-	11/38/38/57	-
24	SF4	B	301	2	-	-	0/6/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	201	EHZ	C15-N2	5.41	1.45	1.33
32	W	201	EHZ	C12-N1	5.20	1.45	1.33
28	F	501	FMN	C9A-C5A	4.83	1.49	1.41
30	P	401	NDP	C5A-C4A	4.31	1.47	1.39
33	q	201	CDL	OB8-CB7	4.25	1.45	1.33
26	B	303	PC1	O31-C31	4.23	1.45	1.33
33	q	201	CDL	OA8-CA7	4.22	1.45	1.33
26	I	301	PC1	O31-C31	4.21	1.45	1.33
29	H	403	3PE	O31-C31	4.20	1.45	1.33
29	H	402	3PE	O31-C31	4.19	1.45	1.33
33	q	201	CDL	OB6-CB5	4.11	1.45	1.34
29	H	402	3PE	O21-C21	4.11	1.45	1.34
29	H	403	3PE	O21-C21	4.11	1.45	1.34
26	B	303	PC1	O21-C21	4.04	1.45	1.34
26	I	301	PC1	O21-C21	4.04	1.45	1.34
33	q	201	CDL	OA6-CA5	4.00	1.45	1.34
30	P	401	NDP	C6N-C5N	3.28	1.39	1.33
28	F	501	FMN	C8-C7	3.11	1.48	1.40
25	B	302	UQ9	C3-C2	-2.80	1.40	1.48
30	P	401	NDP	C5A-C6A	2.67	1.48	1.41
25	H	401	UQ9	C3-C2	-2.67	1.41	1.48
25	H	401	UQ9	C4-C5	-2.58	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	201	EHZ	P1-O7	2.56	1.64	1.54
25	B	302	UQ9	C4-C5	-2.48	1.41	1.48
28	F	501	FMN	C4-N3	-2.48	1.34	1.38
32	W	201	EHZ	O4-C15	-2.44	1.18	1.23
32	W	201	EHZ	O3-C12	-2.44	1.18	1.23
30	P	401	NDP	C8A-N7A	2.41	1.36	1.31
32	W	201	EHZ	C9-S1	2.39	1.81	1.76
32	W	201	EHZ	P1-OP3	-2.25	1.46	1.54
30	P	401	NDP	C5A-N7A	-2.24	1.34	1.39
25	B	302	UQ9	C6-C1	2.21	1.39	1.35
28	F	501	FMN	C4A-N5	2.09	1.34	1.30
28	F	501	FMN	C5A-N5	-2.08	1.35	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	W	201	EHZ	C8-C9-S1	6.36	121.50	113.63
30	P	401	NDP	C5A-C4A-N3A	-6.10	118.80	126.75
30	P	401	NDP	N3A-C4A-N9A	4.73	134.88	127.08
26	B	303	PC1	O21-C21-C22	4.25	120.65	111.50
30	P	401	NDP	C2A-N3A-C4A	3.89	120.94	111.75
26	I	301	PC1	O21-C21-C22	3.86	119.82	111.50
33	q	201	CDL	OA6-CA5-C11	3.83	119.75	111.50
33	q	201	CDL	OB6-CB5-C51	3.80	119.69	111.50
29	H	402	3PE	O21-C21-C22	3.59	119.25	111.50
30	P	401	NDP	PN-O3-PA	-3.42	121.09	132.83
29	H	403	3PE	O21-C21-C22	3.39	118.80	111.50
30	P	401	NDP	C4A-C5A-N7A	-3.35	106.53	110.62
30	P	401	NDP	N3A-C2A-N1A	-3.21	123.59	128.60
32	W	201	EHZ	C14-C13-C12	-3.07	107.24	112.36
32	W	201	EHZ	C13-C12-N1	3.07	121.59	116.42
32	W	201	EHZ	OP3-P1-O9	-2.90	99.34	110.68
30	P	401	NDP	C4A-N9A-C8A	2.87	108.84	105.73
30	P	401	NDP	C5A-N7A-C8A	2.87	107.59	103.51
32	W	201	EHZ	C7-C8-C9	-2.86	107.37	113.89
33	q	201	CDL	OB8-CB7-C71	2.73	120.48	111.91
29	H	403	3PE	O31-C31-C32	2.68	120.31	111.91
26	I	301	PC1	C2-O21-C21	-2.68	111.20	117.79
28	F	501	FMN	O4-C4-C4A	-2.64	119.58	126.60
28	F	501	FMN	C4A-C10-N1	-2.64	118.60	124.73
29	H	402	3PE	O31-C31-C32	2.60	120.06	111.91
33	q	201	CDL	OA8-CA7-C31	2.50	119.76	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I	301	PC1	O31-C31-C32	2.50	119.75	111.91
26	B	303	PC1	O31-C31-C32	2.40	119.44	111.91
32	W	201	EHZ	C5-C6-C7	-2.37	108.03	114.85
30	P	401	NDP	N9A-C8A-N7A	-2.34	110.71	113.91
30	P	401	NDP	C6A-C5A-N7A	2.28	136.26	132.02
26	B	303	PC1	C2-O21-C21	-2.28	112.19	117.79
33	q	201	CDL	CA4-OA6-CA5	-2.27	112.21	117.79
32	W	201	EHZ	C10-S1-C9	2.27	108.93	101.87
28	F	501	FMN	C10-N1-C2	2.21	121.33	116.90
28	F	501	FMN	C4-C4A-N5	2.20	121.36	118.23
32	W	201	EHZ	C11-N1-C12	-2.17	118.81	122.84
32	W	201	EHZ	O3-C12-N1	-2.14	118.98	123.01
32	W	201	EHZ	O6-P1-O9	2.12	112.43	106.47
32	W	201	EHZ	O2-C9-S1	-2.12	119.86	122.61
28	F	501	FMN	C4A-C4-N3	2.11	118.56	113.19
30	P	401	NDP	C3D-C2D-C1D	2.10	105.42	101.43
28	F	501	FMN	O2-C2-N1	-2.08	118.39	121.83
26	B	303	PC1	O21-C21-O22	-2.03	118.79	123.70
28	F	501	FMN	C4-N3-C2	-2.01	121.93	125.64

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	302	UQ9	C7-C8-C9-C11
25	B	302	UQ9	C7-C8-C9-C10
25	B	302	UQ9	C1-C6-C7-C8
25	B	302	UQ9	C5-C6-C7-C8
25	H	401	UQ9	C17-C18-C19-C21
25	H	401	UQ9	C17-C18-C19-C20
25	H	401	UQ9	C9-C11-C12-C13
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	402	3PE	C1-O11-P-O12
29	H	402	3PE	C1-O11-P-O14
29	H	402	3PE	C11-O13-P-O12
29	H	402	3PE	C11-O13-P-O14
29	H	402	3PE	O32-C31-O31-C3
29	H	402	3PE	C32-C31-O31-C3
29	H	403	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
29	H	403	3PE	C1-O11-P-O13
29	H	403	3PE	C1-O11-P-O14
29	H	403	3PE	C11-O13-P-O14
30	P	401	NDP	C2B-O2B-P2B-O2X
30	P	401	NDP	C2N-C3N-C7N-N7N
32	W	201	EHZ	O1-C7-C8-C9
32	W	201	EHZ	C6-C7-C8-C9
32	W	201	EHZ	C7-C8-C9-S1
32	W	201	EHZ	S1-C10-C11-N1
32	W	201	EHZ	C11-C10-S1-C9
32	W	201	EHZ	C16-C17-C20-O6
32	W	201	EHZ	C20-O6-P1-O7
32	W	201	EHZ	C20-O6-P1-O9
32	W	201	EHZ	C20-O6-P1-OP3
33	q	201	CDL	CA2-OA2-PA1-OA3
33	q	201	CDL	OA7-CA5-OA6-CA4
33	q	201	CDL	C11-CA5-OA6-CA4
33	q	201	CDL	CB2-OB2-PB2-OB3
33	q	201	CDL	CB2-OB2-PB2-OB4
33	q	201	CDL	CB2-OB2-PB2-OB5
33	q	201	CDL	CB3-OB5-PB2-OB2
33	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
29	H	402	3PE	C22-C21-O21-C2
25	H	401	UQ9	C25-C24-C26-C27
25	H	401	UQ9	C23-C24-C26-C27
29	H	403	3PE	C32-C31-O31-C3
33	q	201	CDL	C31-CA7-OA8-CA6
29	H	403	3PE	O32-C31-O31-C3
33	q	201	CDL	C51-CB5-OB6-CB4
29	H	402	3PE	O22-C21-O21-C2
33	q	201	CDL	OA9-CA7-OA8-CA6
25	B	302	UQ9	C9-C11-C12-C13
33	q	201	CDL	OB7-CB5-OB6-CB4
26	I	301	PC1	C32-C31-O31-C3
29	H	402	3PE	C1-O11-P-O13
29	H	402	3PE	C11-O13-P-O11
29	H	403	3PE	C11-O13-P-O11
33	q	201	CDL	CA3-OA5-PA1-OA2
33	q	201	CDL	CB6-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
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	402	3PE	C31-C32-C33-C34
33	q	201	CDL	CA2-OA2-PA1-OA5
29	H	402	3PE	C2E-C2F-C2G-C2H
29	H	402	3PE	C3-C2-O21-C21
29	H	403	3PE	C3E-C3F-C3G-C3H
25	H	401	UQ9	C16-C17-C18-C19
29	H	403	3PE	C37-C38-C39-C3A
32	W	201	EHZ	N2-C15-C16-C17
32	W	201	EHZ	C3-C4-C5-C6
32	W	201	EHZ	C5-C6-C7-O1
32	W	201	EHZ	O2-C9-S1-C10
25	B	302	UQ9	C2-C3-O3-C3M
26	I	301	PC1	C11-C12-N-C13
25	H	401	UQ9	C21-C22-C23-C24
30	P	401	NDP	PN-O3-PA-O2A
30	P	401	NDP	O4D-C1D-N1N-C6N
33	q	201	CDL	C1-CA2-OA2-PA1
26	I	301	PC1	C11-C12-N-C15
29	H	403	3PE	C11-O13-P-O12
33	q	201	CDL	CA3-OA5-PA1-OA3
33	q	201	CDL	CB3-OB5-PB2-OB3
25	H	401	UQ9	C2-C3-O3-C3M
32	W	201	EHZ	O4-C15-C16-O5
32	W	201	EHZ	C19-C17-C20-O6
28	F	501	FMN	C5'-O5'-P-O1P
26	I	301	PC1	C1-O11-P-O13
32	W	201	EHZ	C2-C3-C4-C5
29	H	403	3PE	C24-C25-C26-C27
26	B	303	PC1	C1-C2-C3-O31
26	I	301	PC1	C11-C12-N-C14
25	H	401	UQ9	C12-C11-C9-C10
26	I	301	PC1	C32-C33-C34-C35
33	q	201	CDL	CA4-CA3-OA5-PA1
25	H	401	UQ9	C4-C3-O3-C3M
32	W	201	EHZ	N2-C15-C16-O5
32	W	201	EHZ	C18-C17-C20-O6
25	H	401	UQ9	C12-C11-C9-C8
32	W	201	EHZ	C15-C16-C17-C18
32	W	201	EHZ	O5-C16-C17-C18

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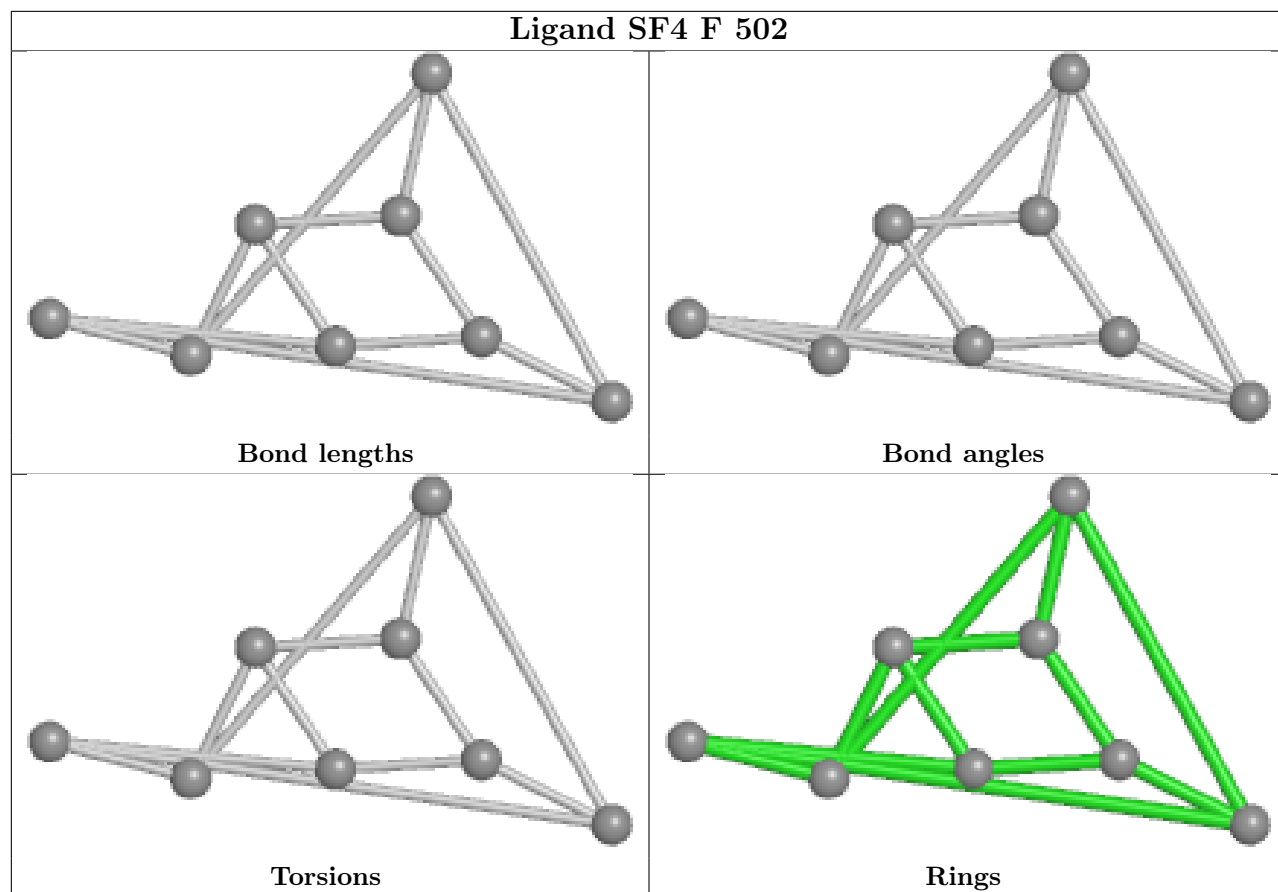
Mol	Chain	Res	Type	Atoms
26	B	303	PC1	C32-C31-O31-C3
26	B	303	PC1	O32-C31-O31-C3
33	q	201	CDL	CB4-CB3-OB5-PB2
26	B	303	PC1	C3-C2-O21-C21
32	W	201	EHZ	O4-C15-C16-C17

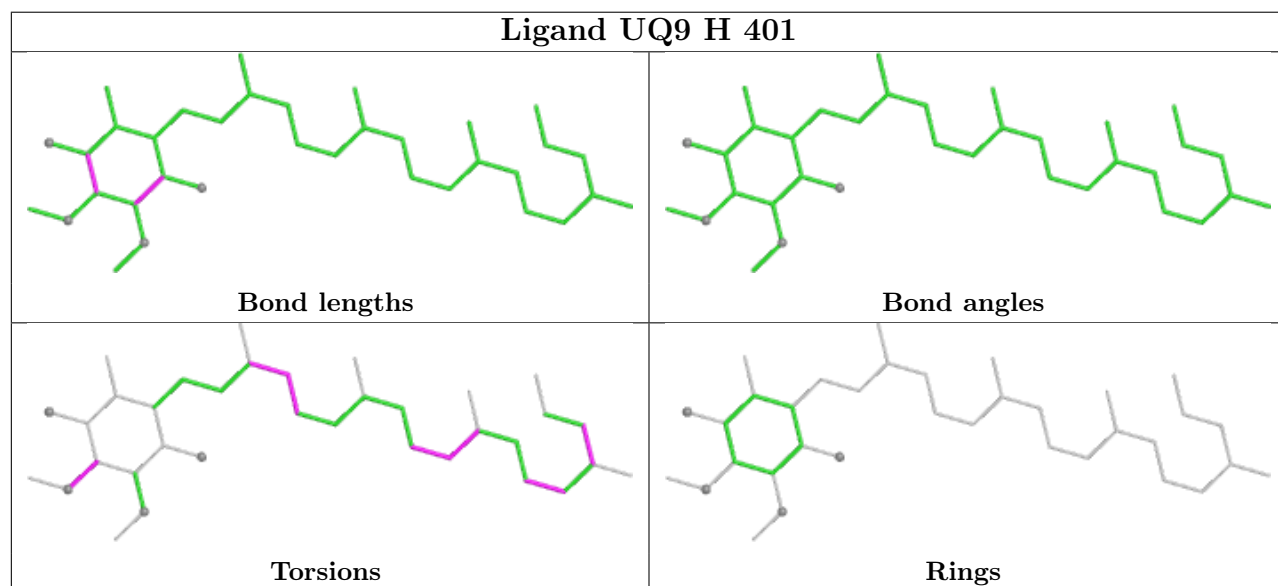
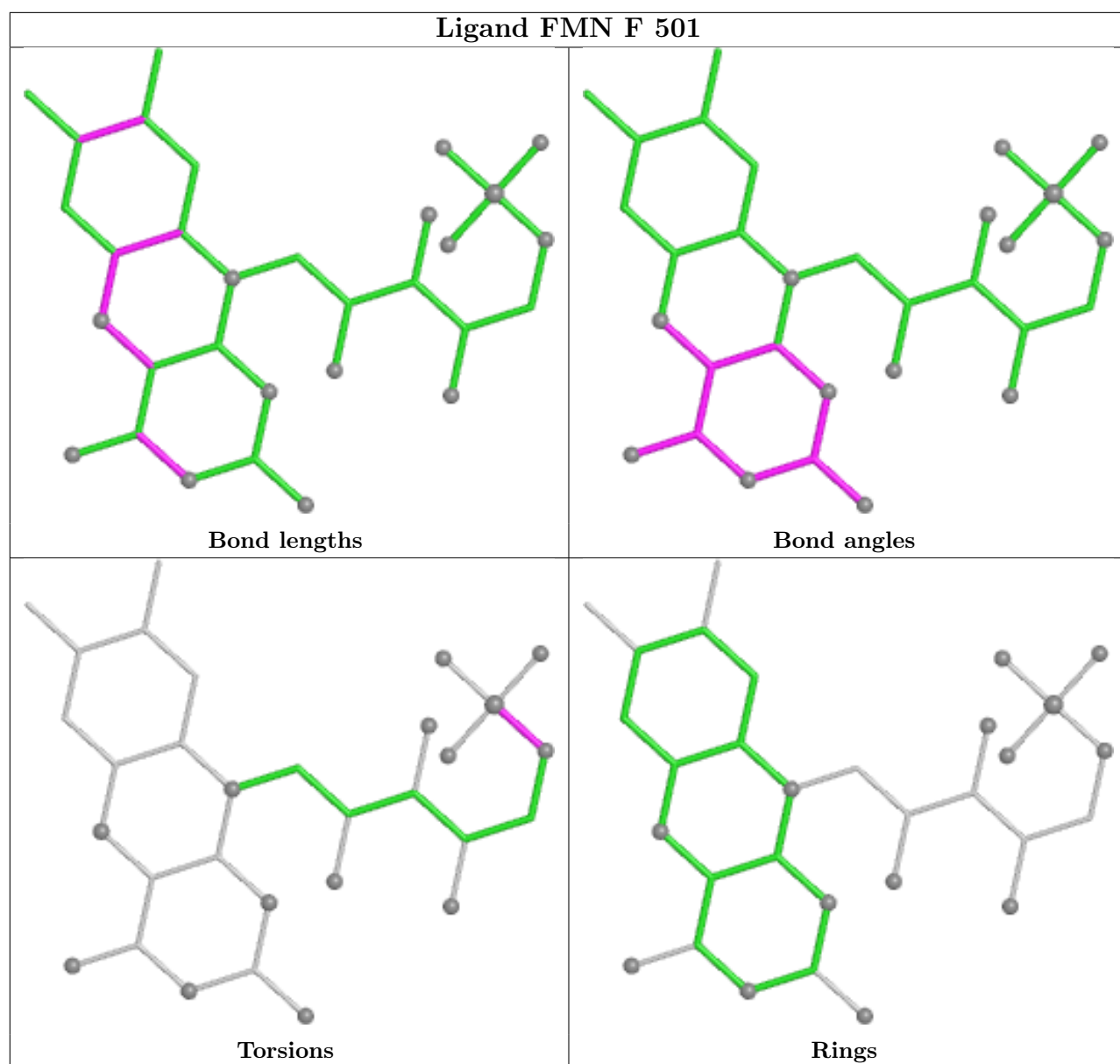
There are no ring outliers.

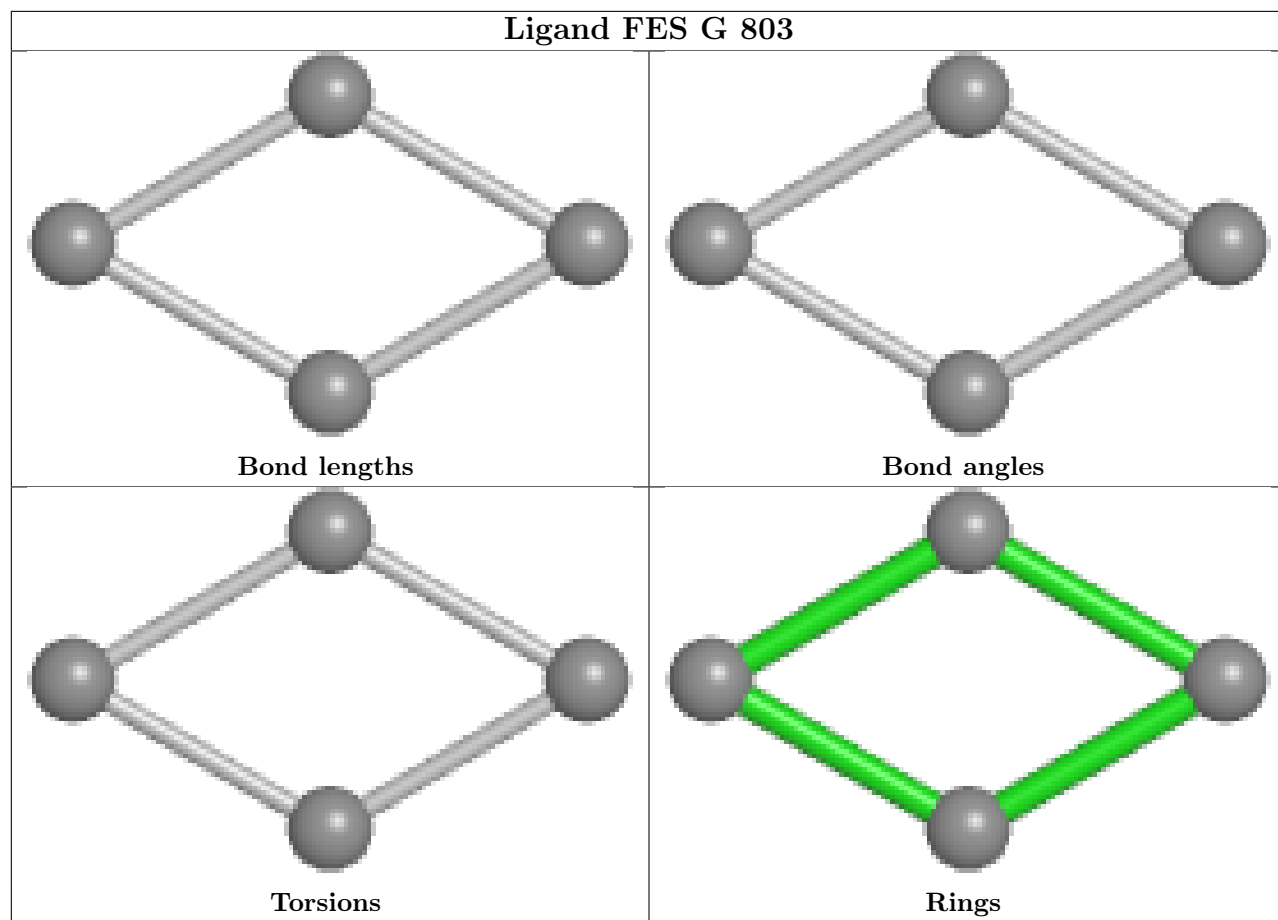
15 monomers are involved in 139 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	F	502	SF4	5	0
25	H	401	UQ9	17	0
27	G	803	FES	5	0
24	I	303	SF4	5	0
26	I	301	PC1	8	0
25	B	302	UQ9	31	0
33	q	201	CDL	22	0
29	H	403	3PE	12	0
29	H	402	3PE	7	0
32	W	201	EHZ	7	0
24	G	802	SF4	2	0
27	E	301	FES	4	0
30	P	401	NDP	5	0
26	B	303	PC1	6	0
24	B	301	SF4	3	0

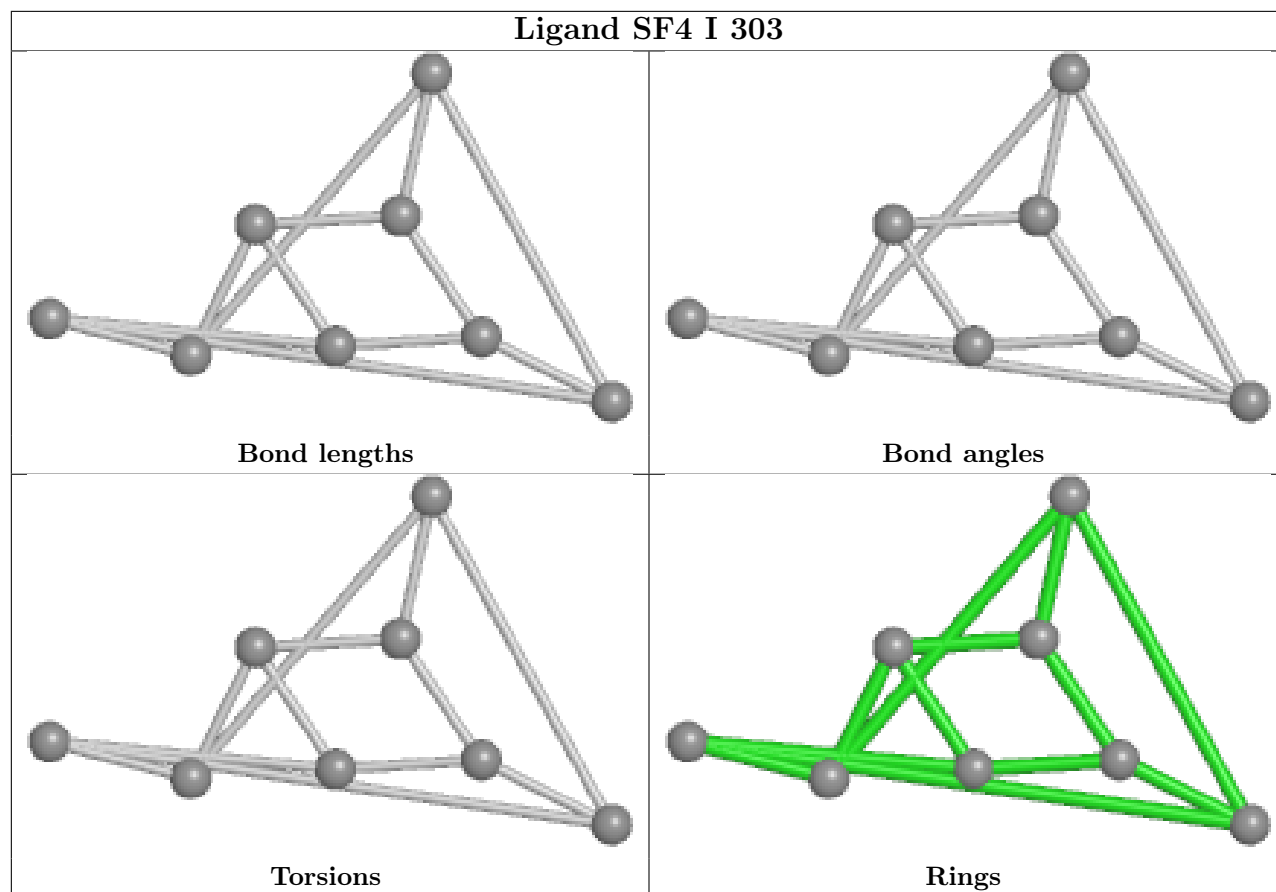
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



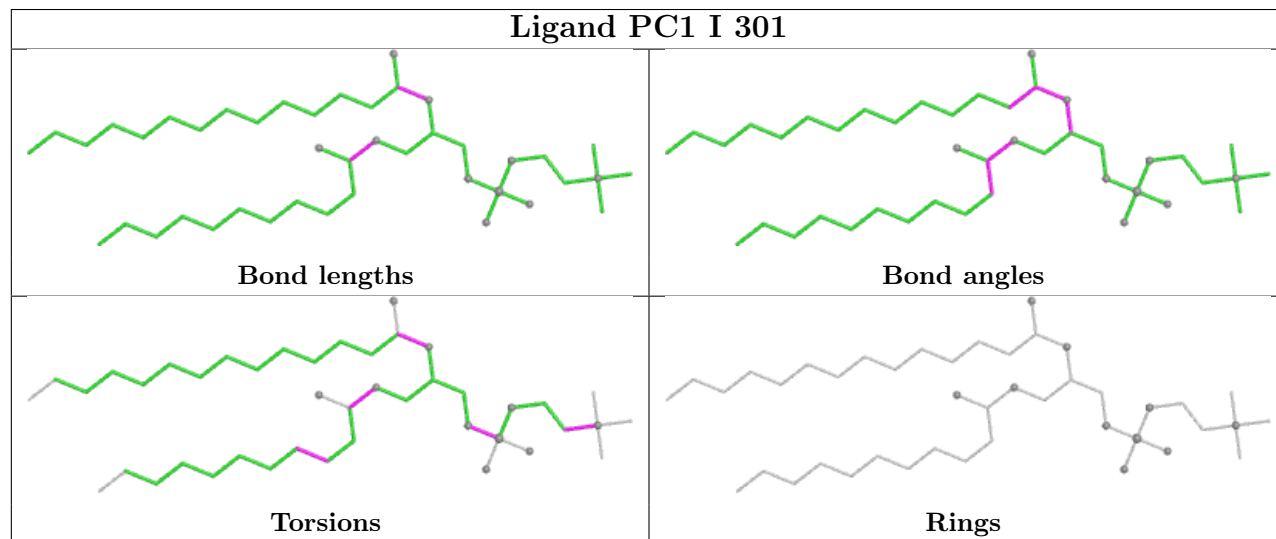


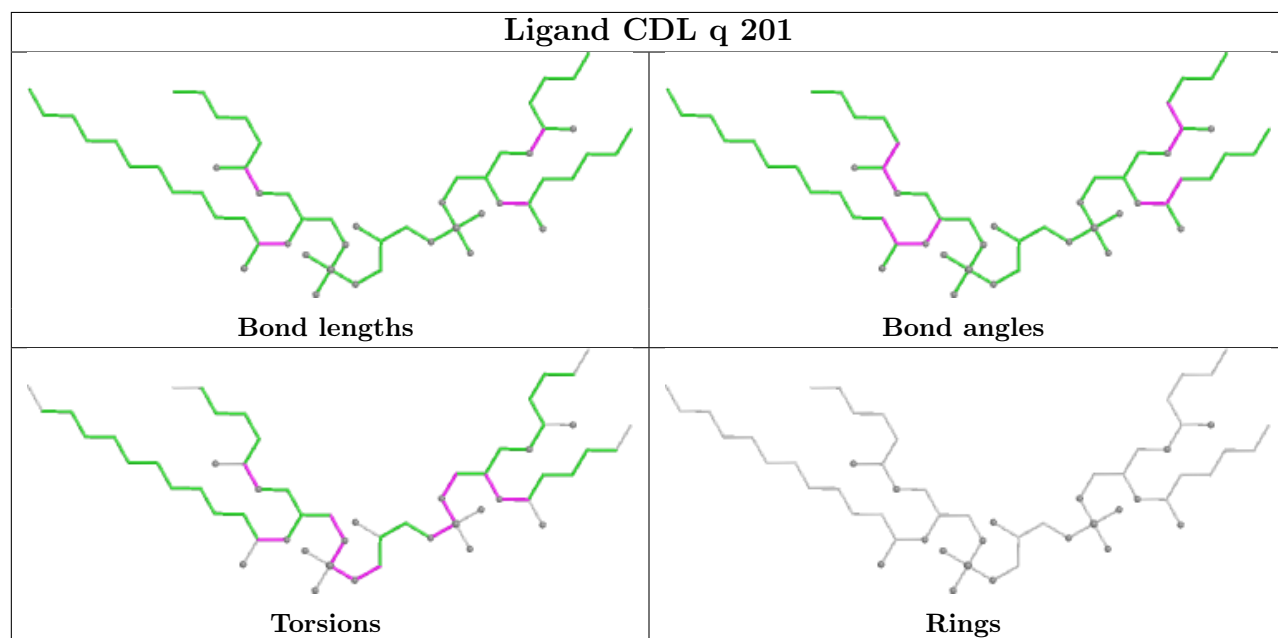
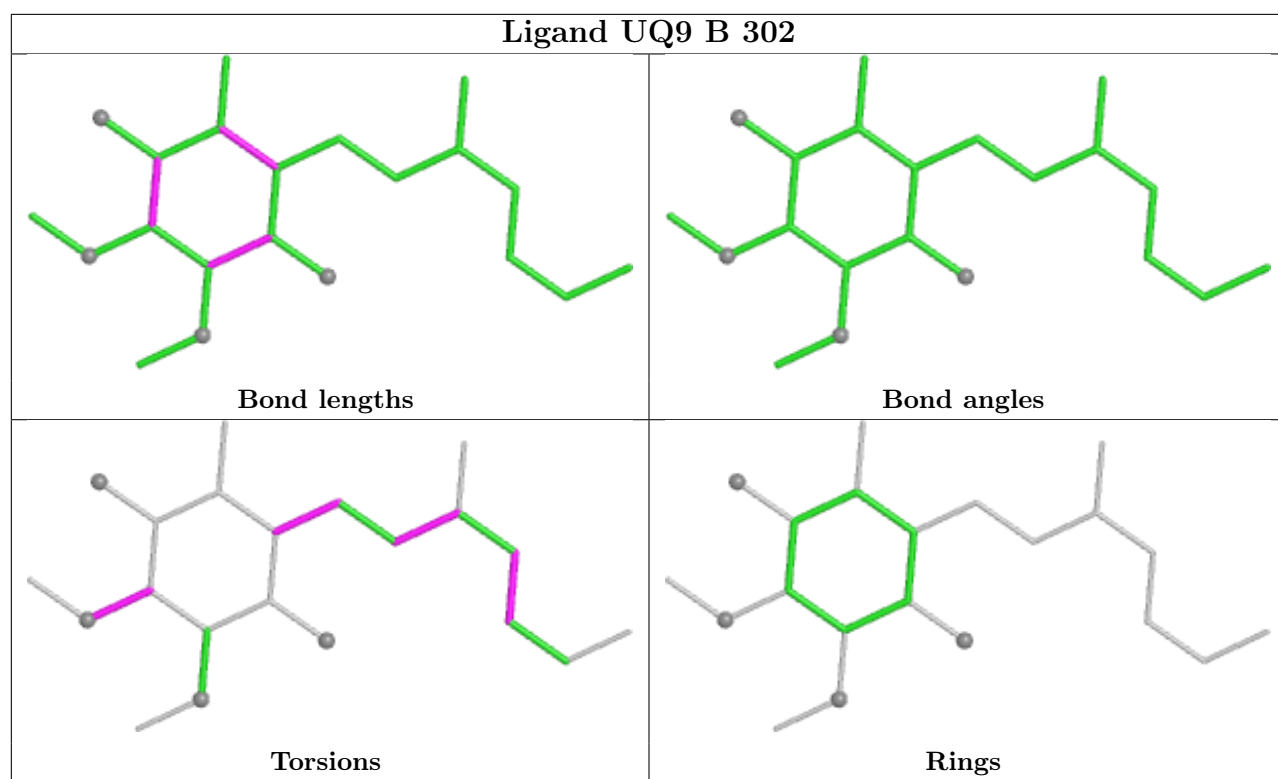


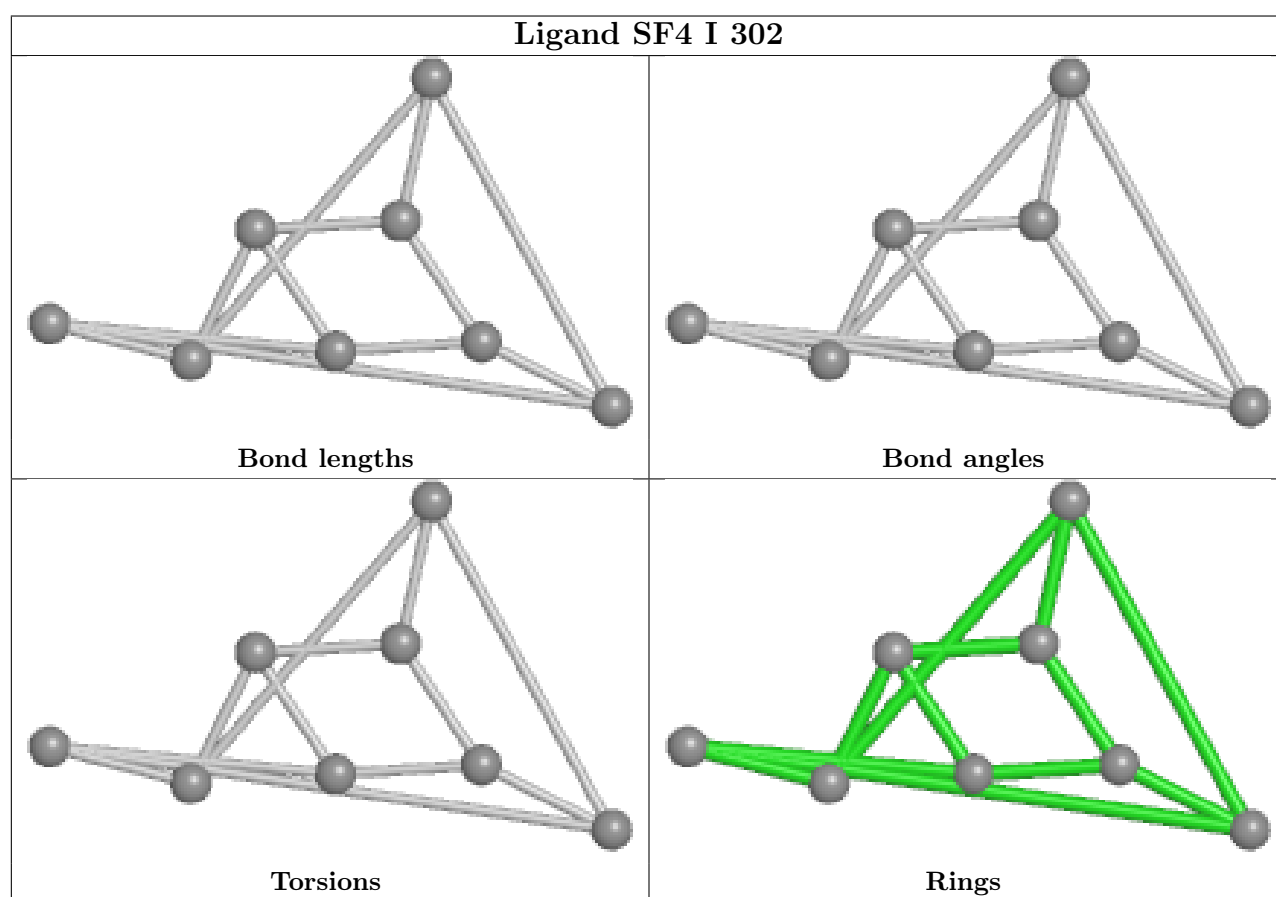
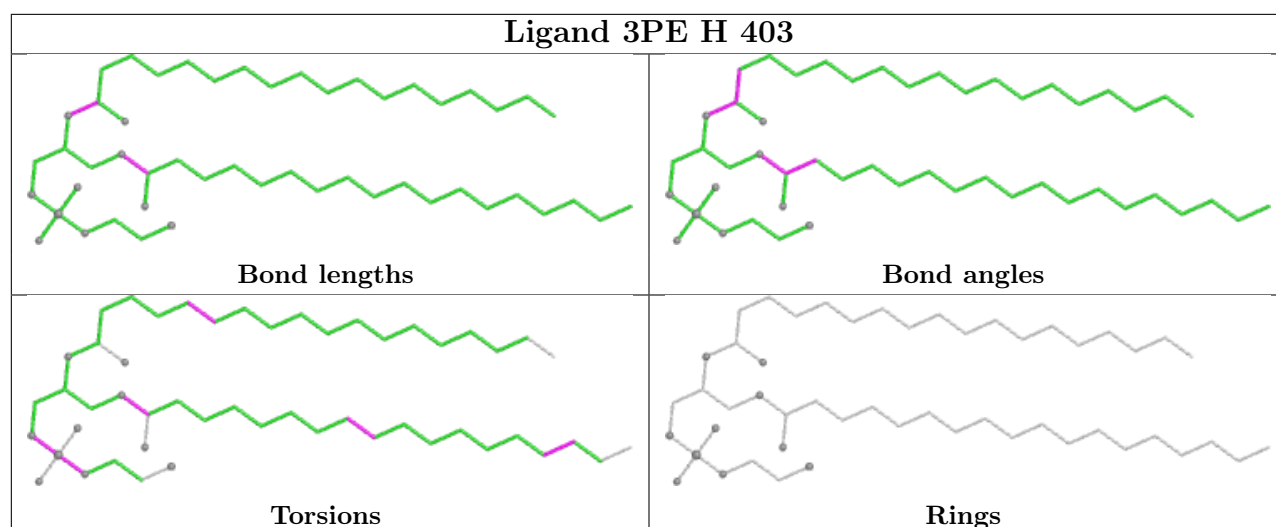
Ligand SF4 I 303



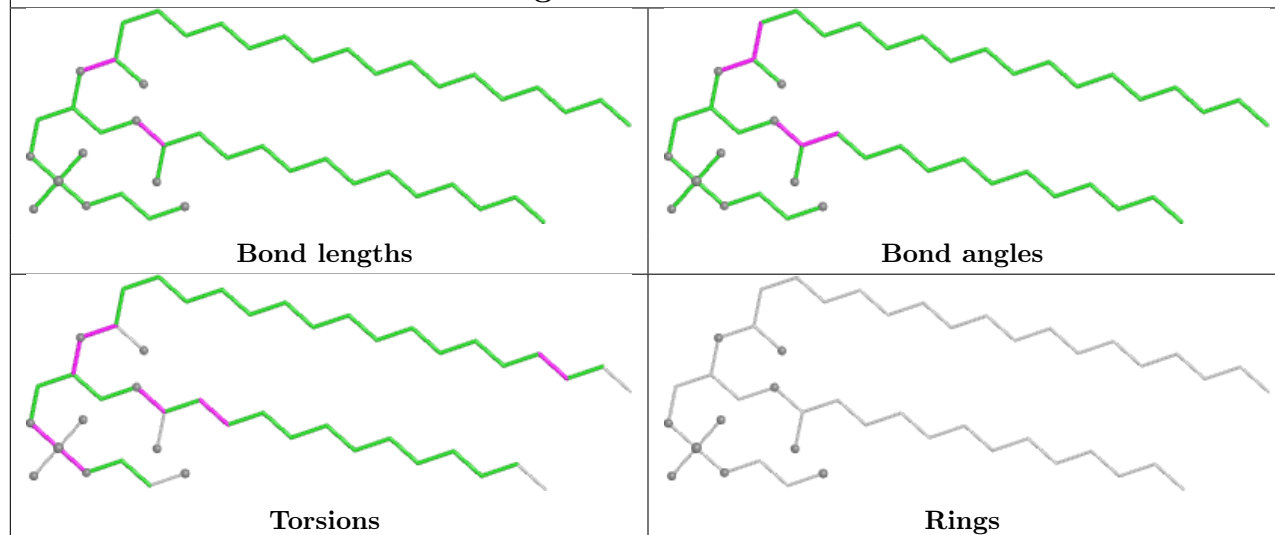
Ligand PC1 I 301



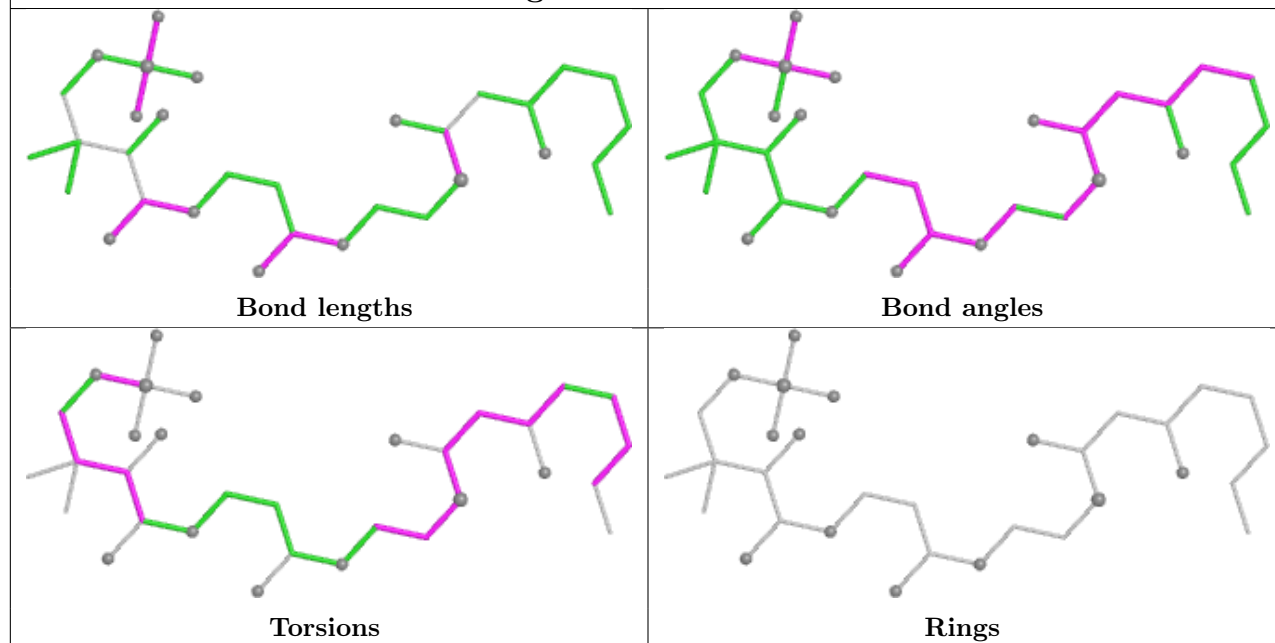


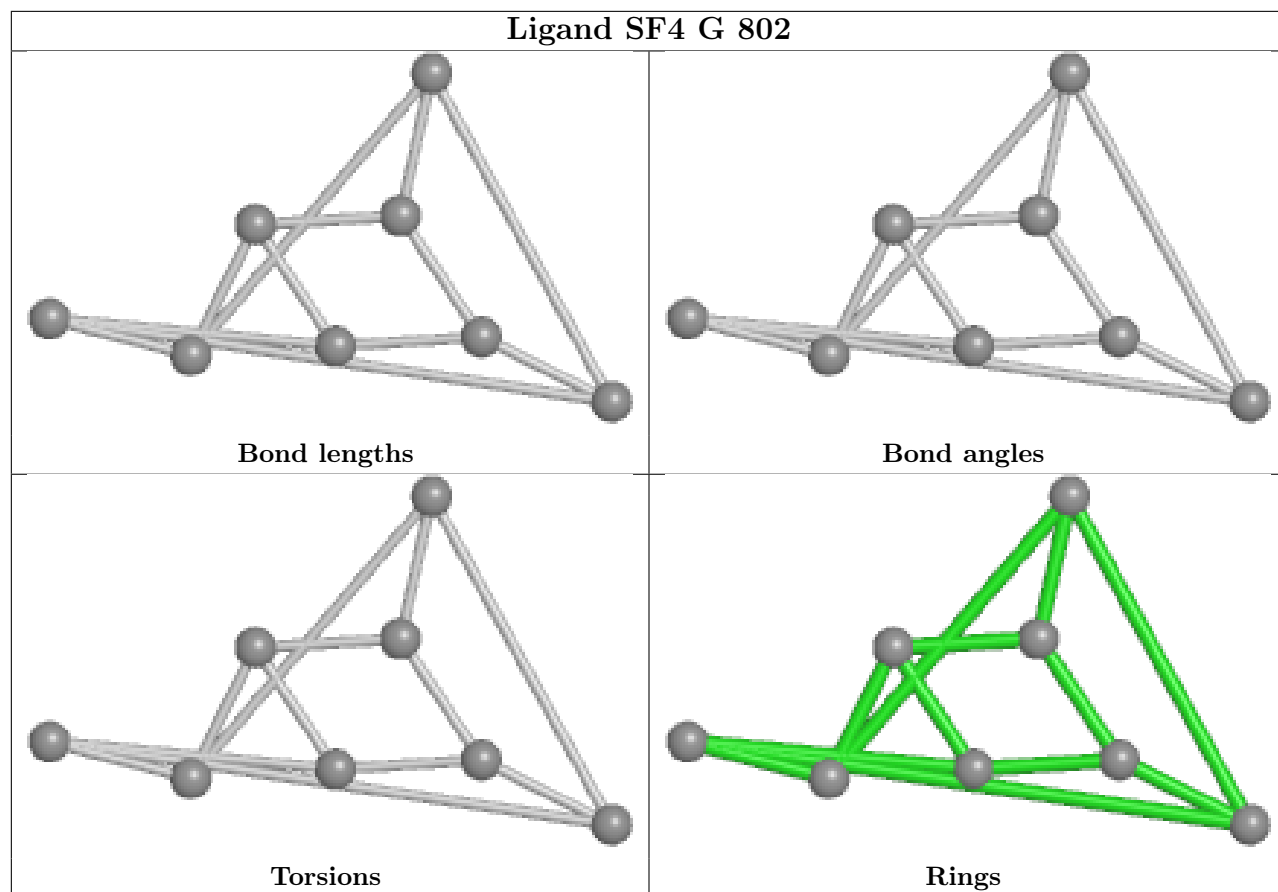


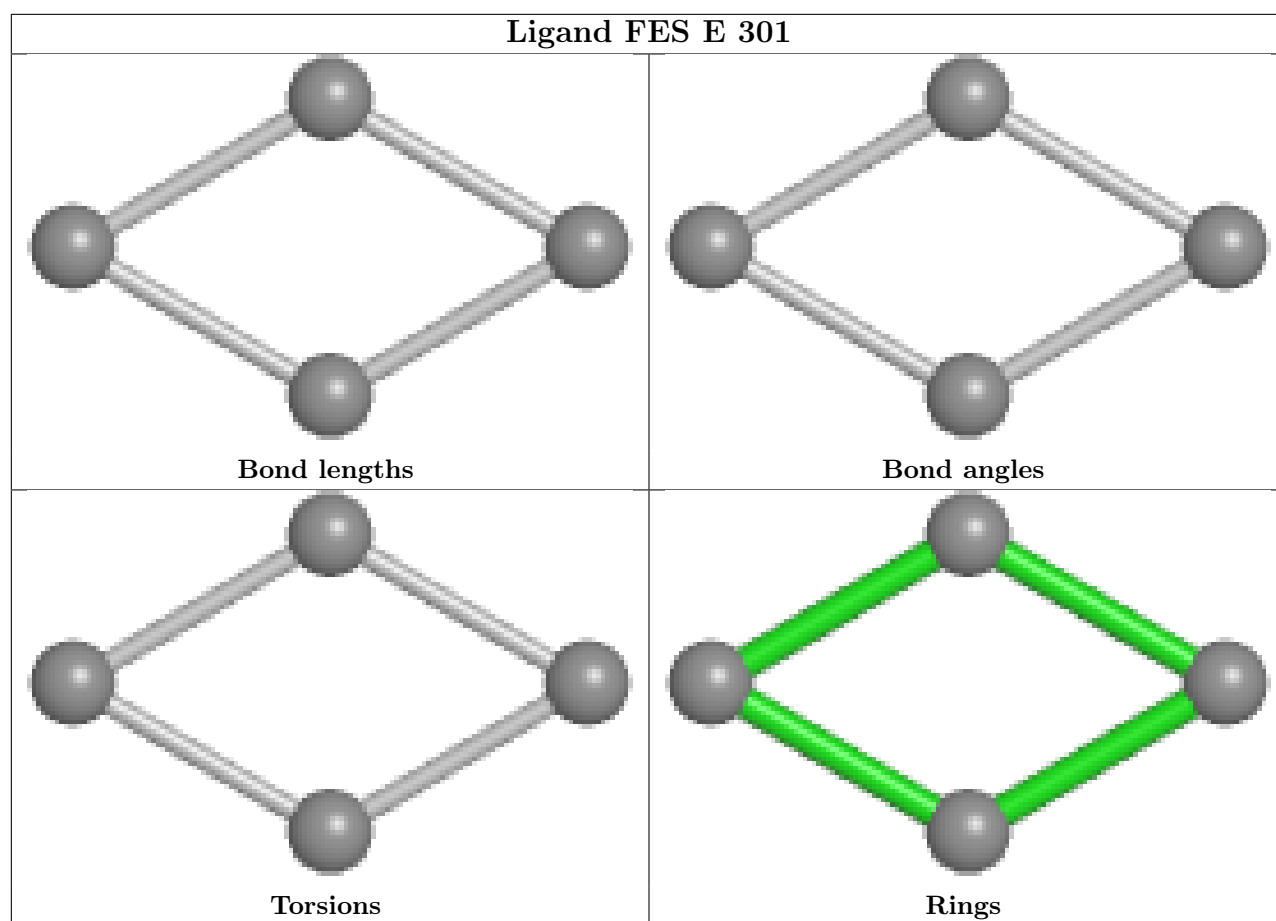
Ligand 3PE H 402

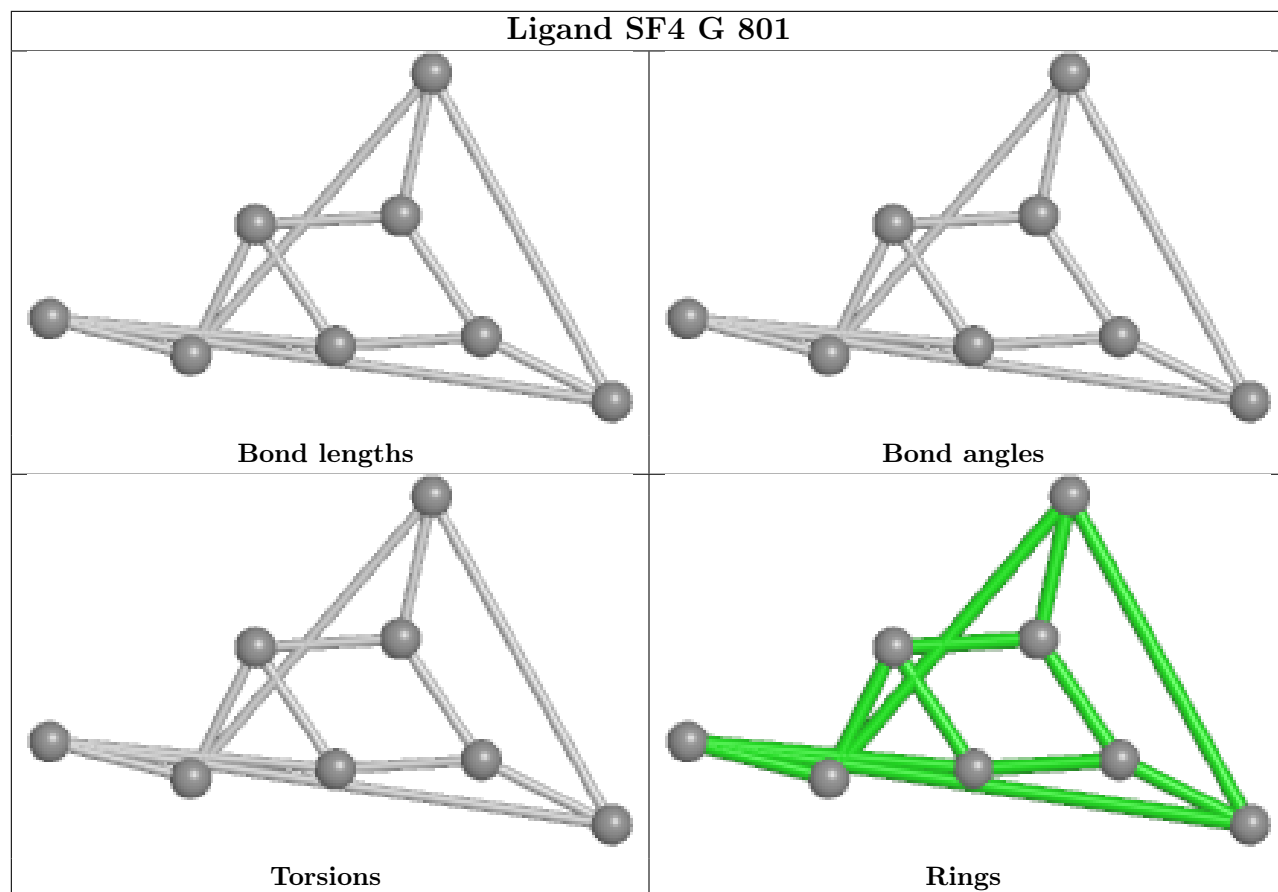


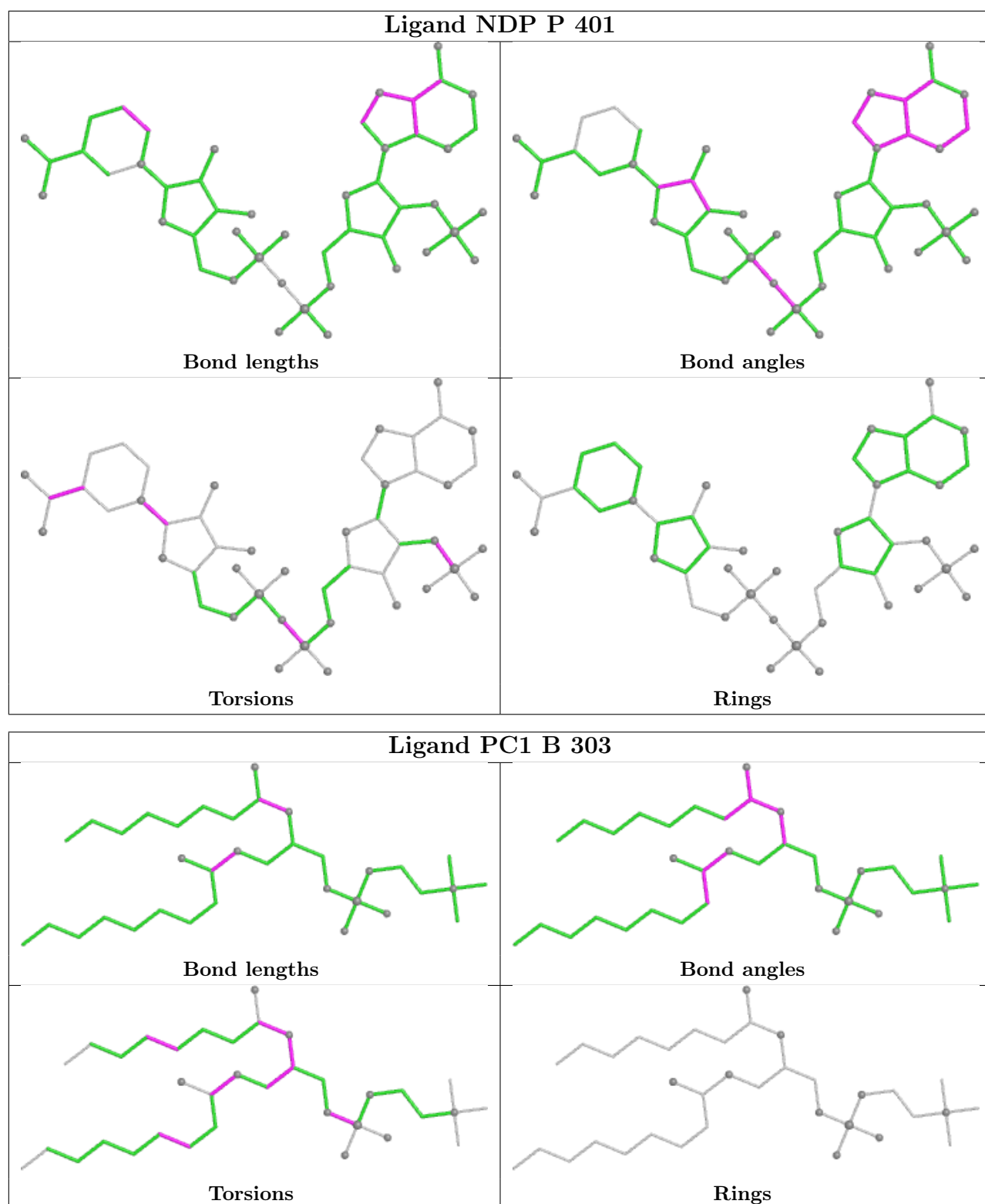
Ligand EHZ W 201

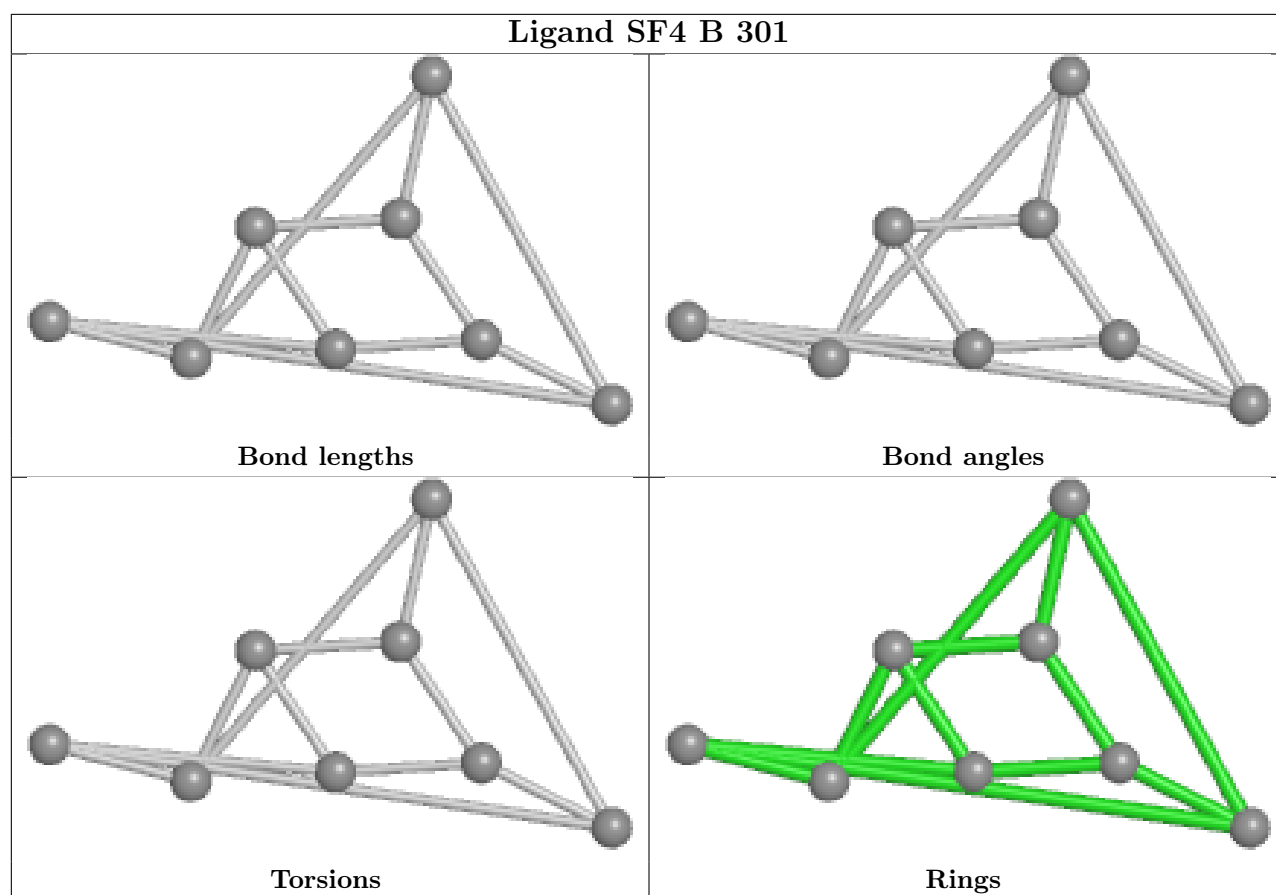












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

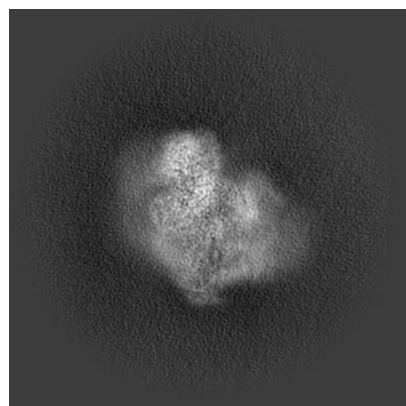
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38520. These allow visual inspection of the internal detail of the map and identification of artifacts.

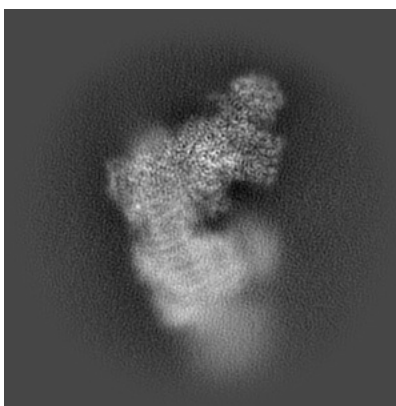
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

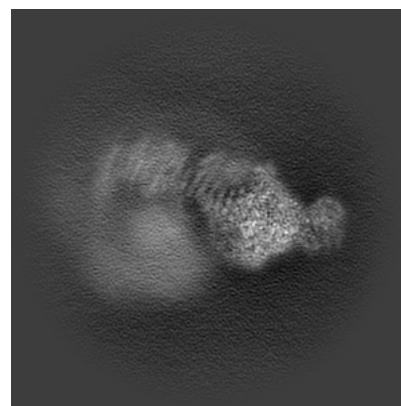
6.1.1 Primary map



X

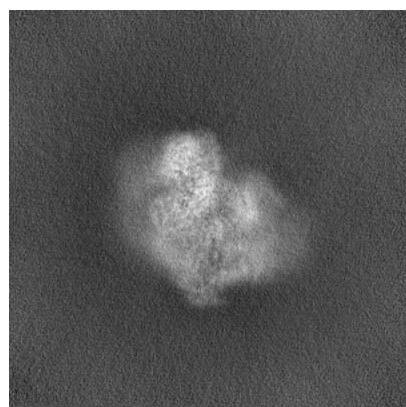


Y



Z

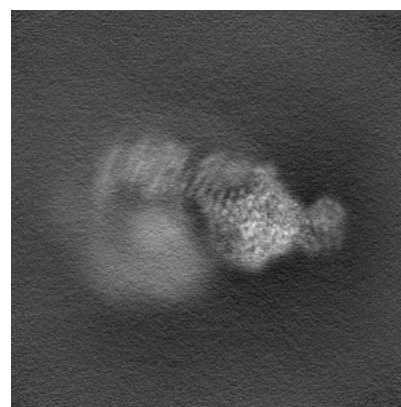
6.1.2 Raw map



X



Y

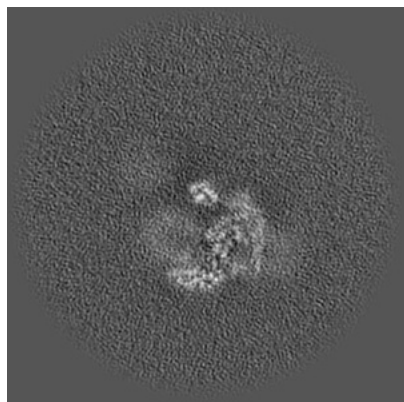


Z

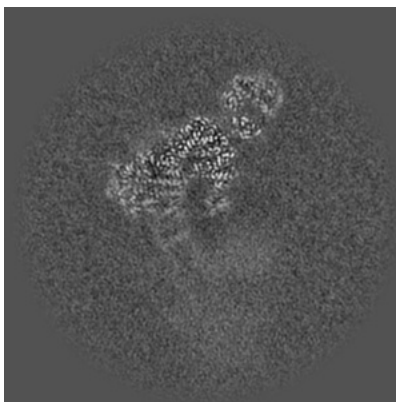
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

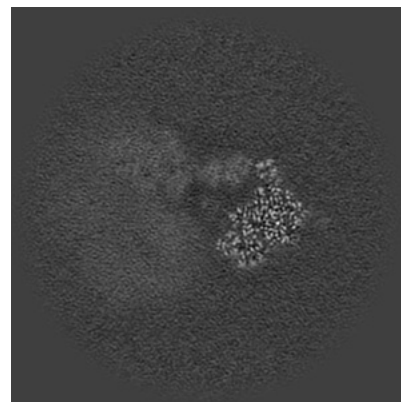
6.2.1 Primary map



X Index: 256

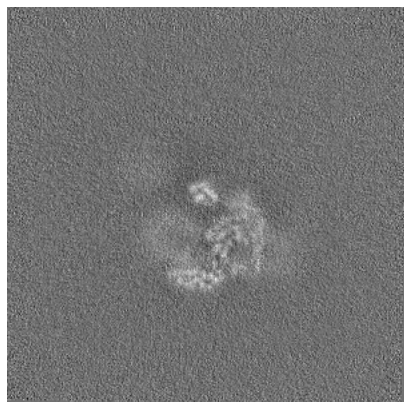


Y Index: 256

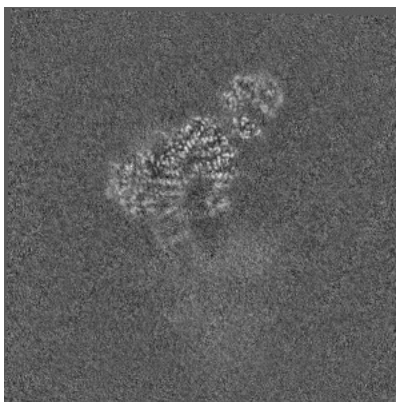


Z Index: 256

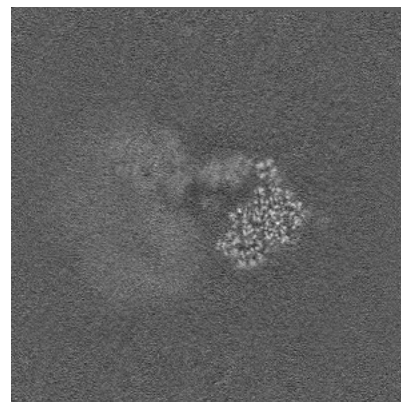
6.2.2 Raw map



X Index: 256



Y Index: 256

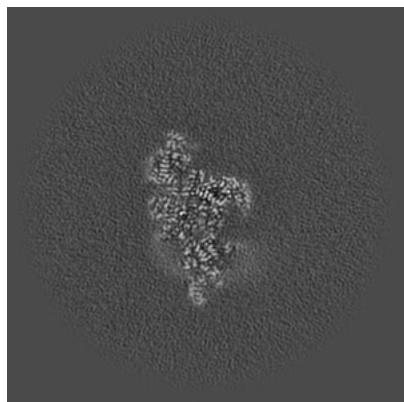


Z Index: 256

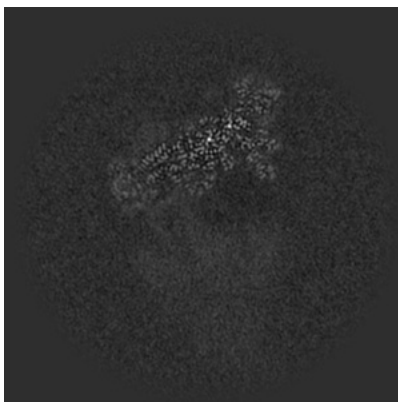
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

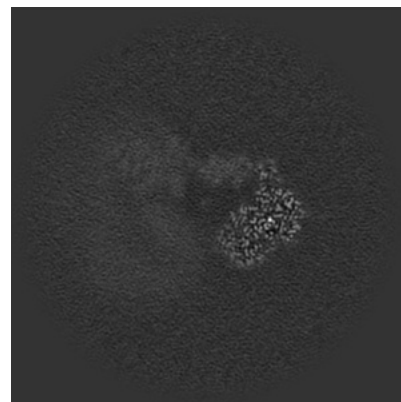
6.3.1 Primary map



X Index: 315

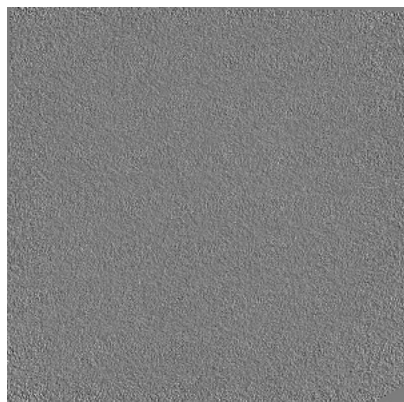


Y Index: 232

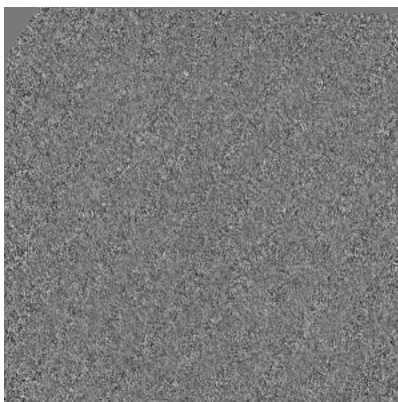


Z Index: 253

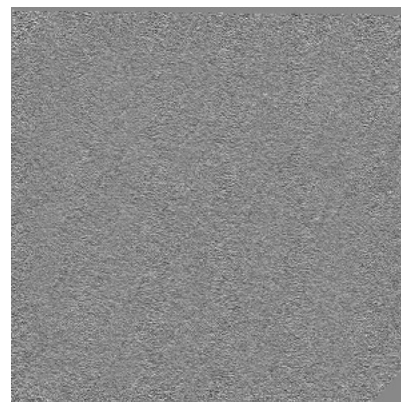
6.3.2 Raw map



X Index: 1



Y Index: 502

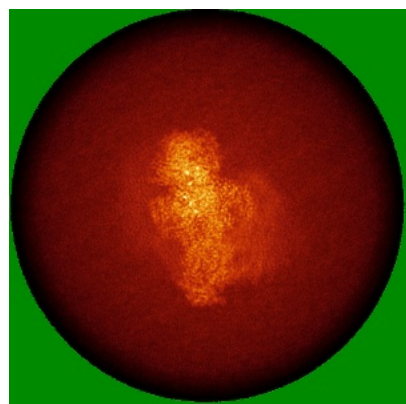


Z Index: 12

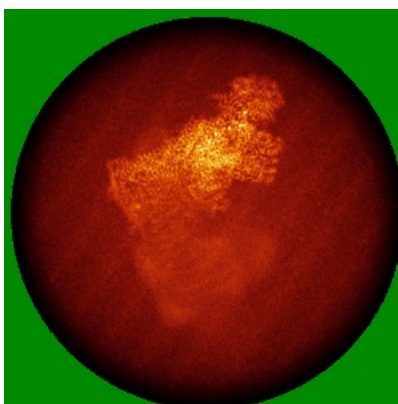
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

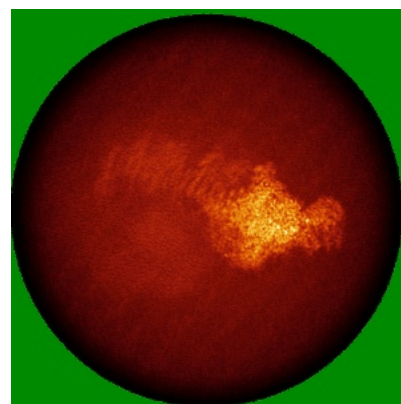
6.4.1 Primary map



X

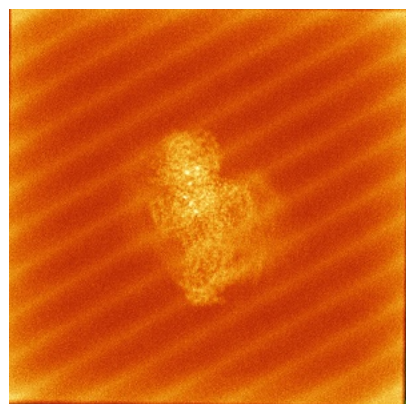


Y

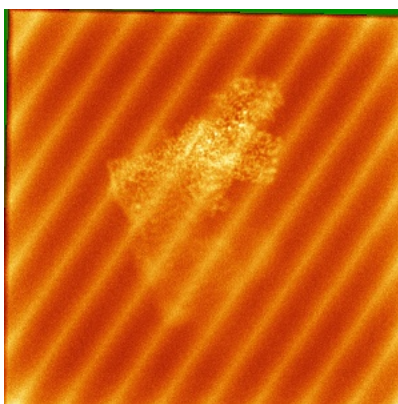


Z

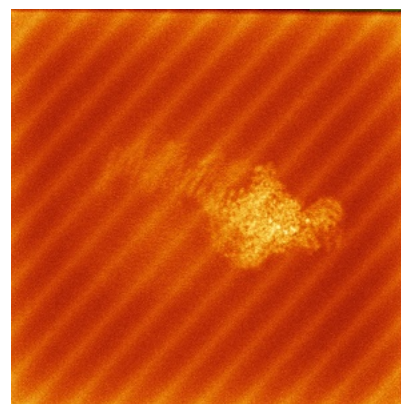
6.4.2 Raw map



X



Y

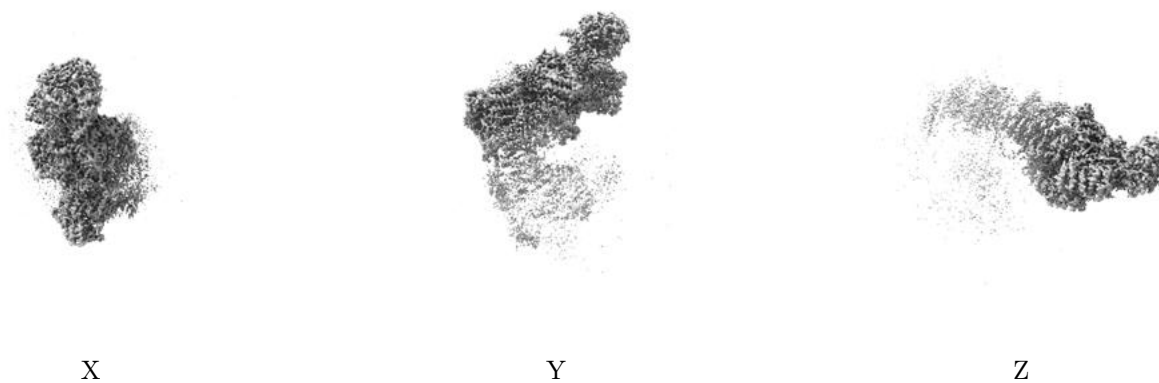


Z

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.

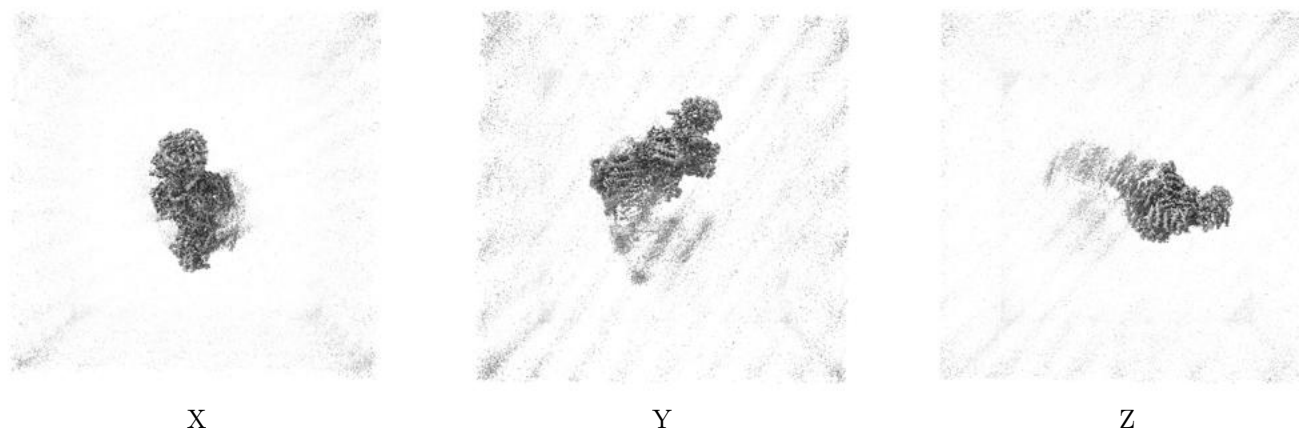
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. 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



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.

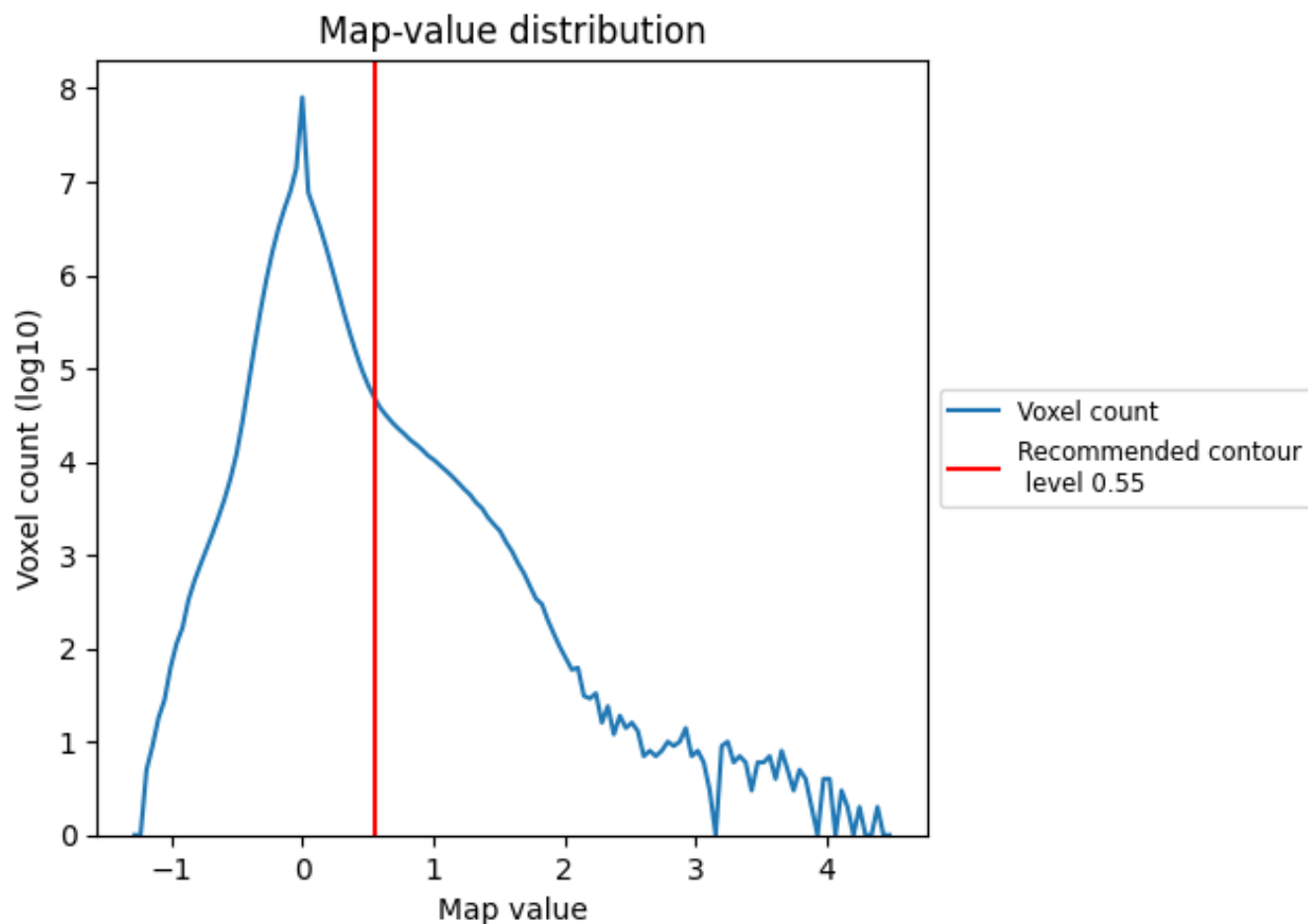
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

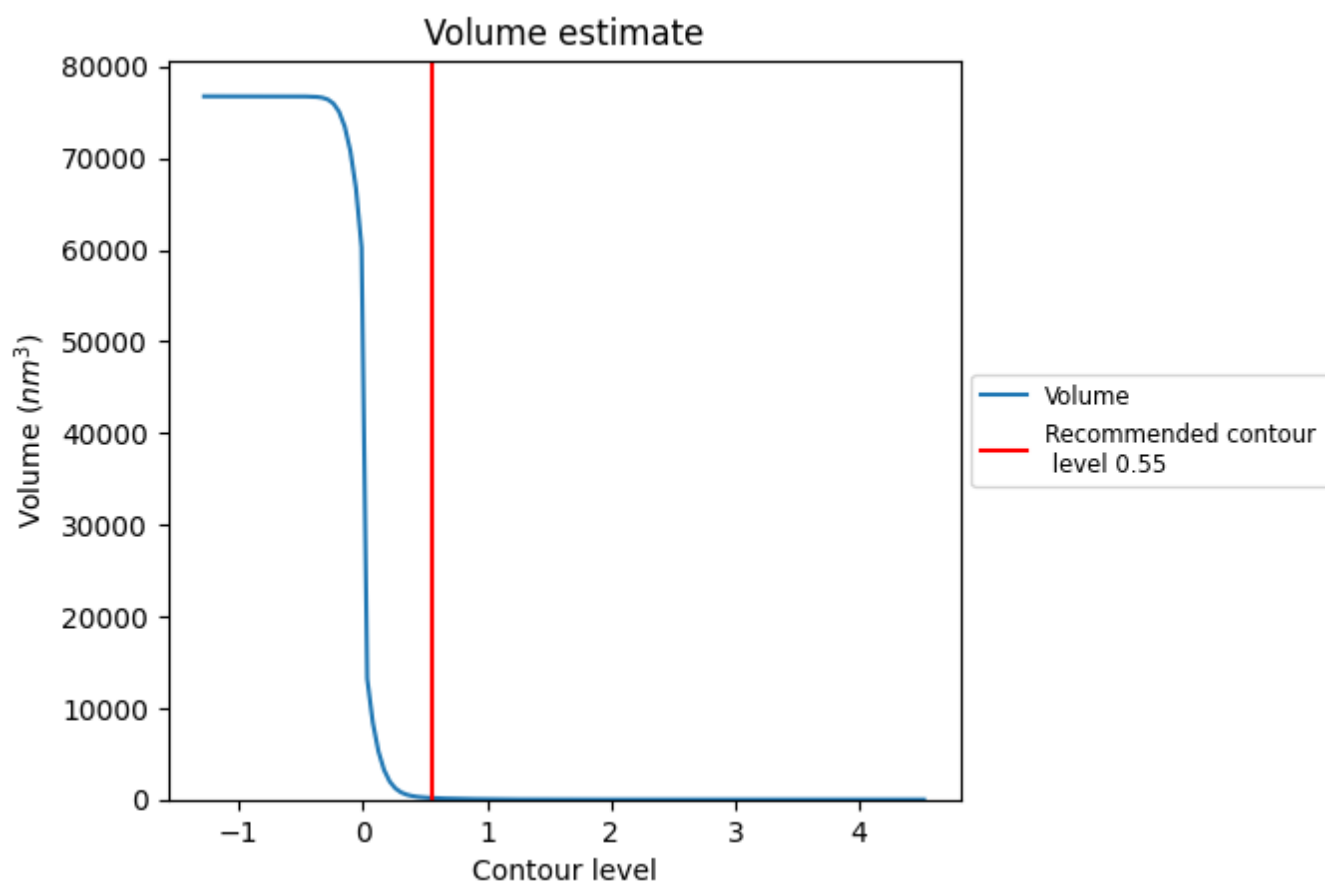
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

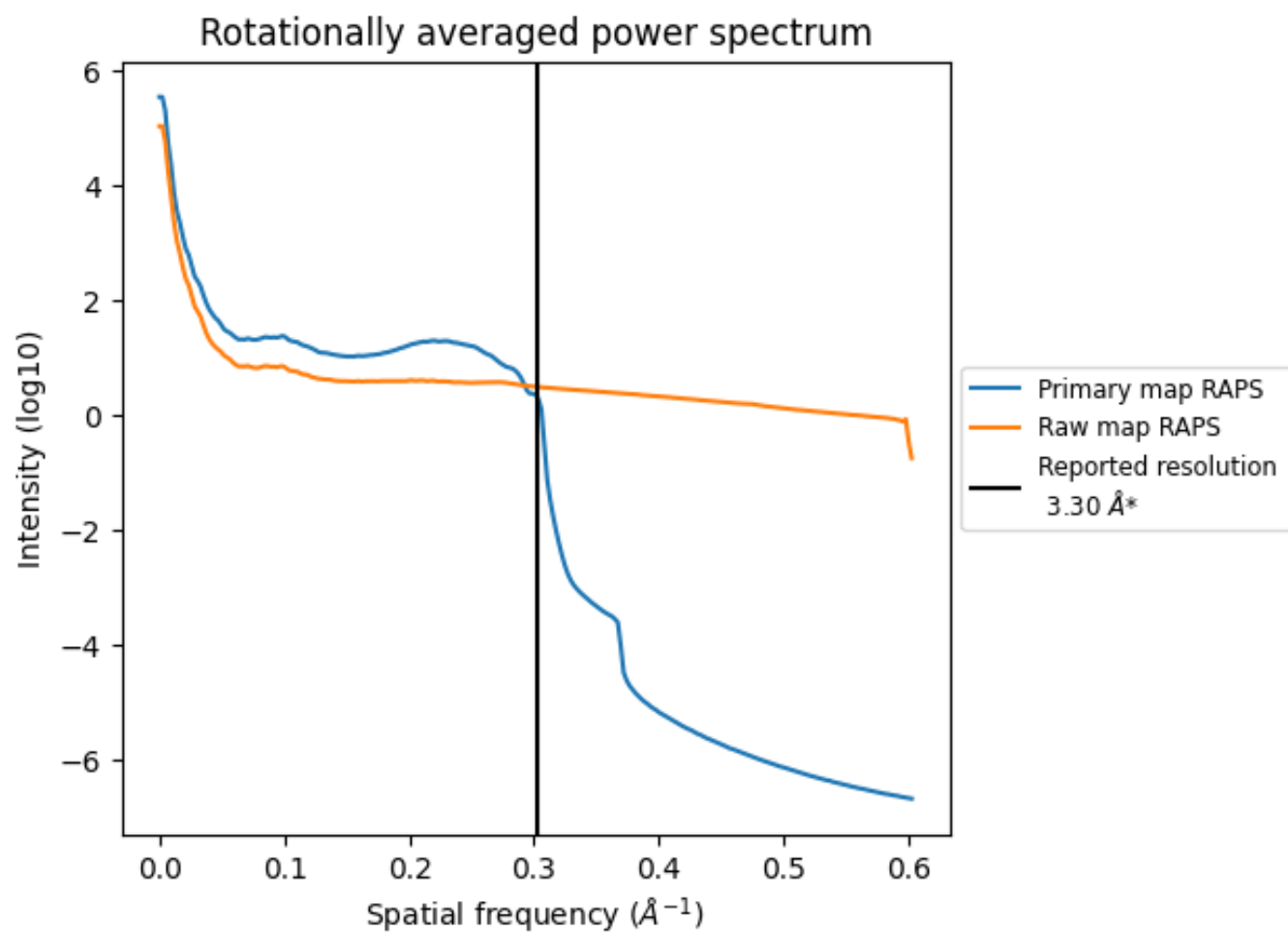
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 178 nm³; this corresponds to an approximate mass of 161 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 ⓘ

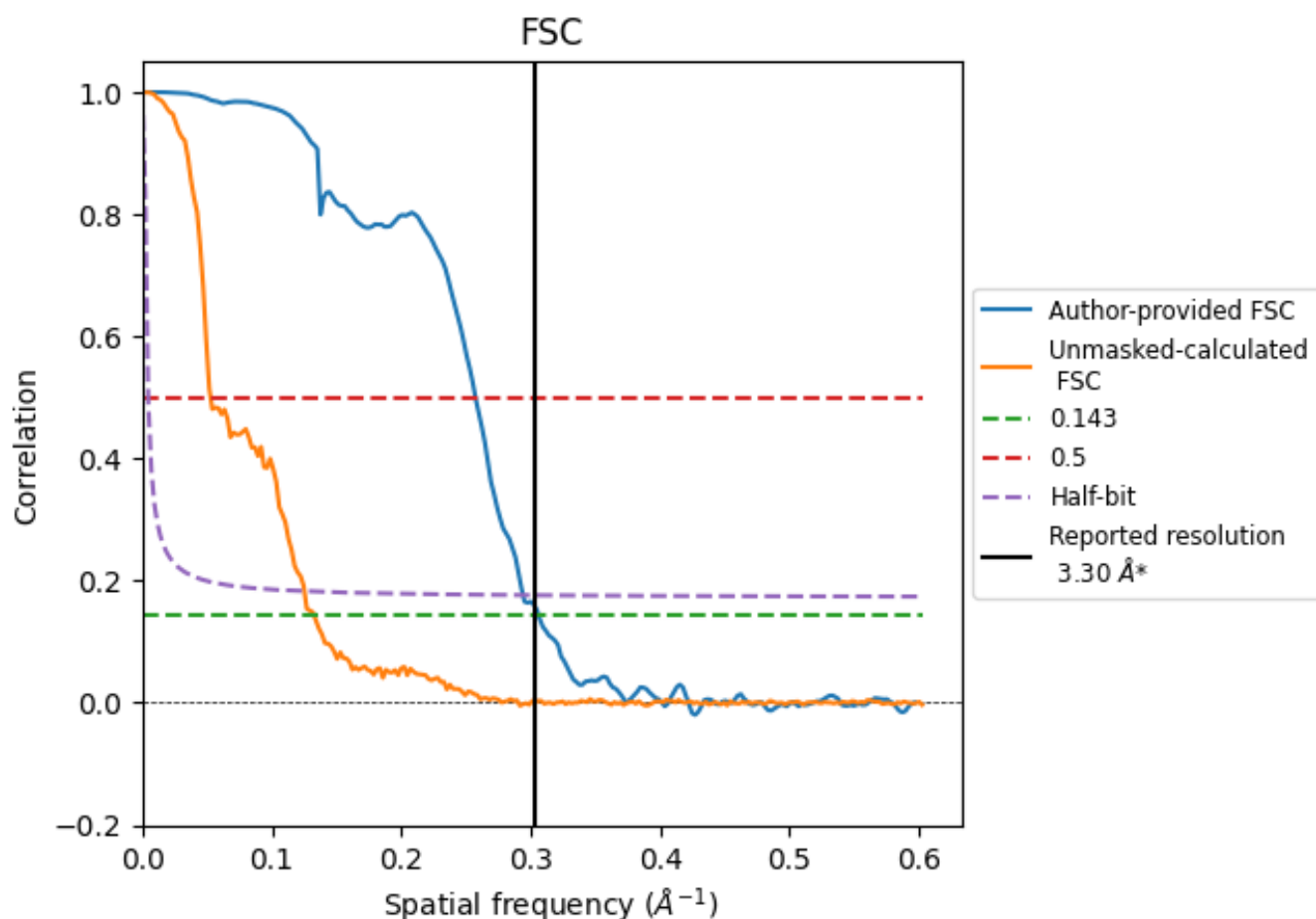


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

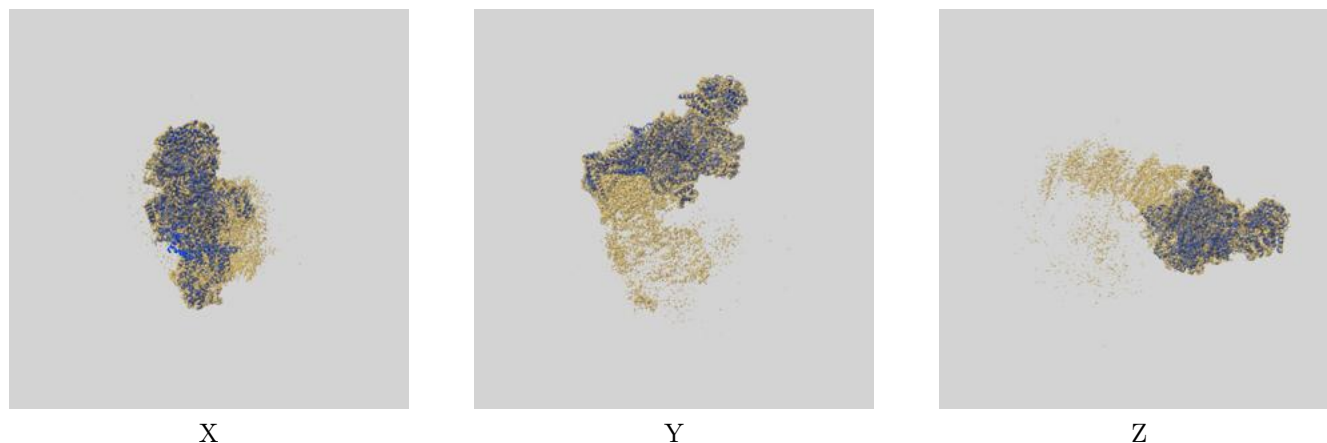
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.89	3.40
Unmasked-calculated*	7.54	18.94	7.98

*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 7.54 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

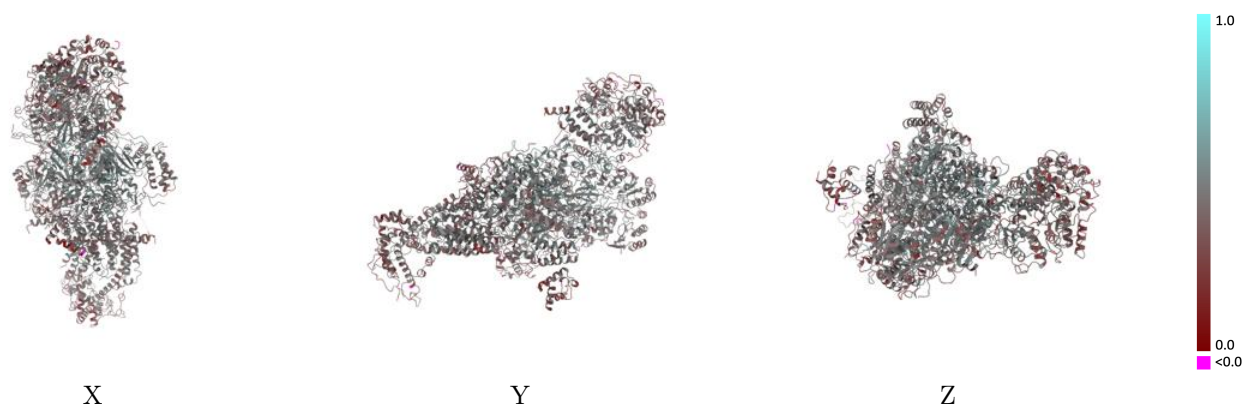
This section contains information regarding the fit between EMDB map EMD-38520 and PDB model 8XNZ. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



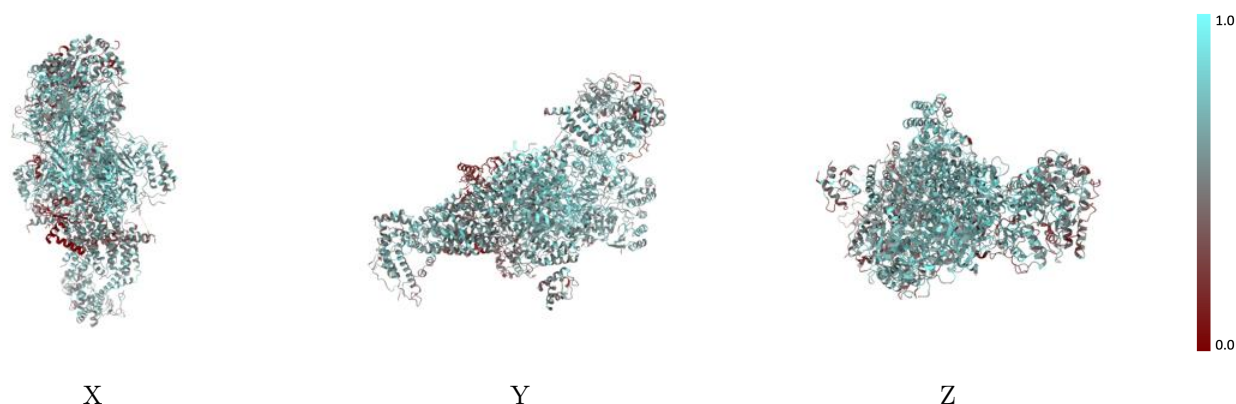
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



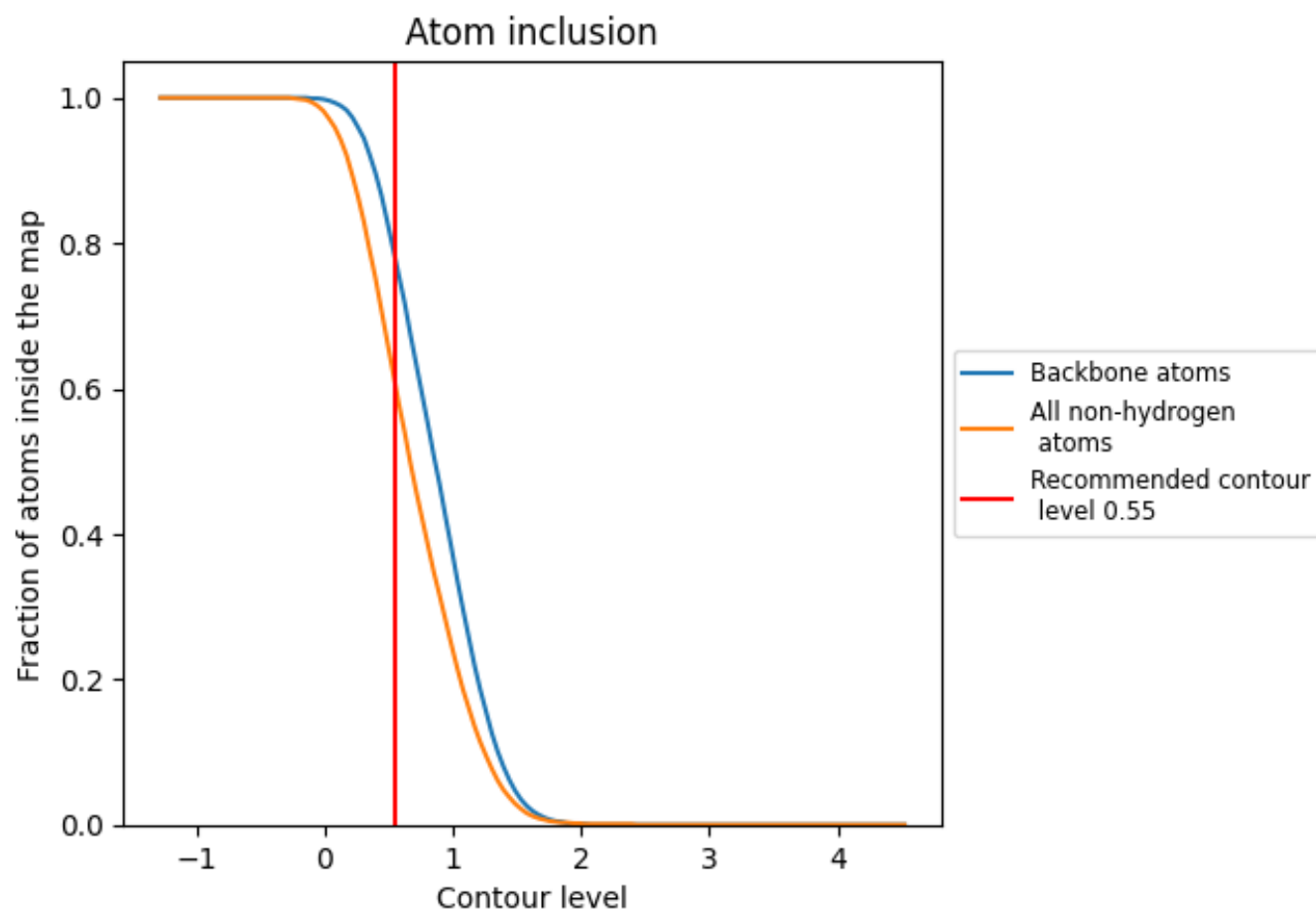
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



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 (0.55).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 60% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6050	 0.4320
A	 0.4730	 0.4260
B	 0.6860	 0.4890
C	 0.7450	 0.5040
D	 0.7380	 0.5060
E	 0.5300	 0.3860
F	 0.6000	 0.4040
G	 0.6810	 0.4550
H	 0.6040	 0.4590
I	 0.7110	 0.4810
P	 0.5690	 0.4040
Q	 0.6280	 0.4620
R	 0.3820	 0.3910
S	 0.6220	 0.4160
T	 0.4320	 0.2960
V	 0.6440	 0.4170
W	 0.6210	 0.4390
X	 0.5600	 0.3570
Z	 0.5670	 0.3800
a	 0.6240	 0.4040
b	 0.5340	 0.3680
q	 0.1880	 0.3500
r	 0.3520	 0.3610
s	 0.2030	 0.3230

