



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 08:03 PM JST

PDB ID : 8XNN / pdb_00008xnn
EMDB ID : EMD-38508
Title : Respiratory complex Peripheral Arm of CI, open form A, focus-refined map of type I, Wild type mouse under thermoneutral temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-12-30
Resolution : 3.60 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:

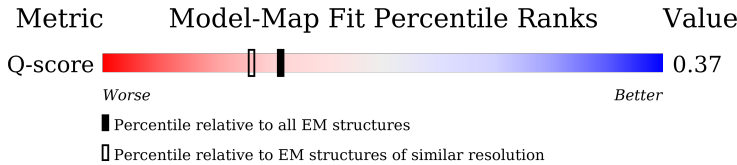
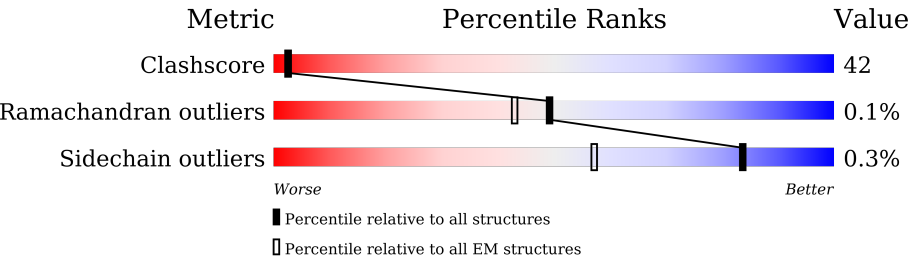
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 3.60 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.



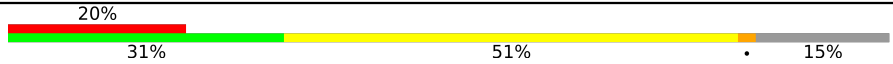
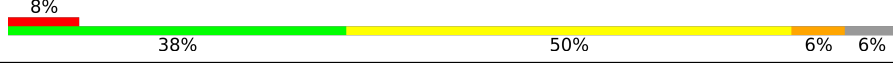
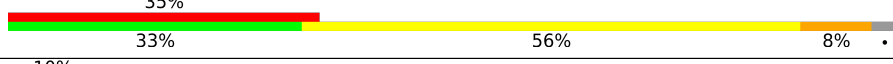
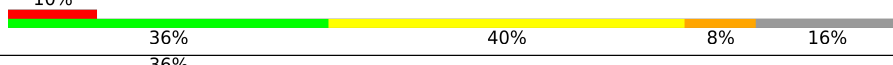
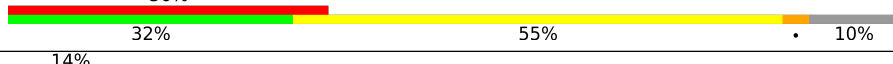
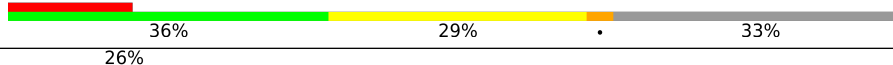
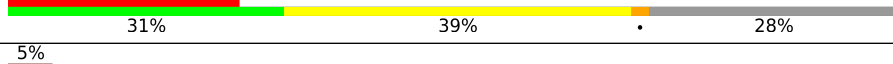
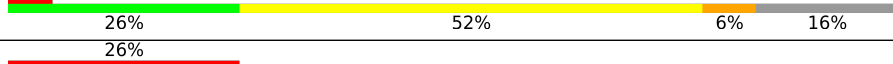
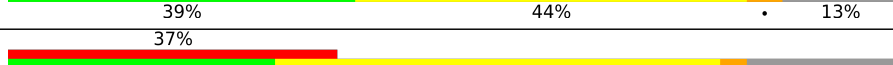
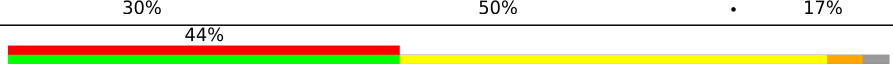
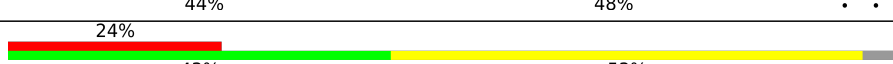
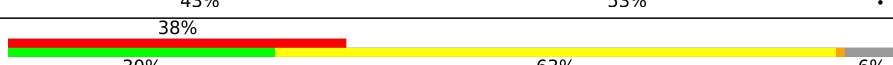
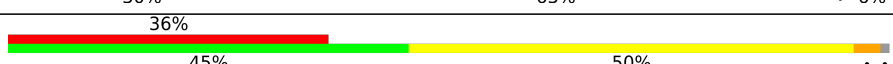
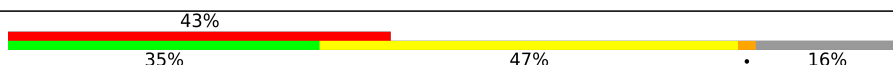
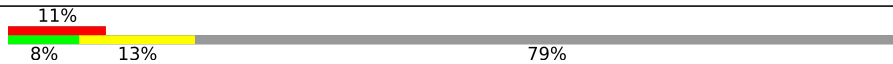
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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
25	SF4	B	301	-	-	X	-
25	SF4	F	502	-	-	X	-
25	SF4	G	802	-	-	X	-
25	SF4	I	302	-	-	X	-
25	SF4	I	303	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	FES	E	301	-	-	X	-
26	FES	G	803	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 34420 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	91	Total	C	N	O	S	0	0
			743	517	103	118	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1258	802	227	215	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	381	Total	C	N	O	S	0	0
			3056	1951	527	556	22		

- 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	426	Total	C	N	O	S	0	0
			3288	2073	588	605	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	310	Total	C	N	O	S	0	0
			2479	1667	376	414	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	143	Total	C	N	O	S	0	0
			1192	766	212	210	4		

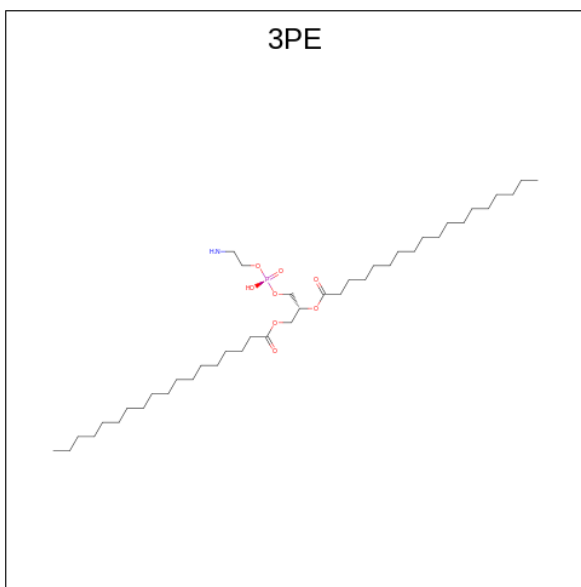
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	95	Total	C	N	O	S	0	0
			764	482	143	136	3		

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

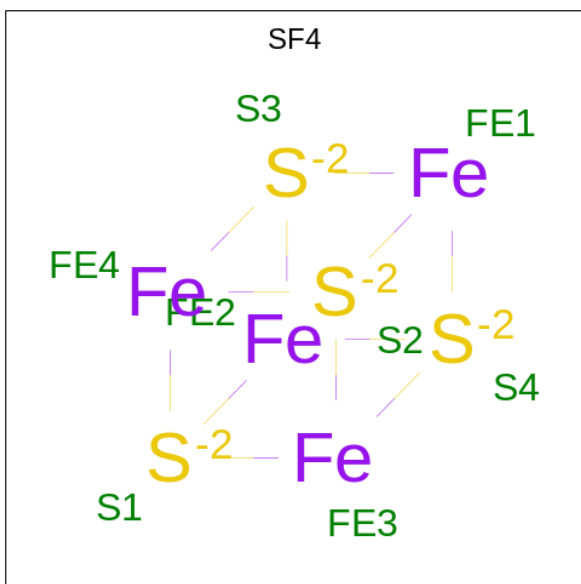
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	22	Total	C	N	O	0	0
			189	124	29	36		

- Molecule 24 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



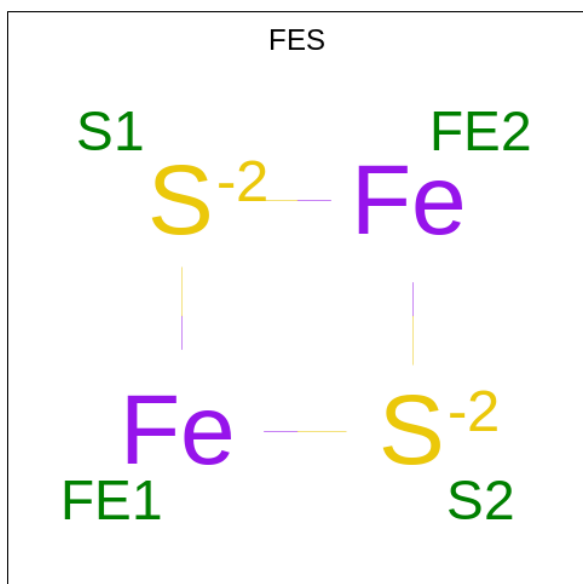
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	b	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



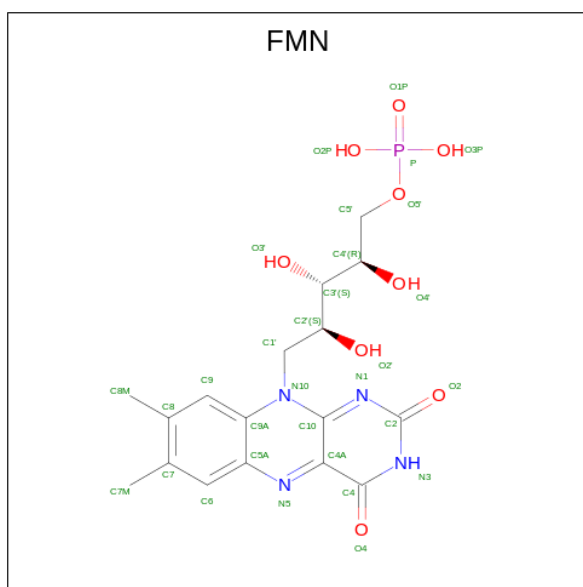
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	Fe	S	0
			8	4	4	
25	F	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



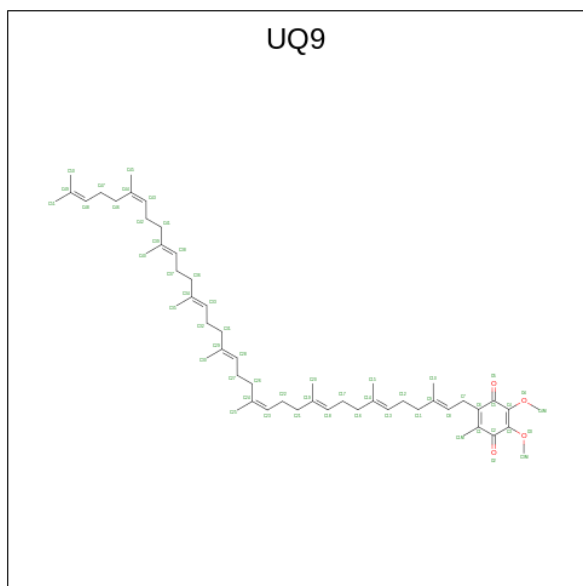
Mol	Chain	Residues	Atoms			AltConf
26	E	1	Total	Fe	S	0
			4	2	2	
26	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 27 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).



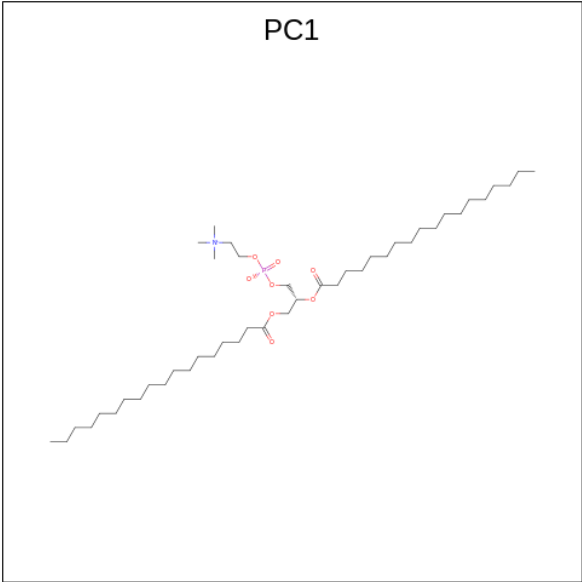
Mol	Chain	Residues	Atoms					AltConf
27	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 28 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



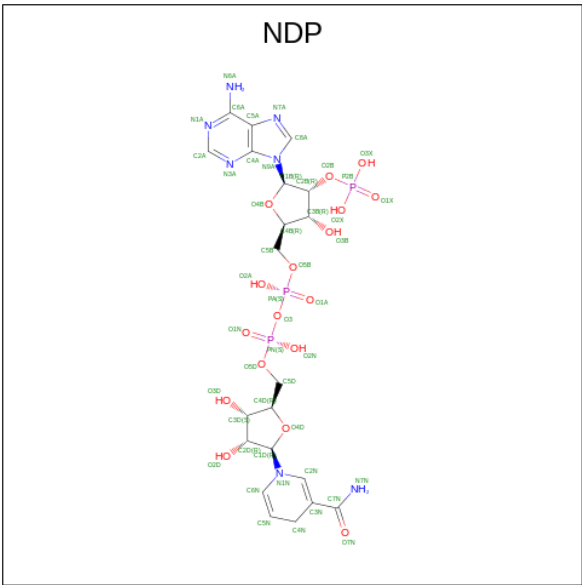
Mol	Chain	Residues	Atoms			AltConf
28	H	1	Total	C	O	0
			35	31	4	

- Molecule 29 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
29	I	1	Total	C	N	O	P	0
			47	37	1	8	1	
29	q	1	Total	C	N	O	P	0
			35	25	1	8	1	

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

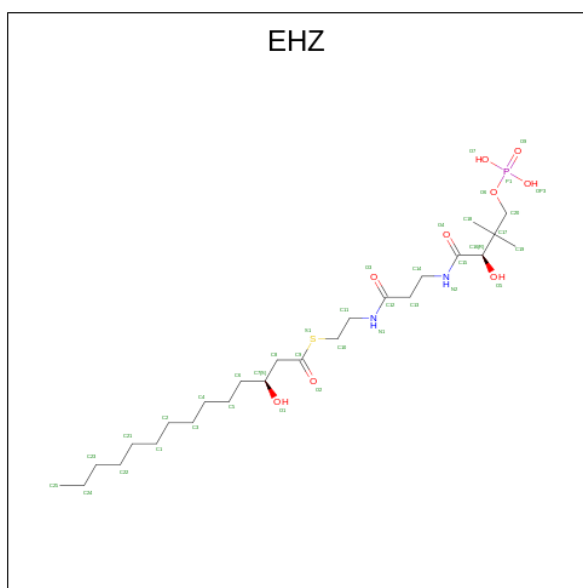


Mol	Chain	Residues	Atoms					AltConf
30	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

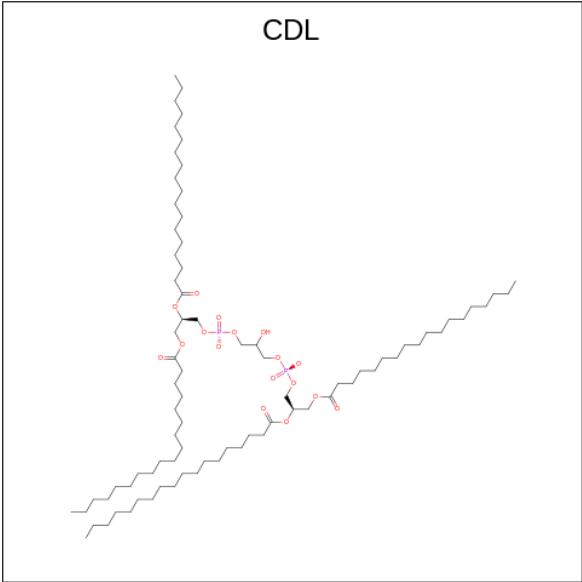
Mol	Chain	Residues	Atoms		AltConf
31	R	1	Total	Zn	0
			1	1	

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

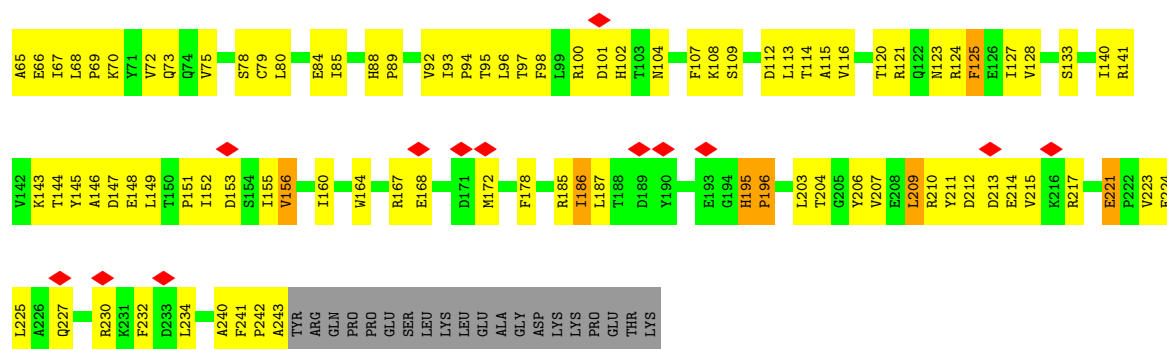


Mol	Chain	Residues	Atoms						AltConf
32	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

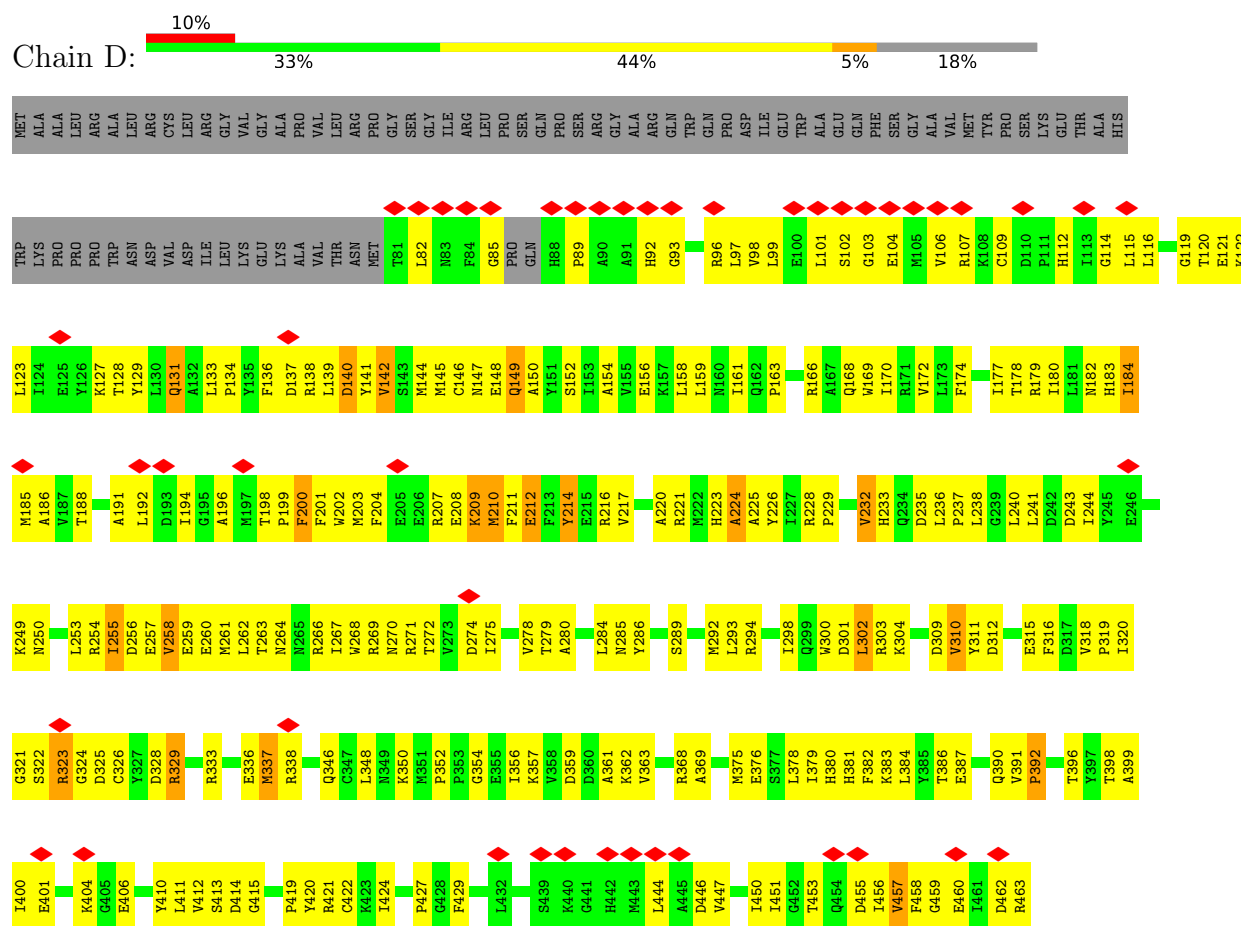
- Molecule 33 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



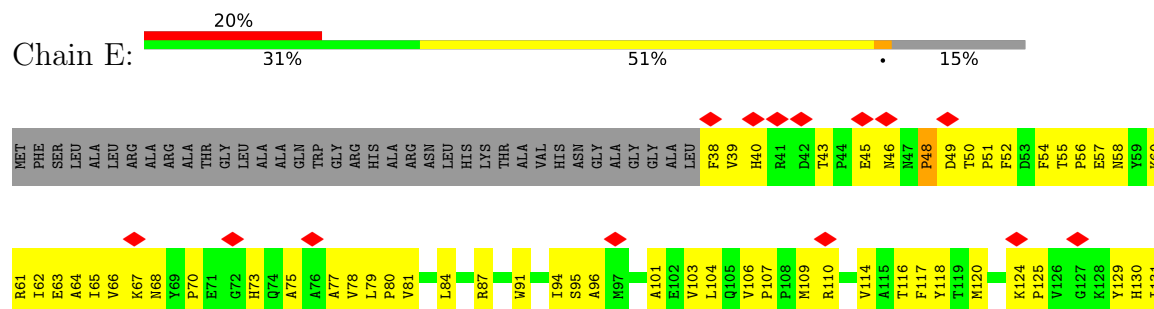
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	q	1	57	38	17	2	0

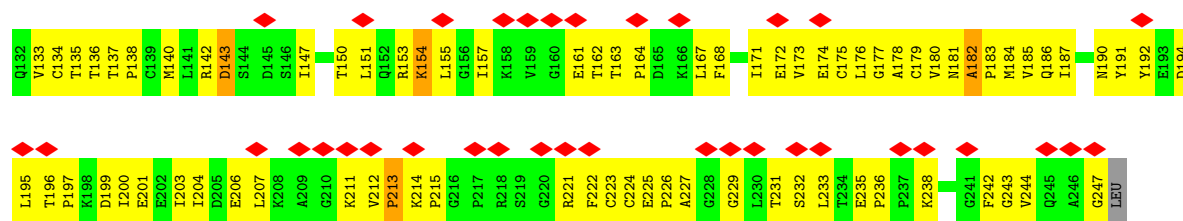


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

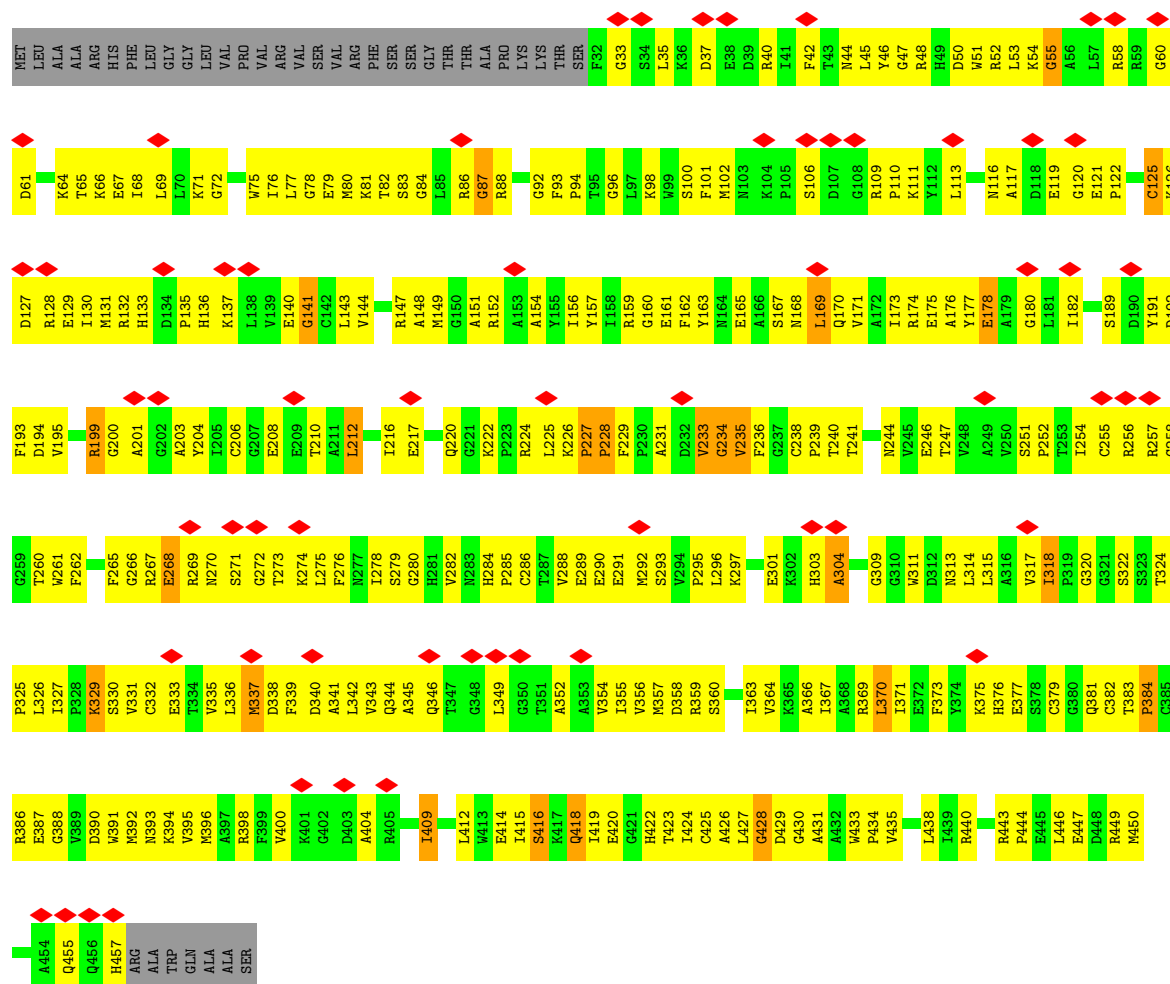


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

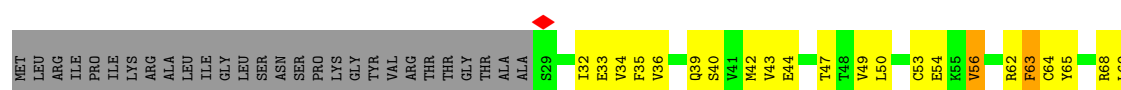


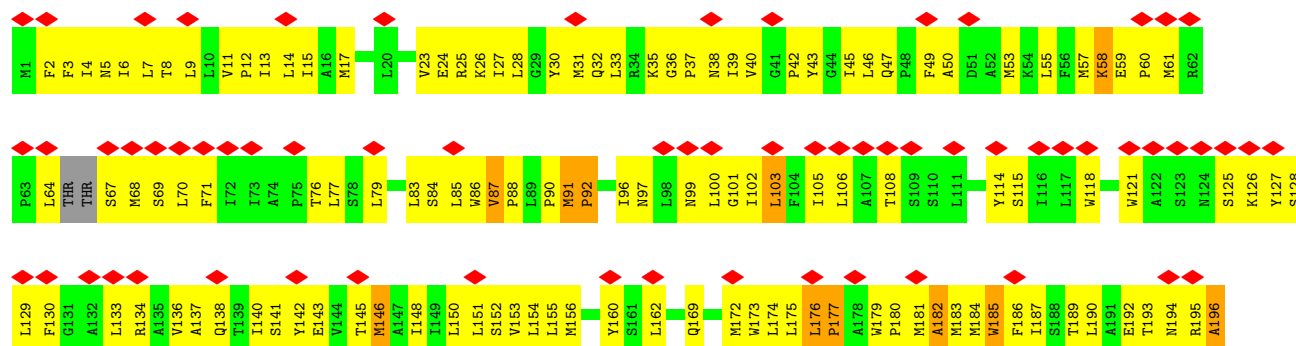
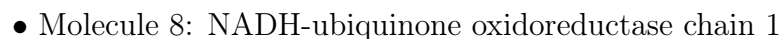


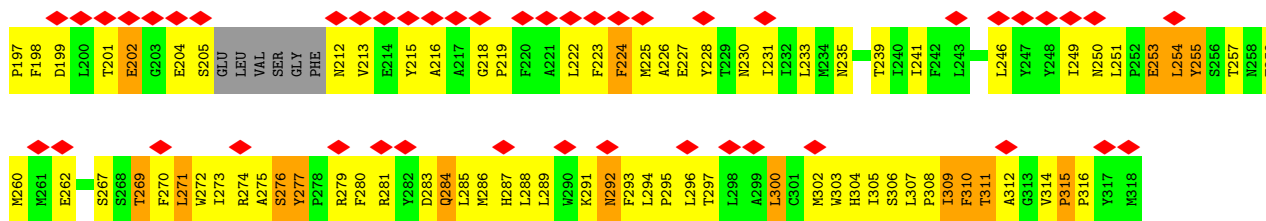
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



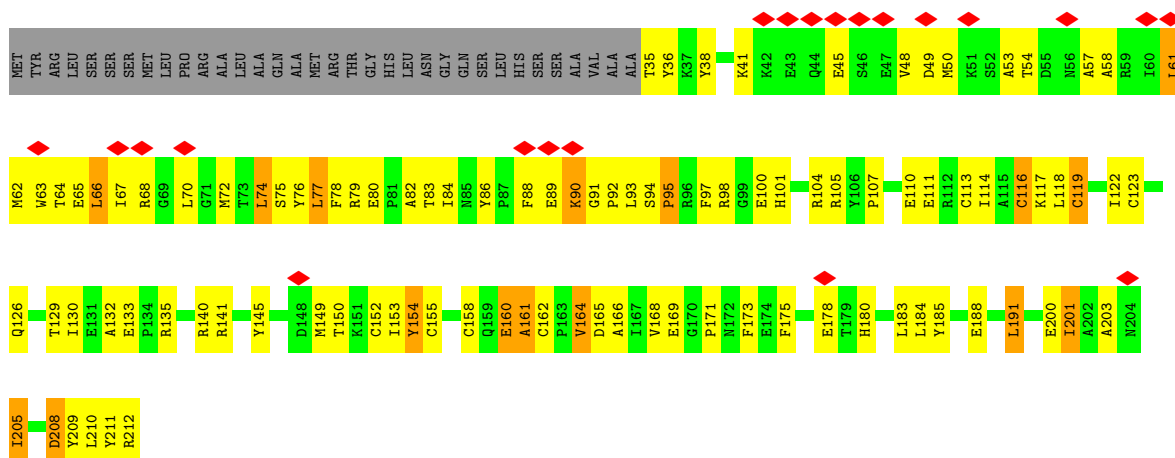
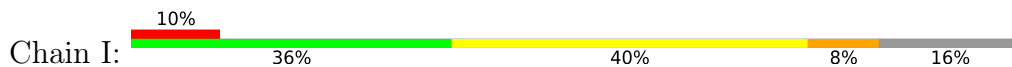
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



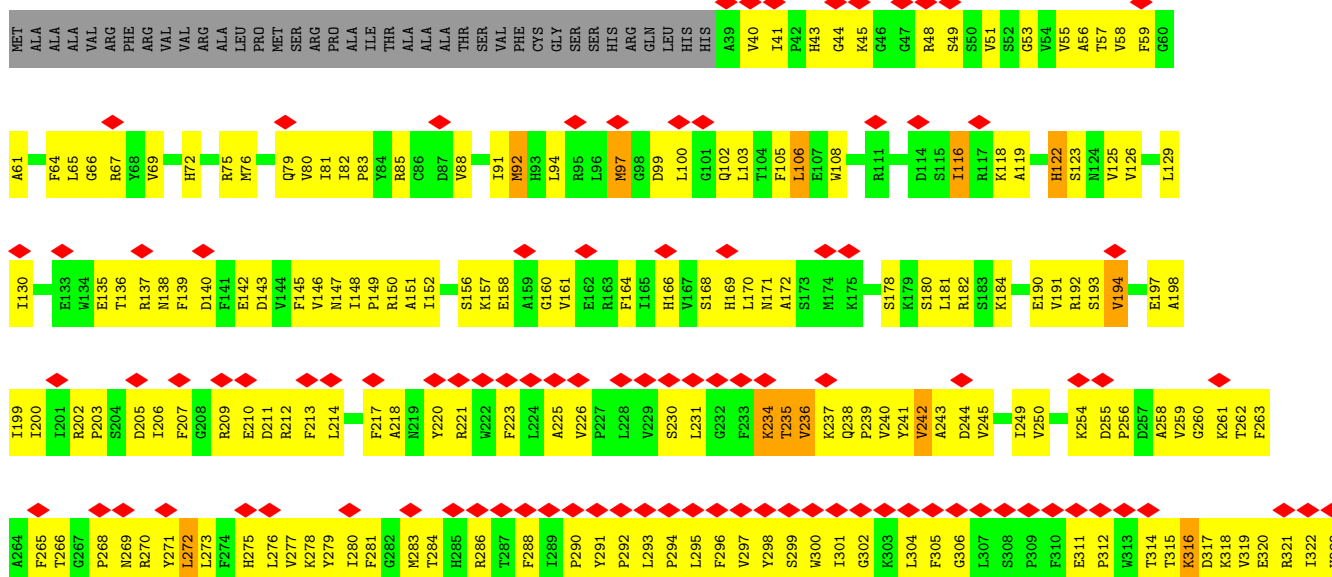




• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

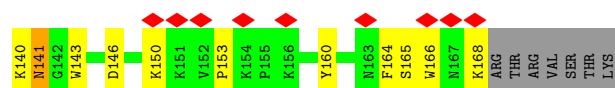
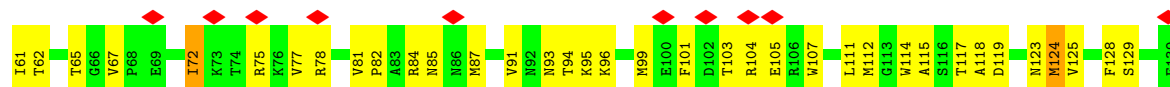
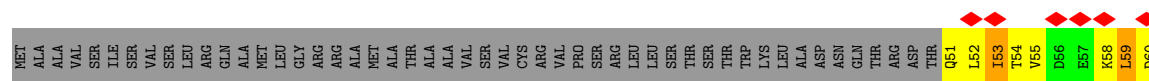


• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial





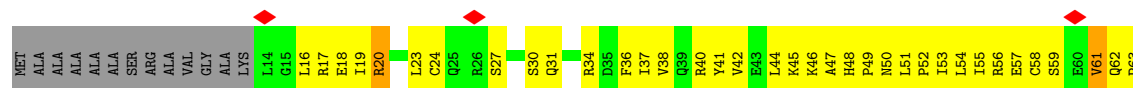
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



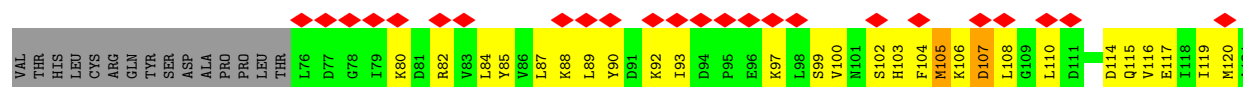
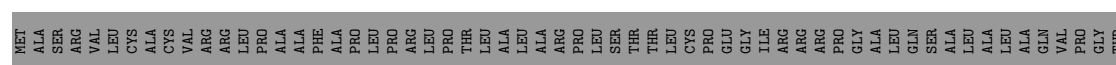
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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

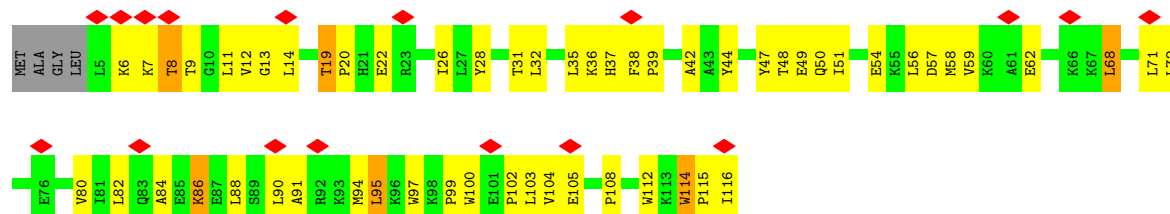


- Molecule 14: Acyl carrier protein, mitochondrial

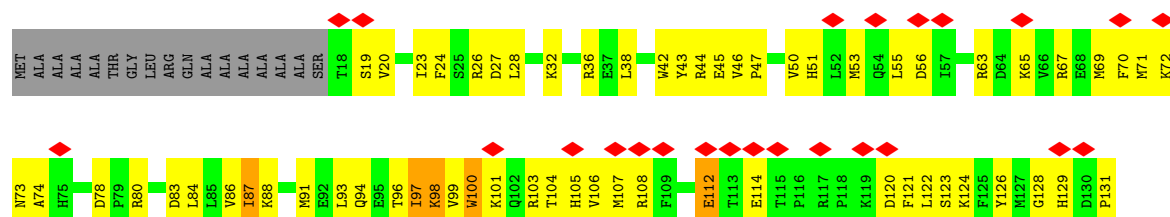




- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



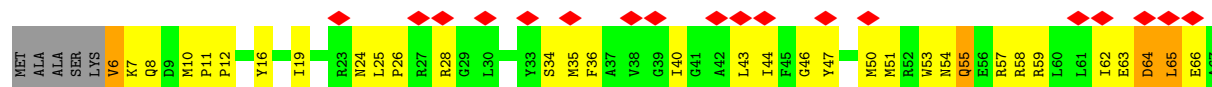
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

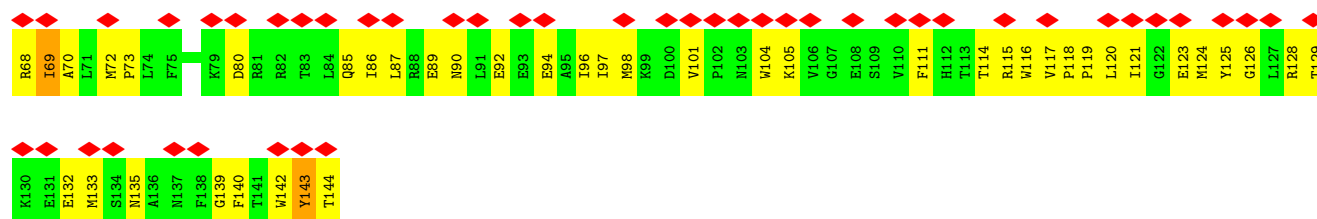


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

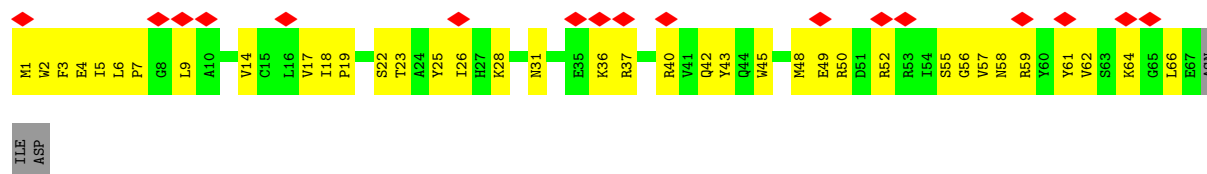


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

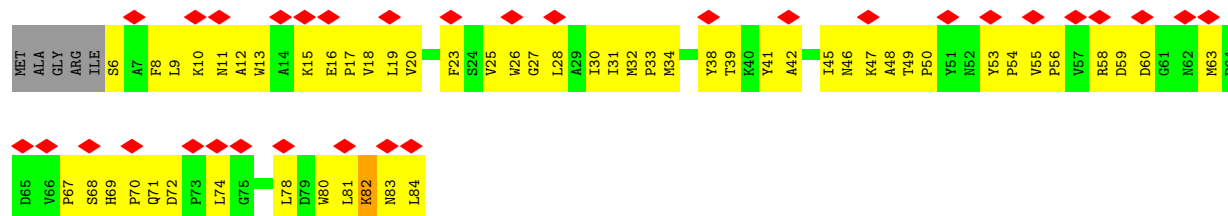




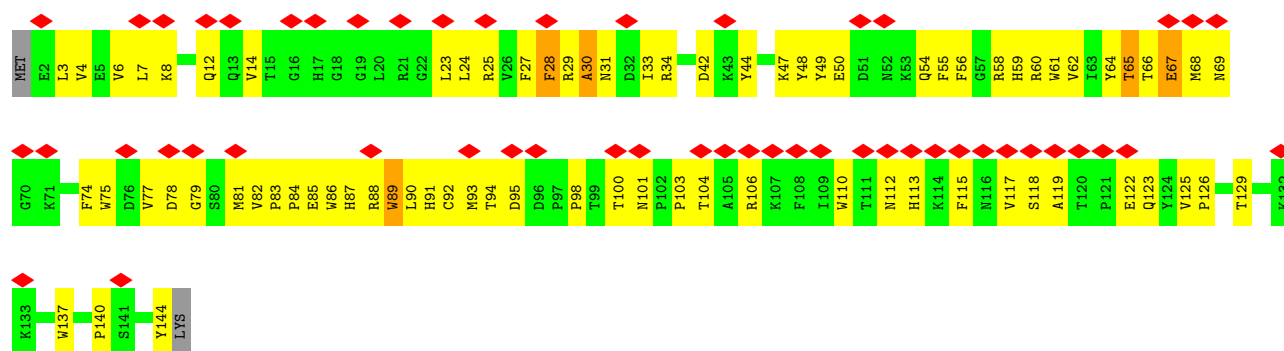
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



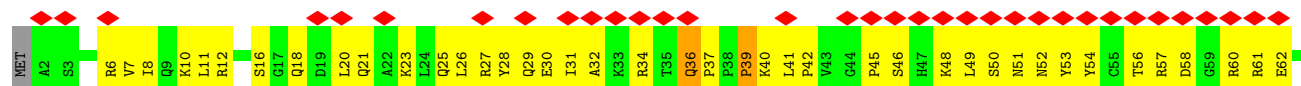
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

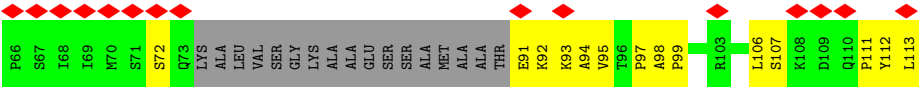


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

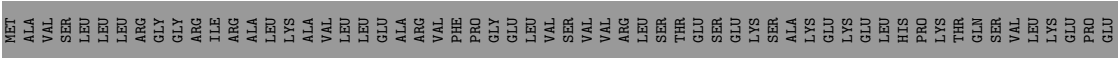


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7





• 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	14488	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.762	Depositor
Minimum map value	-0.854	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.55	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.81	0/763	1.16	7/1042 (0.7%)
2	B	0.93	1/1289 (0.1%)	1.46	20/1744 (1.1%)
3	C	0.88	0/1687	1.26	12/2297 (0.5%)
4	D	0.96	4/3128 (0.1%)	1.49	38/4228 (0.9%)
5	E	0.71	0/1675	1.07	10/2282 (0.4%)
6	F	0.89	5/3363 (0.1%)	1.37	47/4543 (1.0%)
7	G	0.90	8/5374 (0.1%)	1.55	96/7281 (1.3%)
8	H	0.94	2/2553 (0.1%)	1.41	39/3486 (1.1%)
9	I	0.89	0/1461	1.51	20/1974 (1.0%)
10	P	0.75	1/2793 (0.0%)	1.12	18/3787 (0.5%)
11	Q	0.89	1/980 (0.1%)	1.24	8/1324 (0.6%)
12	R	0.66	0/671	0.92	2/903 (0.2%)
13	S	0.87	1/678 (0.1%)	1.37	9/915 (1.0%)
14	T	0.61	0/613	0.91	2/826 (0.2%)
15	V	0.82	0/937	1.38	12/1270 (0.9%)
16	W	0.80	1/993 (0.1%)	1.05	7/1335 (0.5%)
17	X	0.71	0/1191	1.20	13/1605 (0.8%)
18	Z	0.67	1/1183 (0.1%)	1.09	13/1597 (0.8%)
19	a	0.84	0/561	1.11	3/755 (0.4%)
20	b	0.70	0/643	1.01	3/884 (0.3%)
21	q	0.68	0/1234	1.13	10/1681 (0.6%)
22	r	0.61	0/782	1.04	6/1058 (0.6%)
23	s	0.44	0/194	0.69	0/264
All	All	0.84	25/34746 (0.1%)	1.32	395/47081 (0.8%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	234	GLY	CA-C	-10.39	1.40	1.52
6	F	227	PRO	N-CD	10.14	1.61	1.47
6	F	235	VAL	N-CA	-9.69	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	140	ASP	C-O	-7.92	1.14	1.24
11	Q	53	ILE	C-O	7.80	1.33	1.24
8	H	58	LYS	C-N	-7.43	1.21	1.33
7	G	541	PRO	N-CD	-6.76	1.38	1.47
7	G	203	ASP	CA-C	6.73	1.62	1.52
7	G	449	PRO	N-CD	6.69	1.57	1.47
6	F	233	VAL	CA-C	-6.67	1.44	1.52
4	D	140	ASP	CA-C	-6.53	1.44	1.52
7	G	632	ILE	CA-C	-6.46	1.44	1.52
7	G	600	GLU	CA-C	6.42	1.61	1.52
18	Z	63	GLU	C-N	-6.31	1.24	1.33
7	G	127	ASP	CA-C	6.18	1.62	1.52
6	F	384	PRO	N-CD	-6.14	1.39	1.47
2	B	110	PRO	C-O	-6.11	1.16	1.24
4	D	392	PRO	C-O	-5.96	1.20	1.25
7	G	361	VAL	CA-C	5.92	1.60	1.52
8	H	224	PHE	C-N	5.80	1.41	1.33
13	S	95	LEU	CA-C	5.51	1.59	1.52
7	G	683	PRO	N-CD	-5.50	1.40	1.47
16	W	98	LYS	CA-C	-5.41	1.46	1.52
10	P	235	THR	CA-C	5.33	1.59	1.53
4	D	310	VAL	C-O	-5.01	1.16	1.23

All (395) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	174	THR	N-CA-C	-17.51	89.01	114.39
7	G	632	ILE	N-CA-C	-13.65	88.01	107.80
7	G	251	ILE	N-CA-C	13.30	126.79	108.17
6	F	125	CYS	N-CA-C	-12.95	93.43	113.89
7	G	500	ILE	N-CA-C	-12.43	98.84	110.53
2	B	199	GLU	N-CA-C	-12.24	98.02	111.36
10	P	106	LEU	N-CA-C	12.20	128.71	109.07
16	W	98	LYS	N-CA-C	-12.06	89.00	108.41
6	F	171	VAL	N-CA-C	-11.87	99.38	110.53
2	B	80	ASP	N-CA-C	-11.76	98.49	111.07
7	G	204	MET	N-CA-C	-11.64	91.45	109.25
6	F	449	ARG	N-CA-C	-11.59	98.73	111.36
7	G	599	THR	N-CA-C	11.33	126.20	112.38
11	Q	60	ASP	N-CA-C	-11.30	90.37	109.24
8	H	259	PHE	N-CA-C	-11.08	99.28	111.36
7	G	77	MET	N-CA-C	-10.82	97.38	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	105	MET	N-CA-C	-10.82	99.27	111.71
9	I	164	VAL	N-CA-C	-10.61	100.17	113.22
9	I	77	LEU	N-CA-C	-10.51	99.63	111.71
7	G	280	ASP	N-CA-C	10.30	122.51	111.28
7	G	414	PHE	N-CA-C	-10.12	101.43	113.88
9	I	161	ALA	N-CA-C	10.01	122.19	111.28
4	D	114	GLY	N-CA-C	-10.00	100.85	114.95
2	B	195	PRO	N-CA-C	-9.92	98.60	110.70
9	I	166	ALA	N-CA-C	-9.88	100.76	113.12
7	G	325	ARG	N-CA-C	-9.86	100.23	110.97
6	F	141	GLY	N-CA-C	-9.83	101.09	112.50
4	D	311	TYR	N-CA-C	-9.82	98.39	113.02
7	G	654	VAL	N-CA-C	9.78	123.31	111.09
6	F	178	GLU	N-CA-C	-9.76	99.39	111.11
6	F	144	VAL	N-CA-C	-9.71	101.40	110.53
6	F	418	GLN	N-CA-C	-9.60	100.78	111.14
16	W	87	ILE	N-CA-C	-9.54	101.26	110.42
7	G	337	ALA	N-CA-C	-9.54	100.86	114.12
17	X	70	PHE	N-CA-C	-9.47	99.75	111.11
21	q	123	GLN	N-CA-C	9.43	123.91	110.23
18	Z	69	ILE	N-CA-C	-9.28	100.61	110.36
7	G	694	PHE	N-CA-C	9.28	121.39	111.28
7	G	692	LYS	N-CA-C	-9.27	100.55	112.23
7	G	389	THR	N-CA-C	-9.19	96.18	109.96
4	D	323	ARG	N-CA-C	9.14	124.88	112.90
4	D	212	GLU	N-CA-C	-9.10	100.32	111.33
19	a	57	VAL	N-CA-C	-9.05	105.11	113.71
8	H	91	MET	N-CA-C	-9.02	98.47	109.57
18	Z	143	TYR	N-CA-C	8.96	121.93	108.31
7	G	133	GLN	N-CA-CB	8.89	121.66	110.45
2	B	170	TYR	N-CA-C	-8.83	97.79	110.24
7	G	212	LYS	N-CA-C	-8.78	94.58	108.90
7	G	365	ASN	N-CA-C	-8.78	102.13	112.92
9	I	154	TYR	N-CA-CB	-8.68	99.20	111.62
4	D	209	LYS	N-CA-C	-8.65	101.81	111.07
22	r	62	GLU	N-CA-C	-8.58	102.80	113.18
13	S	86	GLU	N-CA-C	-8.57	102.02	111.36
4	D	140	ASP	N-CA-C	-8.43	94.78	108.52
17	X	99	HIS	N-CA-C	-8.42	102.18	111.36
4	D	214	TYR	CB-CA-C	-8.41	97.68	110.88
3	C	108	LYS	N-CA-C	8.38	120.03	111.07
5	E	154	LYS	N-CA-C	-8.35	101.87	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	452	LEU	N-CA-C	-8.35	102.18	111.28
11	Q	54	THR	N-CA-C	8.33	123.29	109.46
7	G	558	GLN	N-CA-C	-8.28	102.21	111.07
7	G	691	ILE	N-CA-C	8.22	123.73	111.89
8	H	196	ALA	N-CA-C	8.20	127.93	109.81
3	C	196	PRO	N-CA-C	8.17	124.89	113.53
1	A	64	LEU	N-CA-C	-8.17	102.33	111.07
7	G	484	ASP	N-CA-C	8.15	121.09	111.71
7	G	500	ILE	N-CA-CB	8.14	121.00	110.57
15	V	86	LYS	N-CA-C	-8.12	102.37	111.14
21	q	118	SER	N-CA-C	8.12	120.85	111.11
9	I	201	ILE	N-CA-C	-8.10	102.54	110.72
7	G	534	VAL	N-CA-C	-8.07	104.72	111.91
1	A	9	ILE	N-CA-C	-8.04	102.42	110.62
13	S	76	THR	N-CA-C	8.04	122.01	108.90
17	X	43	PHE	N-CA-C	-8.00	102.51	111.07
10	P	206	ILE	N-CA-C	7.96	120.96	108.87
8	H	271	LEU	N-CA-C	-7.95	102.55	111.14
7	G	651	PRO	CB-CA-C	-7.94	98.46	111.56
8	H	253	GLU	N-CA-C	7.89	122.01	112.38
15	V	6	LYS	N-CA-C	-7.88	100.13	110.53
9	I	160	GLU	N-CA-C	7.83	124.22	111.37
21	q	28	PHE	N-CA-C	7.83	122.60	112.89
10	P	235	THR	CB-CA-C	-7.81	100.04	112.07
7	G	270	VAL	N-CA-CB	-7.80	100.71	110.31
7	G	389	THR	N-CA-CB	7.78	121.45	109.85
18	Z	143	TYR	CB-CA-C	-7.78	107.60	116.54
9	I	74	LEU	N-CA-C	-7.74	102.84	111.28
4	D	233	HIS	N-CA-C	7.72	119.48	111.14
21	q	89	TRP	N-CA-C	-7.71	102.81	111.14
4	D	184	ILE	N-CA-C	-7.66	102.80	110.62
6	F	58	ARG	N-CA-C	-7.65	103.02	111.36
9	I	119	CYS	N-CA-C	-7.64	103.03	111.36
7	G	56	VAL	N-CA-C	-7.63	103.02	110.72
4	D	257	GLU	N-CA-C	7.62	119.58	111.28
6	F	171	VAL	N-CA-CB	7.59	120.29	110.57
7	G	569	GLN	N-CA-C	7.59	121.98	108.24
22	r	30	GLU	N-CA-C	-7.54	104.98	114.56
9	I	158	CYS	N-CA-C	-7.51	103.09	111.28
7	G	277	MET	N-CA-C	7.49	120.59	109.59
13	S	94	VAL	N-CA-C	7.46	117.58	110.42
7	G	467	LYS	N-CA-C	-7.42	102.35	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	430	GLY	N-CA-C	7.42	121.63	112.73
2	B	80	ASP	N-CA-CB	7.42	120.77	110.01
8	H	309	ILE	N-CA-C	7.40	117.48	110.30
16	W	100	TRP	N-CA-C	-7.39	103.84	114.12
7	G	510	TRP	N-CA-CB	7.38	120.85	109.85
7	G	303	THR	N-CA-C	7.31	122.90	113.18
3	C	195	HIS	CB-CA-C	7.27	117.37	110.17
7	G	661	GLU	N-CA-C	7.25	118.88	110.97
15	V	68	LEU	N-CA-C	-7.25	103.37	111.28
7	G	374	THR	CB-CA-C	-7.23	99.85	111.28
7	G	384	ASN	N-CA-C	-7.23	103.44	111.82
4	D	210	MET	N-CA-C	7.21	119.14	111.28
4	D	177	ILE	N-CA-C	-7.19	103.29	110.62
13	S	20	ARG	N-CA-C	7.16	120.66	107.99
8	H	254	LEU	N-CA-C	-7.15	103.52	111.82
7	G	465	VAL	N-CA-CB	7.15	118.44	110.51
8	H	50	ALA	N-CA-C	7.14	118.71	111.07
6	F	455	GLN	N-CA-C	7.13	118.70	111.07
7	G	461	SER	N-CA-C	7.12	119.95	111.33
4	D	180	ILE	N-CA-C	-7.11	103.37	110.62
7	G	497	VAL	N-CA-C	-7.11	103.37	110.62
4	D	457	VAL	N-CA-C	-7.09	98.19	108.11
4	D	119	GLY	N-CA-C	-7.07	103.48	115.08
9	I	45	GLU	N-CA-C	7.06	120.84	108.56
15	V	95	LEU	N-CA-C	-7.05	103.59	111.28
7	G	217	GLU	N-CA-C	-7.05	101.74	110.41
6	F	169	LEU	N-CA-C	7.02	118.93	111.28
8	H	311	THR	N-CA-C	-7.00	104.31	112.92
8	H	176	LEU	CA-C-N	-6.99	113.60	120.52
8	H	176	LEU	C-N-CA	-6.99	113.60	120.52
7	G	294	TYR	N-CA-C	-6.98	104.58	113.23
10	P	235	THR	CA-C-O	6.98	128.16	121.67
6	F	428	GLY	N-CA-C	-6.98	103.84	112.77
6	F	418	GLN	N-CA-CB	6.97	120.17	110.07
18	Z	34	SER	N-CA-C	-6.96	103.69	111.28
6	F	246	GLU	N-CA-C	-6.96	103.70	111.28
6	F	148	ALA	N-CA-C	-6.94	103.80	111.36
2	B	78	LEU	N-CA-C	6.93	119.86	111.82
7	G	300	GLN	N-CA-CB	6.91	122.51	112.08
7	G	102	ILE	N-CA-C	6.89	119.71	111.09
7	G	362	ASP	N-CA-C	6.89	125.48	110.80
7	G	582	VAL	N-CA-C	6.88	118.39	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	233	VAL	O-C-N	6.88	131.15	123.10
6	F	329	LYS	N-CA-C	6.87	119.65	111.33
12	R	108	GLY	N-CA-C	-6.85	106.01	114.92
6	F	233	VAL	CA-C-O	-6.83	113.22	120.53
7	G	133	GLN	N-CA-C	-6.83	101.18	110.68
8	H	305	ILE	N-CA-C	-6.83	103.36	113.39
8	H	87	VAL	CA-C-N	-6.82	113.17	120.47
8	H	87	VAL	C-N-CA	-6.82	113.17	120.47
8	H	292	ASN	N-CA-C	6.82	118.79	111.36
6	F	244	ASN	N-CA-C	-6.82	100.89	110.50
8	H	300	LEU	N-CA-C	-6.81	104.23	112.54
7	G	268	GLY	N-CA-C	6.81	124.77	115.30
2	B	110	PRO	N-CA-C	6.79	122.82	113.65
10	P	91	ILE	CB-CA-C	-6.79	102.58	111.88
18	Z	63	GLU	O-C-N	-6.74	114.97	122.12
2	B	196	PRO	N-CA-C	-6.72	100.67	111.03
5	E	154	LYS	N-CA-CB	6.72	119.72	109.91
7	G	434	SER	N-CA-C	-6.71	101.03	110.29
4	D	329	ARG	CB-CA-C	6.70	121.92	110.79
8	H	267	SER	N-CA-C	-6.70	104.06	111.36
15	V	114	TRP	N-CA-CB	6.70	120.28	110.30
9	I	208	ASP	N-CA-C	6.67	121.58	113.17
15	V	8	THR	N-CA-C	6.67	118.99	108.79
6	F	344	GLN	N-CA-C	-6.64	103.96	111.07
15	V	86	LYS	N-CA-CB	6.64	119.70	110.07
10	P	116	ILE	N-CA-C	-6.64	104.01	110.72
17	X	129	THR	N-CA-C	6.62	120.82	110.17
3	C	125	PHE	N-CA-CB	-6.61	100.65	110.17
6	F	228	PRO	N-CA-C	-6.60	98.88	112.47
7	G	601	GLY	N-CA-C	6.59	124.79	115.30
11	Q	141	ASN	N-CA-CB	6.59	120.81	110.46
7	G	287	SER	N-CA-C	6.57	119.20	110.53
2	B	79	ASP	N-CA-C	-6.56	103.62	111.69
18	Z	65	LEU	N-CA-C	-6.56	104.21	111.36
7	G	435	PRO	N-CA-C	-6.53	100.25	110.50
6	F	234	GLY	CA-C-N	-6.52	111.77	120.50
6	F	234	GLY	C-N-CA	-6.52	111.77	120.50
9	I	66	LEU	N-CA-C	-6.51	104.26	111.36
2	B	154	GLU	CA-C-N	-6.51	112.43	119.98
2	B	154	GLU	C-N-CA	-6.51	112.43	119.98
9	I	205	ILE	N-CA-C	-6.49	104.16	110.72
7	G	605	GLN	N-CA-C	6.48	119.09	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	92	MET	N-CA-C	-6.48	104.26	111.71
4	D	237	PRO	N-CA-C	-6.47	101.70	111.41
7	G	250	SER	N-CA-C	6.47	116.82	108.34
3	C	125	PHE	N-CA-C	6.47	119.62	110.50
8	H	177	PRO	N-CA-C	-6.46	101.50	111.13
8	H	182	ALA	N-CA-C	-6.46	104.16	111.07
4	D	149	GLN	N-CA-C	-6.45	105.56	113.50
6	F	370	LEU	N-CA-C	-6.44	104.34	111.36
8	H	255	TYR	N-CA-CB	6.44	119.35	110.01
6	F	178	GLU	N-CA-CB	6.43	119.52	109.94
15	V	49	GLU	N-CA-C	-6.41	104.30	111.28
17	X	98	ARG	N-CA-C	6.39	120.34	112.54
7	G	273	ILE	N-CA-C	-6.38	98.33	107.77
15	V	91	ALA	N-CA-C	-6.36	104.35	111.28
2	B	135	GLY	CA-C-O	-6.36	117.87	122.45
14	T	107	ASP	N-CA-C	6.33	122.84	110.56
4	D	302	LEU	N-CA-C	-6.33	105.42	113.01
11	Q	59	LEU	N-CA-C	-6.32	100.81	110.30
15	V	71	LEU	N-CA-C	6.32	118.17	111.28
6	F	415	ILE	N-CA-C	-6.31	104.35	110.72
17	X	99	HIS	N-CA-CB	6.31	119.50	110.16
7	G	176	CYS	N-CA-C	6.31	119.63	110.42
8	H	271	LEU	N-CA-CB	6.31	119.22	110.07
5	E	50	THR	N-CA-CB	6.29	121.57	110.37
6	F	144	VAL	N-CA-CB	6.28	118.61	110.57
8	H	269	THR	N-CA-C	6.28	118.13	111.28
19	a	26	ILE	N-CA-C	-6.27	104.54	113.07
11	Q	141	ASN	N-CA-C	-6.27	105.64	113.28
5	E	182	ALA	CA-C-N	-6.25	112.73	119.98
5	E	182	ALA	C-N-CA	-6.25	112.73	119.98
6	F	255	CYS	N-CA-C	-6.25	104.55	111.36
21	q	65	THR	N-CA-C	6.24	118.09	110.41
10	P	118	LYS	N-CA-C	6.23	119.05	111.82
18	Z	69	ILE	N-CA-CB	6.22	117.41	110.51
7	G	383	SER	N-CA-C	-6.22	106.92	114.75
16	W	97	ILE	CB-CA-C	-6.21	104.41	111.55
7	G	356	ASP	N-CA-CB	6.20	119.24	110.12
2	B	98	ALA	N-CA-C	6.18	117.71	108.31
7	G	451	ILE	N-CA-C	-6.18	104.97	113.00
7	G	420	LYS	N-CA-C	6.15	118.78	111.33
7	G	325	ARG	N-CA-CB	6.14	118.88	109.91
7	G	418	ILE	N-CA-C	-6.14	103.44	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	122	LYS	N-CA-C	-6.13	105.96	113.50
6	F	212	LEU	N-CA-C	-6.13	104.60	111.28
13	S	61	VAL	N-CA-C	-6.12	99.67	108.42
8	H	76	THR	N-CA-C	-6.12	104.61	111.28
8	H	276	SER	N-CA-C	6.11	118.91	111.82
16	W	99	VAL	N-CA-C	6.09	117.18	107.98
6	F	304	ALA	CB-CA-C	-6.08	109.54	116.54
8	H	185	TRP	N-CA-C	-6.08	104.00	112.45
18	Z	65	LEU	N-CA-CB	6.06	119.14	110.16
6	F	268	GLU	CB-CA-C	-6.06	109.57	116.54
7	G	353	ALA	N-CA-C	-6.06	104.60	112.23
13	S	87	VAL	N-CA-C	-6.05	104.44	110.62
1	A	101	GLY	N-CA-C	-6.04	105.50	112.50
4	D	258	VAL	N-CA-C	-6.04	103.35	111.44
21	q	104	THR	N-CA-C	6.02	118.44	109.59
8	H	103	LEU	N-CA-C	-6.01	104.81	111.36
7	G	508	ALA	N-CA-C	6.00	117.82	111.28
4	D	444	LEU	N-CA-C	-6.00	104.74	111.28
4	D	427	PRO	N-CA-C	-6.00	100.12	112.47
4	D	414	ASP	N-CA-C	-5.96	101.11	110.36
20	b	60	ASP	N-CA-C	-5.96	105.26	112.54
7	G	387	LEU	CB-CA-C	-5.95	101.68	111.68
17	X	38	LYS	N-CA-C	-5.95	104.70	111.07
7	G	480	ALA	N-CA-C	-5.93	104.90	111.36
17	X	141	PRO	N-CA-C	-5.92	102.53	111.41
6	F	127	ASP	N-CA-C	5.89	118.48	111.71
9	I	116	CYS	N-CA-C	-5.88	105.60	112.89
16	W	98	LYS	N-CA-CB	5.88	119.56	110.21
8	H	224	PHE	CA-C-N	-5.87	112.42	120.28
8	H	224	PHE	C-N-CA	-5.87	112.42	120.28
2	B	98	ALA	CB-CA-C	-5.83	109.83	116.54
8	H	315	PRO	O-C-N	5.83	123.89	121.15
10	P	122	HIS	N-CA-C	5.83	120.09	112.92
22	r	11	LEU	N-CA-C	-5.82	104.85	111.14
17	X	97	PHE	N-CA-C	5.82	118.57	111.82
7	G	672	ALA	N-CA-C	-5.81	104.95	111.28
13	S	86	GLU	N-CA-CB	5.80	118.75	110.16
15	V	19	THR	N-CA-CB	5.80	120.69	110.37
3	C	209	LEU	N-CA-CB	-5.79	100.75	110.83
21	q	100	THR	N-CA-C	5.79	117.26	111.07
4	D	337	MET	N-CA-C	-5.78	104.98	111.28
7	G	289	LYS	N-CA-C	5.78	117.58	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	212	GLU	N-CA-CB	5.77	118.72	110.06
10	P	97	MET	N-CA-C	-5.77	102.36	110.50
22	r	72	SER	N-CA-C	-5.74	106.11	113.23
17	X	36	CYS	CB-CA-C	-5.73	102.63	111.74
10	P	234	LYS	CB-CA-C	-5.72	103.44	111.80
10	P	272	LEU	N-CA-C	-5.72	101.82	110.28
6	F	393	ASN	N-CA-C	-5.71	104.95	111.07
4	D	192	LEU	N-CA-C	-5.71	105.06	111.28
7	G	615	LEU	N-CA-C	-5.70	106.30	113.20
12	R	44	ARG	N-CA-C	-5.70	106.03	112.87
6	F	416	SER	N-CA-C	5.68	117.93	111.11
10	P	119	ALA	N-CA-C	-5.68	105.01	111.14
13	S	73	GLN	N-CA-C	-5.68	100.45	109.59
6	F	176	ALA	N-CA-C	5.64	118.16	111.33
9	I	191	LEU	N-CA-C	-5.62	105.23	111.36
6	F	409	ILE	N-CA-C	5.61	116.34	110.62
7	G	599	THR	CA-C-N	-5.60	114.21	122.83
7	G	599	THR	C-N-CA	-5.60	114.21	122.83
7	G	530	TYR	N-CA-C	-5.59	102.01	110.28
4	D	455	ASP	CB-CA-C	-5.58	103.96	111.89
6	F	457	HIS	N-CA-CB	-5.58	101.01	110.50
19	a	25	TYR	N-CA-C	-5.56	107.74	114.75
17	X	40	ASN	N-CA-C	-5.56	104.91	110.97
11	Q	124	MET	CA-C-N	-5.53	115.12	122.98
11	Q	124	MET	C-N-CA	-5.53	115.12	122.98
7	G	127	ASP	CA-C-O	5.52	129.01	121.89
8	H	202	GLU	N-CA-C	-5.51	106.61	113.38
5	E	223	CYS	CB-CA-C	-5.49	110.22	116.54
4	D	350	LYS	CB-CA-C	-5.48	103.79	111.85
18	Z	55	GLN	N-CA-C	-5.48	105.31	111.28
7	G	420	LYS	N-CA-CB	-5.46	101.87	110.06
17	X	113	ASP	N-CA-C	-5.46	106.56	113.43
7	G	404	GLY	N-CA-C	5.44	121.43	113.48
7	G	682	ASP	CA-C-N	-5.44	114.16	119.76
7	G	682	ASP	C-N-CA	-5.44	114.16	119.76
7	G	313	LEU	N-CA-C	5.44	118.42	109.72
4	D	200	PHE	CA-CB-CG	5.44	119.24	113.80
2	B	155	PRO	N-CA-C	-5.43	102.15	110.95
2	B	104	MET	N-CA-C	-5.42	107.21	113.88
7	G	363	SER	N-CA-C	-5.42	100.34	109.07
7	G	510	TRP	N-CA-C	-5.40	101.86	109.96
2	B	146	ARG	N-CA-C	-5.40	105.40	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	255	ILE	N-CA-C	-5.40	105.27	110.72
18	Z	50	MET	N-CA-C	-5.39	105.40	111.28
2	B	105	MET	N-CA-CB	5.38	118.51	110.22
4	D	186	ALA	N-CA-C	5.35	117.12	111.28
21	q	30	ALA	N-CA-CB	5.35	118.51	110.53
4	D	131	GLN	CB-CA-C	5.35	120.28	110.11
6	F	199	ARG	N-CA-C	5.35	117.45	109.59
8	H	284	GLN	N-CA-C	-5.33	105.55	111.36
6	F	84	GLY	N-CA-C	-5.33	107.89	115.30
18	Z	64	ASP	N-CA-C	5.33	119.84	113.23
5	E	48	PRO	N-CA-C	5.33	120.77	113.84
7	G	449	PRO	N-CA-CB	5.32	109.14	103.39
4	D	312	ASP	N-CA-C	-5.30	106.98	113.50
5	E	143	ASP	N-CA-C	5.28	118.41	111.28
9	I	160	GLU	N-CA-CB	-5.28	100.74	109.72
11	Q	72	ILE	N-CA-C	-5.28	108.35	113.53
6	F	318	ILE	CA-C-N	5.26	124.89	119.05
6	F	318	ILE	C-N-CA	5.26	124.89	119.05
21	q	67	GLU	N-CA-CB	-5.26	102.20	110.77
6	F	55	GLY	N-CA-C	-5.24	106.43	112.83
7	G	111	LYS	N-CA-C	-5.24	105.62	112.23
8	H	46	LEU	N-CA-C	-5.24	106.66	113.16
7	G	362	ASP	CA-CB-CG	5.24	117.84	112.60
5	E	48	PRO	CB-CA-C	-5.24	104.42	111.85
7	G	356	ASP	N-CA-C	-5.23	105.58	111.28
8	H	310	PHE	N-CA-C	5.23	119.28	113.01
4	D	369	ALA	N-CA-C	5.23	116.98	111.28
7	G	277	MET	N-CA-CB	-5.22	101.66	109.71
7	G	713	ALA	N-CA-C	-5.22	105.48	111.07
10	P	260	GLY	N-CA-C	-5.22	108.42	115.36
18	Z	118	PRO	CA-C-N	-5.22	113.94	120.51
18	Z	118	PRO	C-N-CA	-5.22	113.94	120.51
15	V	84	ALA	N-CA-C	5.22	116.65	111.07
17	X	33	GLY	N-CA-C	-5.21	107.85	114.16
10	P	339	GLY	N-CA-C	5.21	122.50	115.00
7	G	458	GLY	N-CA-C	-5.20	108.15	115.32
7	G	435	PRO	CB-CA-C	-5.20	105.90	111.56
13	S	85	ASP	N-CA-C	5.20	117.85	111.82
7	G	600	GLU	CB-CA-C	-5.19	103.01	111.06
8	H	146	MET	N-CA-C	-5.19	105.52	111.07
10	P	194	VAL	N-CA-CB	5.19	118.37	110.58
7	G	556	THR	N-CA-C	-5.19	101.52	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	103	GLY	N-CA-C	-5.17	100.92	113.18
8	H	277	TYR	N-CA-C	5.17	118.02	110.10
2	B	167	GLY	N-CA-C	-5.17	106.17	112.68
3	C	164	TRP	N-CA-C	5.17	116.99	111.36
22	r	18	GLN	N-CA-C	5.17	117.24	109.23
20	b	82	LYS	N-CA-C	-5.16	103.72	110.53
7	G	63	PHE	CA-C-O	-5.16	115.07	121.06
3	C	79	CYS	N-CA-C	-5.16	107.05	113.19
22	r	36	GLN	N-CA-C	-5.15	102.54	110.01
7	G	172	ILE	N-CA-C	-5.14	98.65	109.34
20	b	63	MET	N-CA-C	5.13	118.91	109.10
8	H	101	GLY	N-CA-C	5.13	118.45	112.50
3	C	156	VAL	N-CA-C	-5.12	104.10	111.17
6	F	60	GLY	N-CA-C	-5.12	105.97	114.48
8	H	196	ALA	CA-C-N	-5.12	113.53	119.47
8	H	196	ALA	C-N-CA	-5.12	113.53	119.47
9	I	95	PRO	N-CA-C	5.11	121.22	113.81
1	A	2	ASN	CA-C-N	-5.11	113.04	120.29
1	A	2	ASN	C-N-CA	-5.11	113.04	120.29
10	P	198	ALA	N-CA-C	-5.11	100.20	108.52
9	I	61	LEU	N-CA-C	5.10	116.65	111.14
1	A	73	LEU	CA-C-N	-5.10	114.46	120.12
1	A	73	LEU	C-N-CA	-5.10	114.46	120.12
6	F	337	MET	CB-CA-C	-5.09	103.00	111.41
7	G	280	ASP	N-CA-CB	-5.09	102.64	110.12
16	W	112	GLU	N-CA-C	5.08	116.90	111.36
7	G	569	GLN	CB-CA-C	-5.08	104.34	112.05
4	D	224	ALA	CA-C-O	-5.07	115.47	120.90
7	G	387	LEU	N-CA-C	-5.07	98.45	107.98
14	T	105	MET	N-CA-C	-5.07	105.75	111.28
3	C	221	GLU	N-CA-C	-5.07	102.37	108.25
7	G	203	ASP	CA-C-O	5.07	127.20	121.32
6	F	366	ALA	N-CA-C	-5.06	105.45	110.97
8	H	254	LEU	N-CA-CB	5.06	118.12	110.28
6	F	87	GLY	N-CA-C	5.05	118.36	112.50
21	q	89	TRP	N-CA-CB	5.05	117.39	110.07
7	G	393	GLY	N-CA-C	-5.04	107.79	115.66
3	C	109	SER	N-CA-C	5.03	118.00	109.76
3	C	186	ILE	CB-CA-C	-5.03	107.44	111.71
5	E	213	PRO	CB-CA-C	-5.02	106.31	112.89
9	I	90	LYS	N-CA-C	5.02	117.58	109.40
4	D	232	VAL	CA-C-O	-5.02	116.35	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	236	VAL	N-CA-C	-5.01	102.35	109.51

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	743	0	801	67	0
2	B	1258	0	1269	138	0
3	C	1641	0	1596	164	0
4	D	3056	0	3028	294	0
5	E	1635	0	1624	148	0
6	F	3288	0	3243	367	0
7	G	5287	0	5323	564	0
8	H	2479	0	2568	357	0
9	I	1431	0	1385	180	0
10	P	2720	0	2740	240	0
11	Q	957	0	949	73	0
12	R	660	0	639	62	0
13	S	667	0	683	68	0
14	T	604	0	596	66	0
15	V	915	0	954	97	0
16	W	970	0	991	88	0
17	X	1164	0	1154	109	0
18	Z	1152	0	1148	108	0
19	a	548	0	562	42	0
20	b	620	0	617	95	0
21	q	1192	0	1145	89	0
22	r	764	0	789	85	0
23	s	189	0	181	20	0
24	A	46	0	69	3	0
24	H	46	0	69	10	0
24	b	46	0	69	13	0
25	B	8	0	0	2	0
25	F	8	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	G	16	0	0	3	0
25	I	16	0	0	15	0
26	E	4	0	0	3	0
26	G	4	0	0	6	0
27	F	31	0	19	3	0
28	H	35	0	43	16	0
29	I	47	0	71	10	0
29	q	35	0	44	6	0
30	P	48	0	26	2	0
31	R	1	0	0	0	0
32	W	32	0	0	0	0
33	q	57	0	58	8	0
All	All	34420	0	34453	2921	0

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

All (2921) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.22
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.28	1.21
8:H:64:LEU:CD2	10:P:359:TYR:HB2	1.72	1.20
4:D:97:LEU:CD2	4:D:99:LEU:HD21	1.74	1.18
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.17
15:V:44:TYR:CE1	15:V:48:THR:HG21	1.77	1.17
8:H:251:LEU:HD12	8:H:251:LEU:O	1.42	1.17
6:F:379:CYS:SG	25:F:502:SF4:FE4	1.38	1.14
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.13
4:D:97:LEU:CG	4:D:99:LEU:HD21	1.78	1.13
8:H:212:ASN:ND2	28:H:401:UQ9:H4M	1.62	1.12
3:C:203:LEU:HD11	4:D:123:LEU:HD23	1.30	1.11
18:Z:144:THR:HG21	19:a:48:MET:SD	1.90	1.11
21:q:59:HIS:ND1	21:q:60:ARG:HG3	1.64	1.11
4:D:97:LEU:HG	4:D:99:LEU:HD21	1.31	1.11
9:I:123:CYS:SG	25:I:302:SF4:FE1	1.42	1.11
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.22	1.10
12:R:80:ASP:OD2	12:R:84:GLY:HA2	1.49	1.10
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.64	1.10
18:Z:144:THR:CG2	19:a:48:MET:SD	2.38	1.10
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:104:PHE:HZ	14:T:115:GLN:HG2	1.08	1.09
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.32	1.09
4:D:97:LEU:HG	4:D:99:LEU:CD2	1.82	1.08
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.08
9:I:152:CYS:SG	25:I:302:SF4:FE2	1.43	1.08
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.35	1.08
7:G:399:VAL:HG21	7:G:462:PHE:CZ	1.88	1.07
8:H:64:LEU:HD21	10:P:359:TYR:CB	1.82	1.07
3:C:102:HIS:HE1	15:V:48:THR:HG22	0.96	1.07
7:G:353:ALA:HA	7:G:636:TYR:OH	1.54	1.07
10:P:299:SER:HB3	10:P:316:LYS:HE3	1.37	1.07
3:C:102:HIS:CE1	15:V:48:THR:HG22	1.88	1.07
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.06
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.06
15:V:44:TYR:CE1	15:V:48:THR:CG2	2.39	1.06
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.38	1.05
5:E:247:GLY:HA2	6:F:64:LYS:HE2	1.36	1.05
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.05
3:C:241:PHE:CD2	22:r:61:ARG:HB2	1.91	1.04
8:H:64:LEU:HD21	10:P:359:TYR:HB2	1.08	1.04
9:I:208:ASP:O	9:I:208:ASP:OD1	1.76	1.04
16:W:101:LYS:HG3	16:W:105:HIS:HB2	1.34	1.04
4:D:238:LEU:HD13	9:I:211:TYR:OH	1.55	1.03
10:P:272:LEU:HG	10:P:375:VAL:HG21	1.36	1.03
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.22	1.03
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.03
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.42	1.02
14:T:104:PHE:CZ	14:T:115:GLN:HG2	1.94	1.01
17:X:48:TRP:CE2	20:b:55:VAL:HG22	1.94	1.01
5:E:247:GLY:CA	6:F:64:LYS:HE2	1.89	1.01
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.75	1.01
8:H:187:ILE:HD12	24:H:402:3PE:H251	1.42	1.01
4:D:259:GLU:HG3	18:Z:25:LEU:HD11	1.43	1.00
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	1.00
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.87	1.00
3:C:241:PHE:HD2	22:r:61:ARG:HB2	1.24	0.99
21:q:78:ASP:OD1	21:q:81:MET:HG3	1.61	0.99
14:T:102:SER:O	14:T:141:PRO:HD3	1.62	0.99
15:V:44:TYR:CZ	15:V:48:THR:HG21	1.97	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:86:ILE:HG23	18:Z:128:ARG:HE	1.24	0.99
7:G:401:LEU:HD11	7:G:466:LEU:HD21	1.39	0.99
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.99
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.99
7:G:401:LEU:HD11	7:G:462:PHE:CE2	1.98	0.98
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	0.98
9:I:113:CYS:SG	25:I:303:SF4:FE3	1.55	0.98
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.98
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.98
9:I:155:CYS:SG	25:I:302:SF4:FE4	1.55	0.97
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.79	0.97
10:P:363:SER:HB3	16:W:51:HIS:CE1	1.98	0.97
4:D:128:THR:HG22	4:D:131:GLN:HG2	1.45	0.97
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.97
3:C:203:LEU:HD21	4:D:123:LEU:HD21	1.47	0.97
4:D:376:GLU:HG3	7:G:121:LEU:HD12	1.47	0.96
7:G:399:VAL:HG21	7:G:462:PHE:HZ	1.30	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.04	0.96
16:W:55:LEU:HB3	16:W:107:MET:CE	1.94	0.96
17:X:132:LYS:HB3	20:b:59:ASP:HB2	1.48	0.96
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.96
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.96
21:q:59:HIS:CE1	21:q:60:ARG:HG3	2.00	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.95
6:F:379:CYS:HG	25:F:502:SF4:FE4	0.65	0.95
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.95
8:H:212:ASN:HD21	28:H:401:UQ9:C4M	1.79	0.95
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.95
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.95
8:H:212:ASN:ND2	28:H:401:UQ9:C4M	2.30	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.94
3:C:102:HIS:HE1	15:V:48:THR:CG2	1.80	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.94
6:F:318:ILE:HG22	6:F:326:LEU:HB3	1.50	0.94
6:F:318:ILE:HD11	6:F:355:ILE:HD12	1.47	0.94
14:T:104:PHE:HE1	14:T:115:GLN:HB2	1.32	0.93
4:D:128:THR:CG2	4:D:131:GLN:HG2	1.98	0.93
4:D:238:LEU:HD11	22:r:39:PRO:HB3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:147:ARG:HD3	6:F:191:TYR:CD2	2.02	0.93
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.92
21:q:25:ARG:O	21:q:29:ARG:HG2	1.69	0.92
6:F:382:CYS:SG	25:F:502:SF4:FE3	1.60	0.92
3:C:203:LEU:HD11	4:D:123:LEU:CD2	2.00	0.92
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.05	0.91
4:D:129:TYR:HE1	4:D:411:LEU:HD21	1.36	0.91
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.91
16:W:55:LEU:HB3	16:W:107:MET:HE1	1.52	0.91
4:D:361:ALA:O	4:D:384:LEU:HD11	1.71	0.91
7:G:399:VAL:CG2	7:G:462:PHE:HZ	1.82	0.91
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.36	0.91
22:r:12:ARG:HB3	22:r:20:LEU:HD21	1.48	0.91
2:B:111:ARG:HB3	4:D:208:GLU:OE1	1.71	0.91
4:D:97:LEU:HD11	4:D:109:CYS:HB3	1.51	0.90
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.53	0.90
7:G:78:CYS:SG	26:G:803:FES:FE2	1.63	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
9:I:67:ILE:HG13	29:I:301:PC1:H251	1.53	0.90
18:Z:87:LEU:HD21	18:Z:119:PRO:HG3	1.53	0.90
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.33	0.90
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.06	0.90
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.90
18:Z:111:PHE:CZ	18:Z:117:VAL:HG21	2.06	0.90
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.01	0.90
6:F:110:PRO:HB3	6:F:152:ARG:CZ	2.02	0.90
6:F:424:ILE:HD11	7:G:73:GLY:O	1.72	0.90
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.53	0.89
8:H:212:ASN:HD21	28:H:401:UQ9:H4M	1.27	0.89
2:B:100:CYS:HB2	2:B:134:ALA:HB1	1.53	0.89
4:D:451:ILE:HG23	4:D:456:ILE:HD11	1.52	0.89
6:F:266:GLY:HA3	6:F:271:SER:HA	1.54	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
7:G:226:CYS:HG	25:G:802:SF4:FE1	0.87	0.89
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.89
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.55	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.88
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.88
2:B:202:LEU:HD23	9:I:86:TYR:CG	2.08	0.88
6:F:314:LEU:HD11	6:F:317:VAL:HG23	1.55	0.88
9:I:152:CYS:HG	25:I:302:SF4:FE2	0.77	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.38	0.88
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.88
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.08	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.56	0.88
10:P:363:SER:HB3	16:W:51:HIS:NE2	1.86	0.88
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.53	0.88
10:P:333:PRO:HB2	10:P:337:ASP:HB2	1.53	0.88
1:A:3:LEU:HD23	24:A:401:3PE:H251	1.56	0.88
3:C:98:PHE:CA	15:V:90:LEU:HD11	2.04	0.88
5:E:134:CYS:HG	26:E:301:FES:FE1	0.68	0.88
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.57	0.88
3:C:240:ALA:HB1	22:r:61:ARG:HD2	1.56	0.88
4:D:146:CYS:SG	4:D:178:THR:OG1	2.32	0.88
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.55	0.88
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.74	0.88
28:H:401:UQ9:H10	28:H:401:UQ9:C6	2.04	0.87
7:G:176:CYS:HG	25:G:802:SF4:FE4	0.66	0.87
6:F:225:LEU:H	11:Q:160:TYR:HE2	1.21	0.87
10:P:296:PHE:CE1	10:P:297:VAL:HG23	2.10	0.87
2:B:91:TRP:CH2	28:H:401:UQ9:H10A	2.09	0.87
2:B:155:PRO:HD3	8:H:59:GLU:HG2	1.55	0.87
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.57	0.87
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.55	0.87
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.88	0.86
14:T:104:PHE:HZ	14:T:115:GLN:CG	1.88	0.86
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.40	0.86
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.86
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.86
8:H:183:MET:HE2	29:I:301:PC1:H2A1	1.56	0.86
4:D:101:LEU:HD23	4:D:106:VAL:HG22	1.57	0.86
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.40	0.86
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.86
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.86
16:W:55:LEU:HD22	16:W:107:MET:HE2	1.58	0.86
6:F:288:VAL:HG21	6:F:303:HIS:HD2	1.41	0.85
7:G:607:LYS:HG3	11:Q:78:ARG:HH12	1.41	0.85
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.85
12:R:72:VAL:HG11	12:R:77:ILE:HD12	1.59	0.85
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.85
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.59	0.84
14:T:117:GLU:HA	14:T:120:MET:HE3	1.60	0.84
3:C:203:LEU:HD21	4:D:123:LEU:CD2	2.06	0.84
6:F:425:CYS:SG	25:F:502:SF4:FE1	1.68	0.84
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.58	0.84
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.84
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.58	0.84
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.84
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.84
14:T:104:PHE:CZ	14:T:115:GLN:CG	2.61	0.84
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.91	0.84
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.83
9:I:123:CYS:HG	25:I:302:SF4:FE1	0.57	0.83
9:I:162:CYS:SG	25:I:303:SF4:FE4	1.71	0.83
14:T:104:PHE:HD1	14:T:110:LEU:HB3	1.41	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.83
4:D:271:ARG:HD2	8:H:281:ARG:CG	2.09	0.83
14:T:93:ILE:HD11	14:T:110:LEU:HD22	1.58	0.83
13:S:48:HIS:CE1	13:S:95:LEU:HD22	2.13	0.83
4:D:280:ALA:CB	15:V:11:LEU:HG	2.09	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
4:D:102:SER:HB2	4:D:107:ARG:HG3	1.61	0.82
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.60	0.82
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.82
4:D:101:LEU:CD2	4:D:106:VAL:HG22	2.09	0.82
9:I:135:ARG:HD2	12:R:61:ILE:HG12	1.60	0.82
4:D:376:GLU:HG3	7:G:121:LEU:CD1	2.09	0.82
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.61	0.82
7:G:114:GLU:OE2	22:r:53:TYR:HA	1.80	0.82
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.61	0.82
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.82
9:I:162:CYS:HG	25:I:303:SF4:FE4	0.54	0.82
7:G:614:GLY:HA2	10:P:41:ILE:CD1	2.10	0.82
8:H:61:MET:SD	8:H:216:ALA:HB3	2.19	0.82
4:D:104:GLU:HB2	8:H:130:PHE:HZ	1.44	0.82
7:G:651:PRO:HG3	13:S:57:GLU:H	1.44	0.82
18:Z:86:ILE:HG23	18:Z:128:ARG:NE	1.95	0.81
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
8:H:251:LEU:O	8:H:251:LEU:CD1	2.28	0.81
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.81
7:G:607:LYS:HG3	11:Q:78:ARG:NH1	1.94	0.81
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.81
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.60	0.81
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.81
7:G:401:LEU:HD11	7:G:462:PHE:HE2	1.41	0.81
14:T:104:PHE:CD1	14:T:110:LEU:HB3	2.16	0.81
7:G:225:ILE:HD11	7:G:285:TRP:CZ3	2.16	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.44	0.81
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.62	0.81
5:E:84:LEU:HD12	23:s:46:LEU:HD13	1.61	0.81
6:F:296:LEU:HB2	6:F:337:MET:HE3	1.61	0.81
4:D:304:LYS:HE2	9:I:35:THR:N	1.96	0.81
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.69	0.81
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.81
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.80
16:W:96:THR:HG22	16:W:101:LYS:HD2	1.64	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
16:W:55:LEU:CD2	16:W:107:MET:HE2	2.10	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
29:I:301:PC1:H2D1	29:I:301:PC1:H291	1.64	0.80
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.80
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.80
4:D:97:LEU:HD21	4:D:99:LEU:HD21	1.62	0.80
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.17	0.80
9:I:211:TYR:CE2	22:r:39:PRO:HG3	2.17	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
20:b:20:VAL:HG13	24:b:201:3PE:H2A1	1.64	0.79
5:E:247:GLY:HA2	6:F:64:LYS:CE	2.12	0.79
7:G:614:GLY:HA2	10:P:41:ILE:HD13	1.63	0.79
14:T:108:LEU:O	14:T:108:LEU:HD23	1.82	0.79
4:D:170:ILE:HD13	4:D:236:LEU:CD1	2.13	0.79
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.13	0.79
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.79
14:T:90:TYR:HD2	14:T:93:ILE:HG12	1.48	0.79
7:G:401:LEU:CD1	7:G:466:LEU:HD21	2.13	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:224:PHE:CE1	8:H:228:TYR:CE1	2.71	0.79
12:R:80:ASP:OD2	12:R:84:GLY:CA	2.27	0.79
6:F:174:ARG:HA	23:s:52:LEU:HD21	1.65	0.79
10:P:44:GLY:HA2	11:Q:107:TRP:CZ3	2.19	0.78
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.13	0.78
7:G:225:ILE:HD11	7:G:285:TRP:HZ3	1.48	0.78
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.78
8:H:17:MET:HE1	8:H:225:MET:HE3	1.66	0.78
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.48	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.66	0.78
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.65	0.78
16:W:101:LYS:HG3	16:W:105:HIS:CB	2.12	0.78
6:F:392:MET:HE1	6:F:416:SER:HA	1.65	0.78
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.78
17:X:48:TRP:CD1	20:b:55:VAL:HG13	2.19	0.78
8:H:91:MET:O	8:H:92:PRO:C	2.27	0.78
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.78
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.78
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.78
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	1.99	0.77
18:Z:111:PHE:CZ	18:Z:117:VAL:CG2	2.66	0.77
4:D:271:ARG:HD2	8:H:281:ARG:HG3	1.67	0.77
7:G:75:CYS:HG	26:G:803:FES:FE1	0.99	0.77
5:E:136:THR:HB	26:E:301:FES:S2	2.24	0.77
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.99	0.77
20:b:20:VAL:HA	24:b:201:3PE:H282	1.67	0.77
1:A:54:LYS:HE3	1:A:113:TRP:HB3	1.65	0.77
3:C:241:PHE:HD2	22:r:61:ARG:CB	1.97	0.77
4:D:128:THR:HG22	4:D:131:GLN:CG	2.14	0.77
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.65	0.77
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.77
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.77
8:H:39:ILE:HD11	29:q:202:PC1:H131	1.65	0.77
4:D:198:THR:CG2	8:H:32:GLN:HE21	1.98	0.77
21:q:85:GLU:OE2	21:q:103:PRO:HD3	1.85	0.77
4:D:129:TYR:CE1	4:D:411:LEU:HD21	2.19	0.76
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.76
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.76
5:E:75:ALA:O	5:E:78:VAL:HG23	1.85	0.76
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.67	0.76
4:D:321:GLY:HA3	4:D:328:ASP:OD1	1.86	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.76
13:S:19:ILE:HB	13:S:53:ILE:CD1	2.15	0.76
3:C:88:HIS:CE1	15:V:105:GLU:HB3	2.20	0.76
10:P:231:LEU:HD13	10:P:292:PRO:HD3	1.66	0.76
4:D:259:GLU:CG	18:Z:25:LEU:HD11	2.16	0.76
5:E:120:MET:HE1	6:F:160:GLY:HA3	1.66	0.76
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.76
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
16:W:55:LEU:HB3	16:W:107:MET:HE2	1.66	0.76
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.21	0.76
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.75
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.21	0.75
6:F:234:GLY:HA3	6:F:238:CYS:O	1.85	0.75
9:I:113:CYS:HG	25:I:303:SF4:FE3	0.45	0.75
7:G:173:MET:HE2	7:G:231:LEU:HD23	1.68	0.75
10:P:143:ASP:HA	10:P:147:ASN:HB2	1.67	0.75
14:T:103:HIS:HB2	14:T:106:LYS:HG2	1.67	0.75
2:B:173:TYR:O	3:C:203:LEU:HD22	1.86	0.75
7:G:88:VAL:HG13	7:G:108:LYS:HE2	1.67	0.75
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.75
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.75
20:b:31:ILE:HA	20:b:34:MET:HE2	1.69	0.75
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.20	0.75
6:F:192:ASP:HB3	23:s:57:LEU:HD11	1.67	0.75
10:P:336:GLU:HG3	10:P:342:PRO:HD3	1.67	0.75
4:D:362:LYS:HE2	22:r:54:TYR:CE2	2.22	0.75
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.15	0.75
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.75
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.21	0.75
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.75
21:q:24:LEU:HD22	21:q:28:PHE:HE2	1.50	0.75
6:F:66:LYS:HZ3	6:F:189:SER:HA	1.50	0.75
7:G:75:CYS:SG	26:G:803:FES:FE1	1.79	0.75
7:G:126:LEU:CD1	12:R:89:PRO:HB3	2.16	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
14:T:103:HIS:ND1	14:T:140:CYS:HB3	2.01	0.75
14:T:104:PHE:CE1	14:T:115:GLN:HB2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:7:PRO:HG3	33:q:201:CDL:H181	1.69	0.75
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.67	0.75
10:P:94:LEU:HA	10:P:97:MET:HE2	1.68	0.75
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.67	0.75
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.74
13:S:19:ILE:HB	13:S:53:ILE:HD12	1.68	0.74
4:D:238:LEU:CD1	22:r:39:PRO:HB3	2.17	0.74
5:E:68:ASN:HD21	23:s:49:ASN:HD21	1.35	0.74
3:C:100:ARG:HH12	15:V:86:LYS:HZ1	1.32	0.74
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.22	0.74
4:D:279:THR:HA	15:V:12:VAL:HG13	1.69	0.74
6:F:288:VAL:HG21	6:F:303:HIS:CD2	2.23	0.74
6:F:318:ILE:CG2	6:F:326:LEU:HB3	2.17	0.74
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.74
4:D:375:MET:HE1	7:G:126:LEU:HA	1.70	0.74
9:I:211:TYR:CZ	22:r:39:PRO:HG3	2.23	0.74
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.74
8:H:295:PRO:HB3	24:b:201:3PE:H3A1	1.69	0.74
1:A:24:LEU:N	1:A:25:PRO:HD2	2.03	0.74
16:W:97:ILE:HG13	16:W:98:LYS:N	2.02	0.74
4:D:326:CYS:HB3	4:D:453:THR:HG21	1.69	0.74
6:F:311:TRP:CH2	6:F:333:GLU:HB3	2.22	0.74
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.74
8:H:96:ILE:HG23	18:Z:143:TYR:OH	1.88	0.74
14:T:110:LEU:HG	14:T:114:ASP:CB	2.17	0.74
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.87	0.74
1:A:25:PRO:HB2	8:H:60:PRO:HD3	1.69	0.74
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.70	0.74
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.74
10:P:44:GLY:HA2	11:Q:107:TRP:CE3	2.23	0.74
2:B:120:VAL:HG11	28:H:401:UQ9:H1MA	1.69	0.74
8:H:224:PHE:CZ	8:H:228:TYR:CE1	2.76	0.74
2:B:163:SER:HB2	9:I:150:THR:O	1.88	0.73
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.73
10:P:351:GLU:HB3	16:W:56:ASP:OD2	1.87	0.73
3:C:203:LEU:CD1	4:D:123:LEU:HD23	2.15	0.73
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.53	0.73
1:A:106:TRP:CE3	24:b:201:3PE:H342	2.24	0.73
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.71	0.73
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.73
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.73
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.22	0.73
10:P:169:HIS:H	10:P:184:LYS:HE3	1.54	0.73
18:Z:6:VAL:HG13	18:Z:7:LYS:H	1.53	0.73
1:A:54:LYS:HG3	1:A:113:TRP:HA	1.71	0.73
6:F:66:LYS:NZ	6:F:189:SER:HA	2.03	0.73
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.73
14:T:120:MET:HG2	16:W:44:ARG:HH11	1.53	0.73
4:D:323:ARG:O	15:V:12:VAL:HG21	1.88	0.73
17:X:48:TRP:CZ2	20:b:55:VAL:HG22	2.23	0.73
4:D:392:PRO:HG3	22:r:60:ARG:O	1.89	0.73
1:A:50:PRO:HD3	8:H:126:LYS:HB2	1.70	0.73
7:G:382:ARG:HD2	13:S:56:ARG:CD	2.18	0.73
17:X:57:LEU:HG	17:X:61:LYS:NZ	2.04	0.73
6:F:273:THR:HG22	6:F:291:GLU:HA	1.70	0.72
18:Z:65:LEU:O	18:Z:69:ILE:HG12	1.89	0.72
2:B:166:ASN:O	9:I:150:THR:HB	1.89	0.72
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.72
10:P:293:LEU:HD12	10:P:294:PRO:HD2	1.69	0.72
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.72
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.72
6:F:382:CYS:HG	25:F:502:SF4:FE3	1.07	0.72
6:F:392:MET:CE	6:F:419:ILE:HD12	2.19	0.72
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.20	0.72
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.72	0.72
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.72
6:F:35:LEU:HD22	6:F:273:THR:HG21	1.72	0.72
8:H:181:MET:CE	8:H:304:HIS:CE1	2.72	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.20	0.72
8:H:17:MET:SD	8:H:225:MET:HB3	2.30	0.72
18:Z:6:VAL:CG1	22:r:40:LYS:HB3	2.19	0.72
1:A:49:LEU:HD12	1:A:50:PRO:HD2	1.72	0.72
2:B:210:ARG:NH1	21:q:78:ASP:HB3	2.05	0.72
9:I:57:ALA:HB2	20:b:13:TRP:O	1.88	0.72
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.72
14:T:140:CYS:SG	14:T:143:GLU:HB2	2.29	0.72
20:b:23:PHE:HD2	24:b:201:3PE:H281	1.54	0.72
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.72
3:C:67:ILE:HD11	15:V:47:TYR:HD2	1.55	0.72
3:C:217:ARG:NH1	16:W:112:GLU:HB2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.72
8:H:306:SER:OG	20:b:33:PRO:HG3	1.90	0.72
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.71
6:F:110:PRO:HD2	6:F:238:CYS:SG	2.30	0.71
7:G:544:MET:HE3	7:G:565:PHE:HE2	1.54	0.71
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.20	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.71
5:E:155:LEU:HB3	5:E:157:ILE:HG22	1.72	0.71
6:F:44:ASN:ND2	6:F:133:HIS:O	2.23	0.71
16:W:42:TRP:CH2	16:W:93:LEU:HA	2.24	0.71
6:F:318:ILE:HG22	6:F:326:LEU:CB	2.20	0.71
3:C:67:ILE:HD11	15:V:47:TYR:CD2	2.25	0.71
4:D:136:PHE:HZ	4:D:422:CYS:SG	2.13	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
8:H:114:TYR:HB3	8:H:118:TRP:CH2	2.25	0.71
8:H:310:PHE:HA	20:b:39:THR:HA	1.72	0.71
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.56	0.71
6:F:318:ILE:O	6:F:318:ILE:HG13	1.90	0.71
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.71
9:I:64:THR:HG22	29:I:301:PC1:H222	1.72	0.71
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.71
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.54	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.78	0.71
9:I:135:ARG:HH11	12:R:61:ILE:HG23	1.55	0.71
1:A:73:LEU:O	1:A:76:PRO:HD2	1.90	0.71
2:B:116:ARG:HG2	8:H:36:GLY:O	1.91	0.70
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.70
2:B:166:ASN:HB2	2:B:190:TYR:HD2	1.55	0.70
22:r:46:SER:C	22:r:52:ASN:HD21	1.99	0.70
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.72	0.70
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.22	0.70
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.73	0.70
10:P:191:VAL:HA	10:P:194:VAL:HG22	1.72	0.70
4:D:198:THR:HG22	8:H:32:GLN:NE2	2.07	0.70
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.70
3:C:100:ARG:HH12	15:V:86:LYS:NZ	1.88	0.70
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.07	0.70
4:D:255:ILE:HG12	4:D:337:MET:HE2	1.72	0.70
5:E:61:ARG:NE	23:s:47:ASP:OD1	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.70
8:H:17:MET:HE1	8:H:225:MET:HB3	1.72	0.70
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.70
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.70
9:I:188:GLU:OE1	12:R:56:ASN:N	2.24	0.70
10:P:170:LEU:O	10:P:171:ASN:OD1	2.09	0.70
4:D:238:LEU:CD1	9:I:211:TYR:OH	2.35	0.70
13:S:16:LEU:HD21	13:S:19:ILE:HD11	1.73	0.70
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.70
17:X:122:LEU:HD21	20:b:81:LEU:HD23	1.73	0.70
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.70
7:G:117:MET:HE3	7:G:143:SER:HA	1.74	0.70
4:D:156:GLU:HG2	4:D:161:ILE:HD11	1.74	0.70
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.55	0.70
10:P:365:GLU:HB2	10:P:367:GLU:OE2	1.92	0.70
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.70
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.44	0.69
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.69
8:H:195:ARG:O	8:H:199:ASP:HB2	1.91	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
6:F:110:PRO:O	6:F:238:CYS:HB3	1.91	0.69
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.69
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.69
7:G:81:GLU:OE2	7:G:108:LYS:HD3	1.92	0.69
7:G:614:GLY:CA	10:P:41:ILE:HD13	2.22	0.69
8:H:42:PRO:HD2	8:H:45:ILE:HG12	1.74	0.69
18:Z:6:VAL:HG13	22:r:40:LYS:HB3	1.75	0.69
10:P:171:ASN:OD1	10:P:171:ASN:O	2.11	0.69
22:r:98:ALA:HB1	22:r:99:PRO:HD2	1.75	0.69
4:D:120:THR:HG21	4:D:139:LEU:HD21	1.74	0.69
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.57	0.69
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.69
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.69
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.08	0.69
6:F:278:ILE:HG12	6:F:304:ALA:HB2	1.73	0.69
7:G:78:CYS:HG	26:G:803:FES:FE2	0.46	0.69
13:S:51:LEU:HD13	13:S:95:LEU:HD12	1.75	0.69
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.69
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.08	0.68
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:104:PHE:HB2	14:T:110:LEU:HB2	1.74	0.68
18:Z:144:THR:HG22	19:a:48:MET:SD	2.30	0.68
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.68
8:H:64:LEU:HD21	10:P:359:TYR:CA	2.23	0.68
9:I:155:CYS:HG	25:I:302:SF4:FE4	1.10	0.68
5:E:233:LEU:H	6:F:37:ASP:CG	2.02	0.68
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.68
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.74	0.68
8:H:64:LEU:HD23	10:P:359:TYR:HB2	1.73	0.68
4:D:156:GLU:HG3	4:D:229:PRO:O	1.93	0.68
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.68
6:F:236:PHE:O	11:Q:166:TRP:HE3	1.76	0.68
8:H:17:MET:CE	8:H:225:MET:HB3	2.23	0.68
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.75	0.68
4:D:142:VAL:HG11	4:D:185:MET:HG2	1.76	0.68
6:F:147:ARG:HD3	6:F:191:TYR:CE2	2.29	0.68
7:G:171:THR:HB	7:G:173:MET:HG3	1.74	0.68
7:G:401:LEU:HD11	7:G:462:PHE:CZ	2.29	0.68
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.23	0.68
9:I:93:LEU:O	21:q:93:MET:HG2	1.94	0.68
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.59	0.68
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.76	0.68
8:H:311:THR:HB	18:Z:51:MET:SD	2.32	0.68
16:W:45:GLU:CD	16:W:97:ILE:HG22	2.19	0.68
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.75	0.68
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.68
7:G:651:PRO:CD	13:S:56:ARG:HB3	2.23	0.68
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.68
13:S:42:VAL:HB	13:S:46:LYS:HE3	1.75	0.68
17:X:48:TRP:CE2	20:b:55:VAL:CG2	2.75	0.68
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.67
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.67
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.67
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.77	0.67
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.60	0.67
3:C:217:ARG:HH12	16:W:112:GLU:HB2	1.58	0.67
14:T:90:TYR:HE2	14:T:110:LEU:HD11	1.58	0.67
10:P:197:GLU:HB3	10:P:259:VAL:CG2	2.24	0.67
18:Z:114:THR:O	18:Z:114:THR:HG22	1.94	0.67
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.24	0.67
7:G:73:GLY:HA2	26:G:803:FES:S1	2.35	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.27	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.67
13:S:20:ARG:HB2	13:S:66:TRP:HB2	1.75	0.67
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.67
22:r:12:ARG:HH21	22:r:20:LEU:CD1	2.07	0.67
10:P:263:PHE:HD2	10:P:333:PRO:O	1.77	0.67
10:P:296:PHE:CZ	10:P:297:VAL:HG23	2.29	0.67
2:B:111:ARG:CB	4:D:208:GLU:OE1	2.40	0.67
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.67
17:X:7:LEU:HD13	18:Z:87:LEU:HB3	1.77	0.67
4:D:451:ILE:CG2	4:D:456:ILE:HD11	2.25	0.67
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.67
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.28	0.67
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.67
8:H:300:LEU:HD23	20:b:25:VAL:HG11	1.76	0.67
10:P:302:GLY:HA2	10:P:314:THR:HG23	1.77	0.67
18:Z:65:LEU:HB3	20:b:50:PRO:O	1.93	0.67
2:B:170:TYR:HB2	9:I:153:ILE:CG2	2.24	0.67
2:B:202:LEU:CD2	9:I:86:TYR:CB	2.73	0.67
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.29	0.67
9:I:68:ARG:HH21	18:Z:26:PRO:HD2	1.59	0.67
9:I:200:GLU:OE2	21:q:93:MET:SD	2.53	0.67
16:W:121:PHE:HA	16:W:124:LYS:HE2	1.76	0.67
6:F:275:LEU:HA	6:F:289:GLU:HA	1.77	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.67
3:C:47:ARG:HG3	3:C:48:PRO:HD2	1.77	0.66
22:r:112:TYR:O	22:r:113:LEU:HB2	1.93	0.66
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.66
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.66
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.60	0.66
2:B:154:GLU:HB3	8:H:59:GLU:CG	2.26	0.66
6:F:233:VAL:HG11	11:Q:164:PHE:HB2	1.76	0.66
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.66
3:C:98:PHE:HE1	15:V:44:TYR:CE1	2.13	0.66
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.94	0.66
18:Z:62:ILE:HD12	20:b:81:LEU:HD22	1.76	0.66
4:D:96:ARG:HG3	4:D:115:LEU:HD11	1.78	0.66
10:P:122:HIS:HB2	12:R:46:VAL:HG12	1.77	0.66
9:I:110:GLU:OE1	12:R:64:ILE:HB	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:320:GLU:O	10:P:324:ILE:HG12	1.96	0.66
4:D:178:THR:HG22	4:D:214:TYR:OH	1.96	0.66
4:D:315:GLU:HB3	4:D:346:GLN:HE22	1.61	0.66
4:D:359:ASP:HB3	7:G:150:ARG:NH2	2.11	0.66
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.77	0.66
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
8:H:17:MET:HE1	8:H:225:MET:CE	2.25	0.66
9:I:62:MET:HE1	18:Z:36:PHE:HA	1.77	0.66
10:P:199:ILE:HD11	10:P:258:ALA:O	1.96	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.30	0.66
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.66
10:P:299:SER:CB	10:P:316:LYS:HE3	2.22	0.66
4:D:211:PHE:O	4:D:214:TYR:HB2	1.96	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
10:P:59:PHE:HB2	10:P:130:ILE:HD11	1.78	0.66
4:D:279:THR:HA	15:V:12:VAL:CG1	2.25	0.65
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.65
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.26	0.65
10:P:262:THR:H	10:P:332:LEU:HD12	1.61	0.65
13:S:16:LEU:HD11	13:S:19:ILE:HD11	1.78	0.65
14:T:97:LYS:HZ3	14:T:108:LEU:N	1.94	0.65
2:B:127:GLN:HE22	8:H:213:VAL:HA	1.59	0.65
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.79	0.65
12:R:40:GLU:HA	12:R:45:ARG:NH1	2.11	0.65
15:V:44:TYR:CE1	15:V:48:THR:HG23	2.30	0.65
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.32	0.65
4:D:102:SER:HB2	4:D:107:ARG:CG	2.26	0.65
4:D:102:SER:CB	4:D:107:ARG:HG3	2.26	0.65
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.65
8:H:134:ARG:HH12	8:H:204:GLU:HG3	1.61	0.65
8:H:283:ASP:OD1	8:H:284:GLN:N	2.29	0.65
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.96	0.65
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65
9:I:68:ARG:NH2	18:Z:26:PRO:O	2.30	0.65
17:X:130:LYS:HG2	20:b:68:SER:HA	1.77	0.65
4:D:384:LEU:CD2	7:G:144:MET:HE1	2.26	0.65
6:F:225:LEU:N	11:Q:160:TYR:HE2	1.95	0.65
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:42:PRO:HD2	8:H:45:ILE:CG1	2.26	0.65
21:q:3:LEU:O	21:q:6:VAL:HG22	1.97	0.65
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.36	0.65
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.73	0.65
10:P:169:HIS:H	10:P:184:LYS:CE	2.09	0.65
17:X:65:GLY:HA2	17:X:68:LEU:HD12	1.78	0.65
1:A:106:TRP:CZ2	8:H:291:LYS:HA	2.32	0.65
6:F:48:ARG:HH11	6:F:48:ARG:HA	1.61	0.65
17:X:141:PRO:O	17:X:142:TYR:HB2	1.96	0.65
7:G:614:GLY:C	10:P:41:ILE:HG21	2.22	0.65
10:P:284:THR:HG23	10:P:356:HIS:HB2	1.79	0.65
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.65
17:X:53:PRO:HB3	18:Z:80:ASP:OD2	1.97	0.65
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.60	0.65
4:D:198:THR:HG22	8:H:32:GLN:CG	2.26	0.65
4:D:198:THR:HG22	8:H:32:GLN:HG3	1.79	0.65
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.65
7:G:449:PRO:HG3	7:G:483:ARG:HH22	1.62	0.65
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.65
13:S:20:ARG:HG2	13:S:54:LEU:HD12	1.79	0.65
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.61	0.64
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.64
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.32	0.64
10:P:226:VAL:HG21	10:P:281:PHE:CZ	2.32	0.64
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.64
6:F:425:CYS:HG	25:F:502:SF4:FE1	0.48	0.64
7:G:152:ARG:HD2	22:r:49:LEU:HA	1.80	0.64
8:H:310:PHE:O	20:b:38:TYR:HB2	1.96	0.64
18:Z:143:TYR:CD1	18:Z:144:THR:N	2.65	0.64
2:B:154:GLU:HB3	2:B:155:PRO:HD3	1.77	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.63	0.64
6:F:379:CYS:SG	25:F:502:SF4:S1	2.96	0.64
8:H:85:LEU:HD21	8:H:108:THR:HB	1.80	0.64
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.64
2:B:95:PHE:HE1	2:B:131:MET:HE2	1.62	0.64
4:D:266:ARG:NH1	24:H:402:3PE:O14	2.30	0.64
4:D:376:GLU:OE1	7:G:151:SER:HB2	1.97	0.64
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.59	0.64
14:T:104:PHE:HE1	14:T:115:GLN:CB	2.07	0.64
4:D:217:VAL:HG22	4:D:226:TYR:CZ	2.33	0.64
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:236:VAL:CG1	10:P:270:ARG:HH21	2.10	0.64
10:P:365:GLU:CB	10:P:367:GLU:OE2	2.46	0.64
13:S:48:HIS:CE1	13:S:95:LEU:CD2	2.80	0.64
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.78	0.64
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.64
7:G:89:VAL:HB	7:G:94:MET:HG3	1.78	0.64
14:T:104:PHE:CE1	14:T:115:GLN:CB	2.80	0.64
17:X:37:ASP:OD1	17:X:38:LYS:N	2.31	0.64
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.80	0.64
5:E:48:PRO:HA	5:E:95:SER:HB2	1.80	0.64
6:F:388:GLY:HA3	6:F:419:ILE:HD11	1.80	0.64
7:G:126:LEU:HD11	12:R:89:PRO:HB3	1.80	0.64
8:H:249:ILE:HD13	17:X:99:HIS:CG	2.32	0.64
13:S:58:CYS:HB2	13:S:61:VAL:HG12	1.78	0.64
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.64
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.64
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.64
7:G:557:ARG:HD3	21:q:144:TYR:CE1	2.32	0.64
10:P:296:PHE:CZ	10:P:297:VAL:CG2	2.81	0.64
3:C:68:LEU:HD13	3:C:95:THR:HG23	1.80	0.64
5:E:58:ASN:HB3	5:E:84:LEU:HD21	1.80	0.64
6:F:293:SER:HA	6:F:338:ASP:HB3	1.78	0.64
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.94	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.32	0.64
10:P:150:ARG:HE	10:P:190:GLU:HG2	1.62	0.64
4:D:156:GLU:HG2	4:D:161:ILE:CD1	2.28	0.64
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.64
21:q:29:ARG:O	29:q:202:PC1:H141	1.97	0.64
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.80	0.63
4:D:384:LEU:HD21	7:G:144:MET:HE1	1.79	0.63
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.63
6:F:425:CYS:SG	25:F:502:SF4:S4	2.96	0.63
14:T:80:LYS:HD3	14:T:100:VAL:HG11	1.79	0.63
21:q:29:ARG:O	29:q:202:PC1:C14	2.46	0.63
2:B:202:LEU:HD21	9:I:86:TYR:CB	2.28	0.63
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.79	0.63
10:P:180:SER:O	10:P:184:LYS:HG3	1.98	0.63
17:X:57:LEU:HG	17:X:61:LYS:HZ3	1.60	0.63
18:Z:6:VAL:HG11	22:r:40:LYS:HD3	1.80	0.63
4:D:139:LEU:O	4:D:460:GLU:N	2.31	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:310:PHE:HB3	20:b:33:PRO:HA	1.80	0.63
2:B:194:CYS:O	25:B:301:SF4:S4	2.56	0.63
2:B:202:LEU:CD2	9:I:86:TYR:HB2	2.29	0.63
4:D:451:ILE:HG23	4:D:456:ILE:CD1	2.28	0.63
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.98	0.63
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.61	0.63
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.79	0.63
6:F:227:PRO:HG3	7:G:94:MET:SD	2.38	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
8:H:186:PHE:CD1	8:H:270:PHE:HE1	2.14	0.63
10:P:363:SER:CB	16:W:51:HIS:NE2	2.60	0.63
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.79	0.63
1:A:7:ILE:HG21	24:A:401:3PE:H292	1.79	0.63
5:E:129:TYR:CE2	5:E:167:LEU:HG	2.33	0.63
6:F:87:GLY:O	6:F:88:ARG:HB2	1.99	0.63
6:F:275:LEU:HG	6:F:289:GLU:HB3	1.80	0.63
6:F:297:LYS:HB2	6:F:333:GLU:HA	1.81	0.63
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.63
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.63
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.63
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.63
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.79	0.63
8:H:181:MET:CE	8:H:304:HIS:ND1	2.62	0.63
8:H:249:ILE:HG21	17:X:99:HIS:CE1	2.33	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
18:Z:65:LEU:O	18:Z:68:ARG:HG2	1.98	0.63
1:A:7:ILE:HG13	24:A:401:3PE:H271	1.81	0.63
2:B:116:ARG:HA	8:H:37:PRO:HA	1.80	0.63
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.24	0.63
17:X:50:GLU:HG2	17:X:138:PRO:HG3	1.79	0.63
2:B:161:MET:HG2	2:B:196:PRO:HG2	1.80	0.63
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.63
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.63	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.81	0.62
12:R:44:ARG:HG2	12:R:47:ARG:NH1	2.14	0.62
3:C:212:ASP:OD2	10:P:75:ARG:NH2	2.32	0.62
4:D:85:GLY:HA2	4:D:89:PRO:HB3	1.81	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.65	0.62
10:P:297:VAL:O	10:P:300:TRP:HB3	1.99	0.62
2:B:98:ALA:O	4:D:141:TYR:CZ	2.52	0.62
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.29	0.62
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.40	0.62
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.34	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
8:H:133:LEU:O	8:H:136:VAL:HG12	1.99	0.62
8:H:138:GLN:O	8:H:142:TYR:HB2	1.99	0.62
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.82	0.62
17:X:18:VAL:HG11	17:X:25:LEU:HD21	1.80	0.62
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.30	0.62
2:B:142:ALA:HB3	2:B:143:PRO:HD3	1.82	0.62
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.62
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.62
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.15	0.62
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.62
4:D:102:SER:HB2	4:D:107:ARG:CD	2.29	0.62
4:D:128:THR:HG23	4:D:131:GLN:HG2	1.81	0.62
4:D:198:THR:HA	8:H:32:GLN:HG2	1.80	0.62
6:F:327:ILE:HG13	6:F:331:VAL:HB	1.81	0.62
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.29	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.30	0.62
4:D:271:ARG:HD2	8:H:281:ARG:HG2	1.82	0.62
5:E:238:LYS:HE2	5:E:242:PHE:CE2	2.34	0.62
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.62
9:I:92:PRO:HG2	21:q:56:PHE:CE2	2.35	0.62
16:W:55:LEU:CB	16:W:107:MET:HE2	2.30	0.62
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.62
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.62
9:I:92:PRO:HA	21:q:91:HIS:O	2.00	0.62
7:G:636:TYR:CD1	7:G:642:VAL:HG22	2.34	0.62
8:H:17:MET:HE3	8:H:225:MET:HG2	1.82	0.62
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.62
7:G:360:LYS:CE	7:G:632:ILE:HB	2.28	0.61
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.61
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.61
6:F:318:ILE:HD11	6:F:355:ILE:CD1	2.28	0.61
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.81	0.61
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.64	0.61
4:D:170:ILE:CD1	4:D:236:LEU:CD1	2.79	0.61
4:D:368:ARG:NH1	9:I:160:GLU:O	2.33	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.61	0.61
7:G:114:GLU:OE2	22:r:54:TYR:N	2.31	0.61
7:G:382:ARG:HD2	13:S:56:ARG:HD3	1.82	0.61
8:H:39:ILE:HG13	21:q:31:ASN:ND2	2.15	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
10:P:169:HIS:HD2	10:P:181:LEU:HD11	1.65	0.61
20:b:11:ASN:O	20:b:15:LYS:N	2.31	0.61
5:E:65:ILE:HD11	23:s:46:LEU:HD22	1.83	0.61
5:E:180:VAL:HG13	5:E:181:ASN:N	2.15	0.61
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.80	0.61
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.35	0.61
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.61
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.61
12:R:72:VAL:CG1	12:R:77:ILE:HD12	2.30	0.61
2:B:95:PHE:CZ	2:B:145:LEU:HA	2.35	0.61
2:B:97:LEU:HD11	2:B:141:MET:HE2	1.82	0.61
4:D:145:MET:HA	4:D:148:GLU:HG2	1.82	0.61
4:D:261:MET:HE1	8:H:276:SER:HA	1.83	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
10:P:240:VAL:HB	10:P:266:THR:O	2.00	0.61
17:X:7:LEU:CD1	18:Z:87:LEU:HB3	2.30	0.61
18:Z:69:ILE:HG23	20:b:54:PRO:HD3	1.81	0.61
33:q:201:CDL:H331	33:q:201:CDL:H722	1.83	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.83	0.61
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.83	0.61
13:S:48:HIS:HE1	13:S:95:LEU:HD22	1.63	0.61
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.61
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.61
17:X:46:CYS:SG	17:X:59:GLU:HG3	2.41	0.61
5:E:91:TRP:CE3	5:E:125:PRO:HB3	2.36	0.61
6:F:87:GLY:H	6:F:92:GLY:HA2	1.64	0.61
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.61
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.61
18:Z:143:TYR:HD1	18:Z:144:THR:H	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.81	0.60
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.36	0.60
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.60
4:D:256:ASP:O	4:D:259:GLU:HB3	2.01	0.60
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.60
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.60
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.66	0.60
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.81	0.60
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.84	0.60
5:E:70:PRO:HB3	23:s:60:PRO:HG3	1.83	0.60
6:F:418:GLN:HE22	7:G:111:LYS:HG3	1.65	0.60
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.60
12:R:72:VAL:HG21	12:R:77:ILE:HD13	1.82	0.60
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.60
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.66	0.60
21:q:84:PRO:HD2	21:q:113:HIS:CD2	2.36	0.60
4:D:97:LEU:HG	4:D:99:LEU:HD23	1.79	0.60
3:C:84:GLU:OE2	3:C:141:ARG:NH1	2.35	0.60
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.14	0.60
4:D:323:ARG:O	15:V:12:VAL:CG2	2.50	0.60
5:E:134:CYS:SG	5:E:175:CYS:HA	2.41	0.60
6:F:69:LEU:HD11	6:F:143:LEU:CD2	2.31	0.60
9:I:188:GLU:OE1	12:R:56:ASN:HB2	2.01	0.60
5:E:150:THR:O	5:E:154:LYS:HG2	2.02	0.60
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.60
7:G:372:PHE:H	7:G:532:PRO:HB2	1.66	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.60
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.30	0.60
16:W:55:LEU:CB	16:W:107:MET:CE	2.75	0.60
2:B:155:PRO:HG2	8:H:58:LYS:HA	1.82	0.60
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.84	0.60
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.67	0.60
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.60
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.60
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.31	0.60
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.83	0.60
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.60
7:G:617:ARG:NH1	16:W:128:GLY:C	2.59	0.60
8:H:239:THR:O	8:H:239:THR:HG22	2.02	0.60
10:P:318:LYS:HG2	10:P:322:ILE:HD11	1.84	0.60
18:Z:144:THR:O	19:a:36:LYS:HD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:GLY:O	2:B:170:TYR:C	2.44	0.60
6:F:270:ASN:HD21	6:F:340:ASP:H	1.50	0.60
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.60
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.83	0.60
10:P:136:THR:CG2	10:P:139:PHE:HB2	2.31	0.60
12:R:97:LYS:HD2	12:R:100:LYS:HB2	1.84	0.60
17:X:37:ASP:HA	17:X:40:ASN:HB2	1.84	0.60
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.60
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.32	0.60
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.60
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.60
9:I:80:GLU:HG3	19:a:1:MET:SD	2.42	0.60
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.84	0.60
22:r:12:ARG:HH21	22:r:20:LEU:HD11	1.65	0.60
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.59
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
7:G:117:MET:HE3	7:G:143:SER:CA	2.32	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
22:r:20:LEU:C	22:r:20:LEU:HD12	2.27	0.59
5:E:63:GLU:O	5:E:67:LYS:HG3	2.02	0.59
5:E:154:LYS:HE3	5:E:201:GLU:HB2	1.83	0.59
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.59
13:S:16:LEU:HD11	13:S:19:ILE:CD1	2.32	0.59
3:C:100:ARG:NH1	15:V:86:LYS:NZ	2.51	0.59
3:C:241:PHE:CD2	22:r:61:ARG:CB	2.75	0.59
4:D:207:ARG:O	4:D:211:PHE:HD1	1.84	0.59
5:E:226:PRO:HG2	5:E:231:THR:H	1.67	0.59
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.59
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.59
8:H:213:VAL:HG22	28:H:401:UQ9:H3M	1.83	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.36	0.59
16:W:42:TRP:CZ2	16:W:93:LEU:HA	2.37	0.59
23:s:57:LEU:HG	23:s:58:PRO:HD2	1.83	0.59
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.59
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.36	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.38	0.59
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.59
10:P:178:SER:O	10:P:182:ARG:HG2	2.02	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PHE:CE1	1:A:60:ILE:HD11	2.38	0.59
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.59
3:C:242:PRO:O	3:C:243:ALA:C	2.45	0.59
6:F:303:HIS:O	6:F:304:ALA:C	2.45	0.59
6:F:414:GLU:OE1	22:r:50:SER:HA	2.02	0.59
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.85	0.59
12:R:32:THR:OG1	12:R:36:GLN:HB3	2.03	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
20:b:8:PHE:HA	20:b:11:ASN:ND2	2.18	0.59
3:C:141:ARG:NH1	4:D:410:TYR:HE1	2.00	0.59
4:D:326:CYS:CB	4:D:453:THR:HG21	2.32	0.59
4:D:411:LEU:HD11	4:D:419:PRO:HB3	1.85	0.59
6:F:318:ILE:HG12	6:F:355:ILE:HB	1.85	0.59
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.81	0.59
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.66	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
10:P:66:GLY:O	10:P:67:ARG:C	2.42	0.59
12:R:45:ARG:HA	12:R:48:PHE:HD2	1.67	0.59
17:X:123:GLY:HA2	18:Z:66:GLU:OE2	2.03	0.59
1:A:60:ILE:O	1:A:61:THR:C	2.45	0.58
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.67	0.58
6:F:87:GLY:HA3	6:F:92:GLY:HA2	1.84	0.58
6:F:314:LEU:O	6:F:329:LYS:HB2	2.03	0.58
6:F:318:ILE:CG1	6:F:355:ILE:HB	2.32	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.16	0.58
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.58
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.67	0.58
6:F:270:ASN:ND2	6:F:340:ASP:H	2.00	0.58
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.58
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.85	0.58
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.58
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.58
21:q:125:VAL:HG23	21:q:125:VAL:O	2.03	0.58
2:B:99:CYS:HB3	4:D:141:TYR:CB	2.33	0.58
4:D:112:HIS:HE1	16:W:100:TRP:CD1	2.22	0.58
6:F:51:TRP:CB	6:F:133:HIS:O	2.52	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
3:C:102:HIS:CE1	15:V:48:THR:CG2	2.68	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	1.84	0.58
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.58
16:W:104:THR:O	16:W:108:ARG:HG3	2.02	0.58
21:q:66:THR:HG22	21:q:67:GLU:OE2	2.03	0.58
4:D:163:PRO:HG2	4:D:168:GLN:HE21	1.68	0.58
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.38	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
7:G:614:GLY:HA2	10:P:41:ILE:HD12	1.84	0.58
10:P:220:TYR:HA	10:P:223:PHE:HD2	1.68	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.86	0.58
6:F:119:GLU:OE1	6:F:125:CYS:HA	2.03	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.84	0.58
10:P:57:THR:HG23	10:P:123:SER:HB2	1.86	0.58
12:R:52:GLN:NE2	12:R:54:GLU:HA	2.19	0.58
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.84	0.58
2:B:202:LEU:CD2	9:I:86:TYR:CG	2.83	0.58
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.58
21:q:129:THR:O	21:q:129:THR:HG22	2.03	0.58
3:C:67:ILE:HD12	15:V:44:TYR:HA	1.85	0.58
4:D:121:GLU:HG2	4:D:424:ILE:HD12	1.86	0.58
4:D:159:LEU:CG	4:D:391:VAL:HG12	2.34	0.58
4:D:217:VAL:HG22	4:D:226:TYR:CE1	2.39	0.58
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.87	0.58
6:F:267:ARG:HH12	6:F:340:ASP:HB3	1.68	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.58
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.58
4:D:159:LEU:HG	4:D:391:VAL:HG12	1.85	0.58
8:H:17:MET:CE	8:H:225:MET:HG2	2.34	0.58
9:I:72:MET:HE1	22:r:16:SER:HB2	1.84	0.58
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.86	0.58
7:G:632:ILE:HG13	7:G:632:ILE:O	2.04	0.58
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.58
20:b:20:VAL:HG22	24:b:201:3PE:H261	1.84	0.58
5:E:227:ALA:HB3	6:F:284:HIS:ND1	2.19	0.57
8:H:17:MET:SD	8:H:225:MET:O	2.63	0.57
18:Z:59:ARG:NH2	20:b:84:LEU:HB3	2.18	0.57
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.68	0.57
21:q:59:HIS:CE1	21:q:60:ARG:CG	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:320:ILE:HG12	9:I:36:TYR:HD2	1.69	0.57
10:P:245:VAL:O	10:P:249:ILE:HG13	2.04	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.05	0.57
2:B:106:HIS:HE1	4:D:207:ARG:HB3	1.69	0.57
8:H:175:LEU:HD21	29:I:301:PC1:H2C1	1.86	0.57
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.85	0.57
5:E:107:PRO:HB2	5:E:110:ARG:HG2	1.87	0.57
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.04	0.57
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.84	0.57
7:G:615:LEU:HG	10:P:41:ILE:HG23	1.86	0.57
10:P:363:SER:O	16:W:51:HIS:CD2	2.58	0.57
12:R:37:VAL:O	12:R:37:VAL:HG13	2.03	0.57
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.34	0.57
3:C:186:ILE:HG13	3:C:187:LEU:N	2.18	0.57
4:D:280:ALA:CB	15:V:11:LEU:CG	2.83	0.57
4:D:320:ILE:O	4:D:320:ILE:HG13	2.03	0.57
6:F:297:LYS:O	6:F:301:GLU:HG2	2.03	0.57
7:G:625:ALA:O	7:G:629:ILE:HG12	2.04	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
10:P:57:THR:HG23	10:P:123:SER:CB	2.33	0.57
3:C:123:ASN:HD22	15:V:108:PRO:HG2	1.69	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.40	0.57
20:b:23:PHE:HE1	24:b:201:3PE:H3A2	1.69	0.57
2:B:91:TRP:CH2	28:H:401:UQ9:H12	2.39	0.57
4:D:154:ALA:HB2	4:D:398:THR:HG21	1.87	0.57
6:F:291:GLU:HG2	6:F:292:MET:O	2.05	0.57
7:G:362:ASP:HB2	13:S:71:PHE:CD1	2.39	0.57
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.57
4:D:170:ILE:CD1	4:D:236:LEU:HD13	2.34	0.57
4:D:375:MET:HE1	7:G:126:LEU:CA	2.35	0.57
6:F:87:GLY:N	6:F:92:GLY:HA2	2.19	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.68	0.57
8:H:180:PRO:HD3	18:Z:43:LEU:HD21	1.87	0.57
8:H:194:ASN:ND2	8:H:201:THR:OG1	2.38	0.57
2:B:92:PRO:HG3	2:B:119:VAL:HG12	1.87	0.57
2:B:112:TYR:CZ	2:B:199:GLU:HG2	2.40	0.57
3:C:151:PRO:HG2	16:W:23:ILE:HG13	1.86	0.57
4:D:203:MET:HE2	4:D:258:VAL:HG13	1.86	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.57
12:R:44:ARG:HG2	12:R:47:ARG:HH12	1.70	0.57
17:X:142:TYR:HA	18:Z:115:ARG:HD3	1.86	0.57
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.87	0.57
2:B:202:LEU:HD23	9:I:86:TYR:CB	2.34	0.57
6:F:270:ASN:HD22	6:F:338:ASP:CG	2.13	0.57
6:F:278:ILE:CD1	6:F:304:ALA:HB1	2.35	0.57
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
2:B:82:ILE:HG23	8:H:57:MET:SD	2.45	0.56
4:D:145:MET:HA	4:D:148:GLU:CG	2.34	0.56
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.35	0.56
5:E:176:LEU:HB2	5:E:184:MET:HE1	1.87	0.56
5:E:247:GLY:C	6:F:64:LYS:HE2	2.30	0.56
6:F:69:LEU:HD11	6:F:143:LEU:HD21	1.87	0.56
8:H:67:SER:C	8:H:69:SER:H	2.13	0.56
21:q:86:TRP:CG	21:q:98:PRO:HG2	2.39	0.56
33:q:201:CDL:H141	33:q:201:CDL:H321	1.87	0.56
1:A:80:GLN:NE2	8:H:315:PRO:O	2.37	0.56
4:D:140:ASP:CB	4:D:147:ASN:HD21	2.07	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.87	0.56
5:E:73:HIS:HB3	6:F:236:PHE:CE1	2.40	0.56
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.87	0.56
6:F:296:LEU:O	6:F:297:LYS:C	2.47	0.56
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
8:H:69:SER:C	8:H:71:PHE:N	2.61	0.56
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.12	0.56
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.56
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.70	0.56
17:X:39:THR:HG23	17:X:40:ASN:N	2.20	0.56
17:X:103:GLN:HA	17:X:106:LYS:HD3	1.87	0.56
17:X:122:LEU:HD23	20:b:82:LYS:HG2	1.88	0.56
18:Z:8:GLN:HG3	22:r:41:LEU:HD12	1.86	0.56
22:r:106:LEU:HD21	22:r:111:PRO:HB2	1.86	0.56
3:C:240:ALA:HB1	22:r:61:ARG:HH11	1.71	0.56
5:E:231:THR:HG21	6:F:303:HIS:HA	1.87	0.56
17:X:53:PRO:HD3	18:Z:116:TRP:CD1	2.40	0.56
2:B:95:PHE:HB3	2:B:97:LEU:CD1	2.35	0.56
2:B:110:PRO:HB3	8:H:33:LEU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:CYS:SG	25:B:301:SF4:S3	3.02	0.56
3:C:209:LEU:HD21	16:W:108:ARG:NH1	2.20	0.56
3:C:240:ALA:HB1	22:r:61:ARG:CD	2.34	0.56
4:D:170:ILE:HD13	4:D:236:LEU:HD11	1.84	0.56
7:G:399:VAL:HG22	7:G:462:PHE:HZ	1.68	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
8:H:77:LEU:HD22	8:H:118:TRP:HZ3	1.71	0.56
10:P:64:PHE:HE1	10:P:209:ARG:O	1.88	0.56
9:I:82:ALA:HA	22:r:26:LEU:HD21	1.88	0.56
10:P:145:PHE:O	10:P:149:PRO:HG2	2.05	0.56
10:P:315:THR:HG22	10:P:317:ASP:H	1.69	0.56
17:X:47:ARG:NH2	17:X:53:PRO:HG3	2.21	0.56
20:b:67:PRO:HB3	20:b:74:LEU:HB2	1.87	0.56
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.06	0.56
7:G:360:LYS:HB2	7:G:632:ILE:CD1	2.22	0.56
8:H:17:MET:SD	8:H:225:MET:CA	2.93	0.56
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.56
14:T:90:TYR:CE2	14:T:110:LEU:HD11	2.39	0.56
17:X:124:GLN:C	17:X:125:LEU:HD12	2.31	0.56
18:Z:85:GLN:O	18:Z:89:GLU:HG3	2.06	0.56
22:r:106:LEU:HD21	22:r:111:PRO:CB	2.36	0.56
2:B:154:GLU:HB3	8:H:59:GLU:HB2	1.88	0.56
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.36	0.56
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.36	0.56
7:G:62:ARG:H	7:G:142:GLN:HE22	1.53	0.56
9:I:88:PHE:CZ	21:q:30:ALA:HA	2.40	0.56
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.56
17:X:5:VAL:HG13	17:X:7:LEU:HG	1.87	0.56
10:P:323:HIS:ND1	10:P:323:HIS:O	2.39	0.55
10:P:363:SER:CB	16:W:51:HIS:CE1	2.84	0.55
13:S:27:SER:N	13:S:34:ARG:HH22	2.05	0.55
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.35	0.55
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.36	0.55
14:T:146:ASP:O	14:T:149:ALA:HB3	2.06	0.55
21:q:56:PHE:HD2	22:r:27:ARG:HH11	1.53	0.55
4:D:271:ARG:NH1	8:H:279:ARG:O	2.38	0.55
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.87	0.55
6:F:382:CYS:HA	7:G:74:ASN:O	2.04	0.55
8:H:4:ILE:O	8:H:8:THR:HG23	2.05	0.55
4:D:380:HIS:O	4:D:384:LEU:HG	2.07	0.55
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.55
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.69	0.55
10:P:375:VAL:HG12	10:P:377:TYR:HB3	1.87	0.55
14:T:85:TYR:O	14:T:89:LEU:HD13	2.07	0.55
20:b:69:HIS:HB3	20:b:72:ASP:OD1	2.05	0.55
2:B:154:GLU:O	2:B:155:PRO:C	2.48	0.55
5:E:226:PRO:HD3	6:F:46:TYR:CE2	2.40	0.55
6:F:154:ALA:HB2	6:F:193:PHE:HZ	1.71	0.55
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.55
8:H:69:SER:C	8:H:71:PHE:H	2.13	0.55
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.45	0.55
14:T:93:ILE:HA	14:T:108:LEU:HD21	1.88	0.55
2:B:194:CYS:HB2	9:I:153:ILE:O	2.06	0.55
4:D:217:VAL:CG2	4:D:226:TYR:CZ	2.89	0.55
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
8:H:127:TYR:O	8:H:130:PHE:HB3	2.07	0.55
10:P:140:ASP:OD1	10:P:142:GLU:HB2	2.06	0.55
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.36	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
7:G:399:VAL:CG2	7:G:462:PHE:CE1	2.87	0.55
12:R:43:TYR:O	12:R:46:VAL:HG22	2.07	0.55
3:C:62:GLU:O	3:C:66:GLU:HG3	2.06	0.55
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.42	0.55
4:D:310:VAL:HG23	4:D:310:VAL:O	2.06	0.55
6:F:51:TRP:CZ3	6:F:168:ASN:HB3	2.41	0.55
7:G:655:ARG:NH1	13:S:59:SER:CB	2.70	0.55
10:P:237:LYS:HE3	10:P:322:ILE:O	2.07	0.55
19:a:31:ASN:HD21	19:a:36:LYS:HB2	1.71	0.55
20:b:8:PHE:CG	20:b:9:LEU:N	2.74	0.55
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.55
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.64	0.55
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.61	0.55
5:E:221:ARG:HH21	5:E:227:ALA:HB2	1.72	0.55
6:F:147:ARG:CD	6:F:191:TYR:CE2	2.90	0.55
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.55
8:H:126:LYS:HG3	8:H:127:TYR:H	1.72	0.55
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.55
12:R:58:ASN:HB3	12:R:63:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:40:ILE:O	18:Z:44:ILE:HG12	2.07	0.55
21:q:3:LEU:O	21:q:7:LEU:HG	2.07	0.55
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.88	0.55
1:A:113:TRP:HH2	8:H:287:HIS:CD2	2.25	0.55
3:C:98:PHE:HB2	15:V:94:MET:CE	2.37	0.55
4:D:128:THR:HG22	4:D:131:GLN:CD	2.31	0.55
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.55
7:G:655:ARG:NH1	13:S:59:SER:HB3	2.21	0.55
8:H:70:LEU:HD22	8:H:121:TRP:HD1	1.72	0.55
28:H:401:UQ9:H4MA	28:H:401:UQ9:H3MB	1.89	0.55
12:R:45:ARG:HA	12:R:48:PHE:CD2	2.41	0.55
16:W:53:MET:HB2	16:W:55:LEU:HG	1.89	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.54
6:F:424:ILE:CG1	7:G:76:ARG:HD3	2.37	0.54
8:H:43:TYR:CE2	21:q:27:PHE:HZ	2.25	0.54
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.89	0.54
10:P:58:VAL:O	10:P:83:PRO:HD2	2.08	0.54
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.22	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.54
18:Z:143:TYR:HD1	18:Z:144:THR:N	2.04	0.54
19:a:1:MET:HB2	19:a:3:PHE:CZ	2.42	0.54
3:C:104:ASN:ND2	22:r:94:ALA:HB1	2.22	0.54
4:D:158:LEU:HD12	4:D:411:LEU:HD23	1.90	0.54
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.54
8:H:316:PRO:HA	18:Z:58:ARG:NH1	2.22	0.54
18:Z:92:GLU:O	18:Z:96:ILE:HG13	2.07	0.54
21:q:49:TYR:HB2	21:q:61:TRP:CE2	2.42	0.54
4:D:136:PHE:HZ	4:D:422:CYS:HG	1.55	0.54
4:D:264:ASN:O	9:I:65:GLU:OE1	2.25	0.54
6:F:102:MET:SD	6:F:149:MET:HB2	2.48	0.54
6:F:388:GLY:CA	6:F:419:ILE:HD11	2.37	0.54
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
10:P:207:PHE:CE1	10:P:214:LEU:HD22	2.43	0.54
10:P:236:VAL:HG13	10:P:270:ARG:HH21	1.71	0.54
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.54
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.71	0.54
4:D:202:TRP:HH2	4:D:261:MET:HG3	1.73	0.54
4:D:293:LEU:HD22	4:D:300:TRP:HB3	1.89	0.54
5:E:84:LEU:HD12	23:s:46:LEU:CD1	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:278:ILE:HG12	6:F:304:ALA:CB	2.38	0.54
8:H:9:LEU:O	8:H:13:ILE:HG12	2.06	0.54
8:H:183:MET:HE2	29:I:301:PC1:H271	1.88	0.54
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.71	0.54
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.90	0.54
14:T:84:LEU:O	14:T:88:LYS:HG3	2.07	0.54
14:T:115:GLN:O	14:T:119:ILE:HG12	2.08	0.54
19:a:58:ASN:HB2	19:a:61:TYR:CD2	2.43	0.54
3:C:64:VAL:HG11	3:C:85:ILE:CD1	2.33	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
7:G:617:ARG:HH12	16:W:128:GLY:C	2.15	0.54
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.71	0.54
17:X:64:ASN:O	17:X:68:LEU:HG	2.07	0.54
2:B:170:TYR:CB	9:I:153:ILE:HG21	2.36	0.54
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.90	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
4:D:150:ALA:HB2	4:D:400:ILE:HG12	1.90	0.54
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.42	0.54
5:E:177:GLY:O	5:E:178:ALA:HB3	2.08	0.54
6:F:87:GLY:CA	6:F:92:GLY:HA2	2.37	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
7:G:651:PRO:HG3	13:S:57:GLU:N	2.18	0.54
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.72	0.54
11:Q:165:SER:HB2	11:Q:168:LYS:HG2	1.89	0.54
13:S:47:ALA:O	13:S:49:PRO:HD3	2.08	0.54
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.54
4:D:240:LEU:HG	4:D:244:ILE:CD1	2.38	0.54
5:E:62:ILE:HD11	5:E:84:LEU:HD22	1.90	0.54
5:E:116:THR:O	7:G:199:GLY:HA2	2.07	0.54
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.54
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
8:H:17:MET:SD	8:H:225:MET:CB	2.96	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
10:P:44:GLY:H	11:Q:105:GLU:CD	2.15	0.54
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.90	0.54
2:B:116:ARG:O	8:H:39:ILE:HG22	2.08	0.54
2:B:153:PRO:HB2	8:H:58:LYS:HG3	1.90	0.54
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.54
5:E:199:ASP:O	5:E:203:ILE:HG13	2.08	0.54
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:332:CYS:HA	6:F:335:VAL:HG12	1.90	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.54
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.54
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
10:P:306:GLY:HA2	10:P:312:PRO:HB3	1.90	0.54
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.54
14:T:93:ILE:HG23	14:T:108:LEU:CD1	2.38	0.54
18:Z:143:TYR:O	18:Z:144:THR:HB	2.08	0.54
22:r:54:TYR:CZ	22:r:58:ASP:HB3	2.42	0.54
2:B:161:MET:CG	2:B:196:PRO:HG2	2.37	0.54
5:E:91:TRP:CZ2	5:E:125:PRO:HD3	2.43	0.54
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.54
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.90	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.08	0.54
18:Z:140:PHE:HD1	19:a:45:TRP:HB2	1.72	0.54
4:D:172:VAL:HG21	4:D:310:VAL:HG23	1.90	0.53
4:D:446:ASP:OD2	8:H:281:ARG:NH2	2.41	0.53
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
8:H:307:LEU:HD11	18:Z:47:TYR:CG	2.42	0.53
16:W:23:ILE:HG23	16:W:24:PHE:N	2.22	0.53
17:X:17:GLU:HG3	17:X:64:ASN:HD22	1.73	0.53
17:X:124:GLN:O	20:b:70:PRO:HB2	2.08	0.53
18:Z:120:LEU:HB2	18:Z:123:GLU:HG3	1.89	0.53
22:r:36:GLN:HB3	22:r:37:PRO:HD2	1.90	0.53
1:A:112:GLU:C	1:A:113:TRP:CG	2.86	0.53
2:B:166:ASN:O	2:B:166:ASN:OD1	2.25	0.53
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.43	0.53
7:G:62:ARG:H	7:G:142:GLN:NE2	2.05	0.53
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.53
7:G:611:THR:CG2	11:Q:105:GLU:HA	2.22	0.53
8:H:77:LEU:HD23	8:H:115:SER:HB3	1.91	0.53
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.44	0.53
12:R:48:PHE:CD1	12:R:53:LYS:HB2	2.43	0.53
21:q:50:GLU:HA	21:q:59:HIS:O	2.07	0.53
5:E:226:PRO:HD3	6:F:46:TYR:CZ	2.44	0.53
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:42:TRP:CD2	16:W:93:LEU:HD13	2.44	0.53
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.53
4:D:159:LEU:HD21	4:D:391:VAL:HG12	1.89	0.53
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.53
10:P:142:GLU:HA	10:P:146:VAL:HG12	1.90	0.53
2:B:182:ASP:OD1	2:B:183:ARG:N	2.41	0.53
5:E:118:TYR:HE1	6:F:206:CYS:SG	2.31	0.53
6:F:286:CYS:SG	6:F:304:ALA:HA	2.47	0.53
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.53
8:H:153:VAL:HG11	8:H:241:ILE:HG23	1.90	0.53
8:H:180:PRO:CD	18:Z:43:LEU:HD21	2.39	0.53
10:P:272:LEU:CG	10:P:375:VAL:HG21	2.25	0.53
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.53
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.08	0.53
19:a:42:GLN:O	19:a:43:TYR:C	2.50	0.53
1:A:69:ILE:O	1:A:73:LEU:HG	2.08	0.53
3:C:63:TYR:HE1	15:V:47:TYR:CG	2.26	0.53
3:C:101:ASP:OD1	15:V:86:LYS:HE3	2.08	0.53
7:G:364:ASP:C	7:G:364:ASP:OD1	2.52	0.53
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.53
7:G:617:ARG:HH12	16:W:129:HIS:N	2.06	0.53
18:Z:59:ARG:HH21	20:b:84:LEU:HB3	1.72	0.53
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.53
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.53
8:H:126:LYS:O	8:H:129:LEU:HB3	2.07	0.53
28:H:401:UQ9:H10	28:H:401:UQ9:C1	2.38	0.53
9:I:209:TYR:HA	9:I:212:ARG:CG	2.39	0.53
20:b:8:PHE:O	20:b:9:LEU:C	2.50	0.53
22:r:6:ARG:O	22:r:10:LYS:HG3	2.09	0.53
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.90	0.53
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.42	0.53
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.39	0.53
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.39	0.53
11:Q:53:ILE:O	16:W:20:VAL:HG22	2.09	0.53
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.53
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.42	0.53
18:Z:129:THR:HB	18:Z:132:GLU:HG3	1.91	0.53
3:C:234:LEU:O	4:D:387:GLU:HG3	2.08	0.53
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.91	0.53
6:F:119:GLU:OE1	6:F:125:CYS:CA	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.53
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.53
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.53
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.74	0.53
10:P:231:LEU:HD13	10:P:292:PRO:CD	2.37	0.53
16:W:42:TRP:CZ2	16:W:93:LEU:CA	2.91	0.53
17:X:70:PHE:O	17:X:74:ILE:HG13	2.09	0.53
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.53
4:D:289:SER:HA	4:D:293:LEU:HD13	1.91	0.53
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.53
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.39	0.53
9:I:49:ASP:O	9:I:50:MET:C	2.50	0.53
10:P:172:ALA:H	10:P:202:ARG:NH2	2.06	0.53
18:Z:126:GLY:HA2	18:Z:133:MET:HE2	1.91	0.53
21:q:31:ASN:HD21	29:q:202:PC1:H151	1.73	0.53
1:A:103:ALA:O	1:A:107:THR:HG23	2.08	0.52
2:B:199:GLU:HB2	9:I:173:PHE:HE2	1.74	0.52
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.52
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.52
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.52
12:R:43:TYR:O	12:R:46:VAL:HG13	2.09	0.52
18:Z:105:LYS:HD2	18:Z:105:LYS:N	2.24	0.52
20:b:23:PHE:CD2	24:b:201:3PE:H281	2.40	0.52
21:q:44:TYR:OH	21:q:112:ASN:CG	2.53	0.52
2:B:163:SER:HA	2:B:166:ASN:OD1	2.10	0.52
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.27	0.52
4:D:139:LEU:O	4:D:459:GLY:C	2.53	0.52
5:E:52:PHE:CD2	5:E:96:ALA:HA	2.44	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.45	0.52
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.10	0.52
3:C:51:ASP:OD1	3:C:54:HIS:HB3	2.08	0.52
6:F:109:ARG:HB3	6:F:238:CYS:SG	2.50	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:133:VAL:HA	5:E:185:VAL:HG12	1.90	0.52
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.91	0.52
9:I:54:THR:HG22	20:b:13:TRP:HE1	1.74	0.52
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.52
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.91	0.52
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.73	0.52
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.52
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.52
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.90	0.52
3:C:63:TYR:HB2	22:r:95:VAL:CG2	2.40	0.52
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.06	0.52
4:D:390:GLN:HG3	4:D:415:GLY:O	2.09	0.52
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.52
7:G:161:GLU:O	7:G:163:LYS:HE3	2.10	0.52
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.52
10:P:236:VAL:HG11	10:P:270:ARG:HH21	1.75	0.52
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.52
6:F:86:ARG:NH1	6:F:339:PHE:HB2	2.24	0.52
7:G:33:GLU:HB3	7:G:98:LYS:HE2	1.92	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.52
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.91	0.52
8:H:199:ASP:O	8:H:279:ARG:HD2	2.10	0.52
14:T:90:TYR:CD2	14:T:93:ILE:HG12	2.38	0.52
2:B:101:ALA:O	2:B:104:MET:HG2	2.10	0.52
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.44	0.52
4:D:303:ARG:HH11	4:D:401:GLU:HG2	1.75	0.52
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.52
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.52
17:X:137:LEU:HA	20:b:58:ARG:HH22	1.75	0.52
2:B:199:GLU:HB2	9:I:173:PHE:CE2	2.44	0.52
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.52
6:F:192:ASP:HB3	23:s:57:LEU:CD1	2.38	0.52
6:F:288:VAL:HG11	6:F:303:HIS:CB	2.40	0.52
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.52
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.52
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.52
10:P:157:LYS:O	10:P:158:GLU:C	2.53	0.52
16:W:23:ILE:HG23	16:W:24:PHE:H	1.74	0.52
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.28	0.52
5:E:183:PRO:HG2	5:E:194:ASP:HA	1.92	0.52
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.46	0.52
6:F:288:VAL:HG11	6:F:303:HIS:HB3	1.91	0.52
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.52
7:G:614:GLY:HA2	10:P:41:ILE:HG21	1.91	0.52
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.91	0.52
10:P:265:PHE:HD1	10:P:334:GLY:HA3	1.74	0.52
12:R:40:GLU:HA	12:R:45:ARG:HH12	1.75	0.52
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.52
19:a:4:GLU:O	19:a:7:PRO:HD2	2.09	0.52
20:b:48:ALA:O	20:b:49:THR:C	2.53	0.52
4:D:172:VAL:HG21	4:D:310:VAL:CG2	2.40	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.10	0.51
8:H:17:MET:CE	8:H:225:MET:CB	2.88	0.51
18:Z:111:PHE:CE1	18:Z:117:VAL:HG21	2.45	0.51
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.91	0.51
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.51
21:q:101:ASN:OD1	21:q:101:ASN:O	2.29	0.51
2:B:92:PRO:HG3	2:B:119:VAL:CG1	2.40	0.51
4:D:202:TRP:CH2	4:D:261:MET:HG3	2.45	0.51
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.51
6:F:238:CYS:O	6:F:239:PRO:C	2.51	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.51
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.51
14:T:104:PHE:CE1	14:T:115:GLN:CG	2.94	0.51
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.93	0.51
2:B:95:PHE:HZ	2:B:148:VAL:HB	1.75	0.51
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.40	0.51
4:D:348:LEU:O	18:Z:11:PRO:HB3	2.09	0.51
5:E:179:CYS:HA	26:E:301:FES:S1	2.50	0.51
5:E:196:THR:O	5:E:197:PRO:C	2.54	0.51
7:G:275:PRO:HB3	7:G:286:ILE:HG23	1.91	0.51
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.41	0.51
8:H:137:ALA:O	8:H:141:SER:HB2	2.09	0.51
10:P:336:GLU:CG	10:P:342:PRO:HD3	2.38	0.51
10:P:353:LEU:HA	10:P:356:HIS:HD2	1.74	0.51
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.51
12:R:50:ASP:O	12:R:51:ARG:HG3	2.10	0.51
16:W:42:TRP:CE3	16:W:93:LEU:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:56:CYS:HA	17:X:135:ARG:HH12	1.76	0.51
2:B:114:MET:HE3	2:B:119:VAL:CG1	2.40	0.51
2:B:202:LEU:HD23	9:I:86:TYR:CD1	2.45	0.51
4:D:179:ARG:HG2	4:D:183:HIS:CD2	2.45	0.51
4:D:320:ILE:CD1	9:I:36:TYR:CD2	2.93	0.51
6:F:66:LYS:HZ3	6:F:189:SER:CA	2.21	0.51
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.51
7:G:81:GLU:O	7:G:103:LEU:HB2	2.09	0.51
8:H:99:ASN:OD1	19:a:40:ARG:HG3	2.11	0.51
18:Z:86:ILE:HA	18:Z:128:ARG:HH21	1.74	0.51
2:B:115:ASP:OD1	8:H:25:ARG:NH2	2.42	0.51
2:B:161:MET:HE2	2:B:196:PRO:HD2	1.92	0.51
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.25	0.51
4:D:174:PHE:CZ	4:D:240:LEU:HD21	2.45	0.51
4:D:274:ASP:H	4:D:325:ASP:CB	2.24	0.51
5:E:180:VAL:HG11	5:E:224:CYS:HB3	1.93	0.51
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.51
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.51
8:H:85:LEU:CD2	8:H:108:THR:HB	2.41	0.51
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.93	0.51
9:I:58:ALA:HB2	18:Z:36:PHE:CZ	2.45	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
10:P:45:LYS:HB2	11:Q:118:ALA:CB	2.41	0.51
10:P:305:PHE:HB2	10:P:314:THR:HG22	1.92	0.51
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.51
14:T:130:ILE:HG23	14:T:147:TYR:HE2	1.75	0.51
16:W:65:LYS:HE3	16:W:69:MET:HE2	1.92	0.51
21:q:65:THR:OG1	21:q:66:THR:N	2.44	0.51
21:q:85:GLU:CD	21:q:103:PRO:HG3	2.36	0.51
2:B:189:ILE:HD12	2:B:207:GLN:HB3	1.93	0.51
4:D:235:ASP:HA	4:D:356:ILE:HG21	1.91	0.51
6:F:267:ARG:HD3	6:F:338:ASP:OD2	2.10	0.51
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.51
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.46	0.51
10:P:207:PHE:HE1	10:P:214:LEU:HD22	1.76	0.51
19:a:14:VAL:O	19:a:18:ILE:HG13	2.10	0.51
21:q:8:LYS:O	21:q:12:GLN:HG2	2.10	0.51
4:D:179:ARG:NH2	4:D:303:ARG:HD3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.51
7:G:239:THR:HA	9:I:132:ALA:O	2.11	0.51
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.51
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.51
10:P:65:LEU:HD23	10:P:129:LEU:HD22	1.93	0.51
10:P:172:ALA:H	10:P:202:ARG:HH21	1.59	0.51
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.92	0.51
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.36	0.51
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.51
9:I:210:LEU:HD22	22:r:39:PRO:HD2	1.92	0.51
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.51
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.51
5:E:129:TYR:HE2	5:E:167:LEU:HG	1.74	0.51
6:F:42:PHE:CE2	6:F:275:LEU:HD11	2.46	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
8:H:137:ALA:O	8:H:141:SER:CB	2.59	0.51
9:I:88:PHE:O	21:q:62:VAL:HG12	2.10	0.51
9:I:152:CYS:SG	25:I:302:SF4:S3	3.09	0.51
10:P:135:GLU:CG	10:P:140:ASP:HA	2.41	0.51
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.51
18:Z:66:GLU:HA	18:Z:69:ILE:HG12	1.93	0.51
1:A:81:THR:O	20:b:46:ASN:ND2	2.44	0.51
6:F:279:SER:O	6:F:355:ILE:HA	2.11	0.51
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
10:P:300:TRP:O	10:P:304:LEU:HG	2.11	0.51
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.41	0.51
18:Z:72:MET:SD	20:b:53:TYR:HB2	2.51	0.51
4:D:159:LEU:CD2	4:D:391:VAL:HG12	2.41	0.50
4:D:263:THR:O	4:D:263:THR:HG22	2.11	0.50
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.76	0.50
6:F:270:ASN:HD22	6:F:338:ASP:HB2	1.76	0.50
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.50
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.50
8:H:90:PRO:O	8:H:91:MET:C	2.50	0.50
8:H:145:THR:HG22	8:H:289:LEU:HD11	1.92	0.50
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.50
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.50
10:P:209:ARG:N	10:P:352:VAL:HG22	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:315:THR:HB	10:P:318:LYS:HB2	1.92	0.50
4:D:255:ILE:HG22	4:D:338:ARG:NH2	2.26	0.50
4:D:399:ALA:HB1	4:D:406:GLU:HG3	1.94	0.50
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.24	0.50
6:F:225:LEU:HB3	6:F:227:PRO:CD	2.37	0.50
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.50
14:T:82:ARG:HD2	14:T:125:GLU:OE2	2.10	0.50
18:Z:69:ILE:CG2	20:b:54:PRO:HD3	2.40	0.50
18:Z:90:ASN:O	18:Z:94:GLU:HB2	2.12	0.50
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.50
1:A:113:TRP:CH2	8:H:287:HIS:HD2	2.29	0.50
6:F:78:GLY:O	6:F:82:THR:HG23	2.12	0.50
6:F:109:ARG:HH21	6:F:239:PRO:HG3	1.76	0.50
6:F:315:LEU:HA	6:F:359:ARG:CZ	2.42	0.50
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.50
10:P:234:LYS:HG2	10:P:234:LYS:O	2.10	0.50
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.50
18:Z:28:ARG:HG3	18:Z:28:ARG:O	2.11	0.50
22:r:48:LYS:HB2	22:r:52:ASN:HD22	1.76	0.50
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.94	0.50
4:D:97:LEU:O	4:D:99:LEU:HG	2.11	0.50
5:E:131:ILE:HA	5:E:187:ILE:HA	1.93	0.50
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.47	0.50
7:G:277:MET:HE1	11:Q:153:PRO:HD3	1.94	0.50
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.50
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.50
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.50
20:b:11:ASN:OD1	20:b:12:ALA:N	2.44	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.94	0.50
4:D:92:HIS:O	4:D:458:PHE:HE2	1.94	0.50
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.50
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.41	0.50
6:F:280:GLY:O	6:F:356:VAL:HB	2.11	0.50
10:P:238:GLN:HB2	10:P:270:ARG:HG2	1.94	0.50
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.50
14:T:97:LYS:NZ	14:T:107:ASP:C	2.69	0.50
3:C:73:GLN:NE2	15:V:112:TRP:HE1	2.09	0.50
4:D:98:VAL:HG21	4:D:112:HIS:CE1	2.47	0.50
4:D:333:ARG:HH12	4:D:453:THR:HA	1.77	0.50
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.92	0.50
5:E:39:VAL:CG2	7:G:205:GLN:HE22	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:414:GLU:OE2	22:r:51:ASN:N	2.29	0.50
7:G:35:PHE:O	7:G:101:ASN:HA	2.10	0.50
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.50
8:H:224:PHE:CE2	28:H:401:UQ9:H12A	2.46	0.50
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.50
4:D:163:PRO:HG2	4:D:168:GLN:NE2	2.27	0.50
6:F:42:PHE:HE2	6:F:275:LEU:HD11	1.75	0.50
6:F:204:TYR:CE1	27:F:501:FMN:H6	2.47	0.50
7:G:643:ARG:O	7:G:644:ASN:C	2.55	0.50
8:H:126:LYS:HG3	8:H:127:TYR:N	2.27	0.50
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.50
15:V:44:TYR:CD1	15:V:48:THR:HG23	2.46	0.50
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.47	0.50
3:C:97:THR:O	15:V:90:LEU:HD12	2.12	0.50
3:C:210:ARG:HD2	10:P:48:ARG:HD3	1.94	0.50
5:E:120:MET:HE2	6:F:201:ALA:HA	1.94	0.50
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
7:G:140:GLN:HG3	7:G:141:ASP:OD1	2.10	0.50
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.50
8:H:182:ALA:HB1	24:H:402:3PE:C2I	2.42	0.50
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.50
10:P:212:ARG:O	10:P:213:PHE:C	2.55	0.50
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.50
4:D:133:LEU:HB3	4:D:134:PRO:HD3	1.94	0.50
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.50
6:F:295:PRO:HA	6:F:336:LEU:HA	1.93	0.50
8:H:8:THR:O	8:H:12:PRO:HG2	2.11	0.50
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.11	0.50
17:X:57:LEU:CG	17:X:61:LYS:NZ	2.75	0.50
20:b:23:PHE:CE2	24:b:201:3PE:H252	2.47	0.50
22:r:48:LYS:O	22:r:49:LEU:HB2	2.12	0.50
3:C:210:ARG:CD	10:P:48:ARG:HD3	2.42	0.49
6:F:391:TRP:HH2	7:G:118:GLU:OE2	1.92	0.49
8:H:173:TRP:CZ2	8:H:262:GLU:OE2	2.65	0.49
8:H:224:PHE:CE1	8:H:228:TYR:CD1	3.00	0.49
28:H:401:UQ9:H10	28:H:401:UQ9:C5	2.42	0.49
9:I:36:TYR:HE2	9:I:38:TYR:CZ	2.29	0.49
10:P:59:PHE:CB	10:P:130:ILE:HD11	2.42	0.49
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.49
17:X:70:PHE:CE2	17:X:74:ILE:HD11	2.46	0.49
1:A:58:VAL:O	1:A:59:ALA:C	2.53	0.49
1:A:106:TRP:HD1	1:A:111:LEU:HD12	1.76	0.49
2:B:104:MET:HE1	2:B:132:ILE:HD12	1.92	0.49
4:D:209:LYS:HG2	22:r:27:ARG:NH2	2.27	0.49
5:E:247:GLY:O	6:F:64:LYS:HE2	2.12	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
7:G:617:ARG:NH1	16:W:129:HIS:N	2.60	0.49
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.49
12:R:38:TYR:CE1	12:R:44:ARG:HD2	2.47	0.49
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.47	0.49
6:F:293:SER:CA	6:F:338:ASP:HB3	2.42	0.49
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
7:G:632:ILE:O	7:G:632:ILE:CG1	2.60	0.49
8:H:85:LEU:HD23	8:H:105:ILE:HA	1.93	0.49
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.40	0.49
9:I:54:THR:CG2	20:b:13:TRP:HE1	2.26	0.49
12:R:43:TYR:C	12:R:45:ARG:N	2.69	0.49
18:Z:58:ARG:CB	20:b:45:ILE:HD11	2.42	0.49
21:q:55:PHE:CD2	22:r:26:LEU:HD22	2.47	0.49
21:q:74:PHE:HD2	21:q:75:TRP:CD2	2.31	0.49
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.42	0.49
5:E:68:ASN:ND2	23:s:49:ASN:HD21	2.07	0.49
5:E:180:VAL:HG13	5:E:181:ASN:H	1.77	0.49
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.49
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.49
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.94	0.49
12:R:81:GLY:HA2	12:R:88:HIS:CD2	2.47	0.49
16:W:103:ARG:O	16:W:104:THR:C	2.54	0.49
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.94	0.49
17:X:78:CYS:C	17:X:81:PRO:HD2	2.36	0.49
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.43	0.49
2:B:95:PHE:CZ	2:B:148:VAL:HB	2.47	0.49
3:C:104:ASN:O	22:r:97:PRO:HD3	2.12	0.49
4:D:324:GLY:O	4:D:329:ARG:NH1	2.45	0.49
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:140:ILE:O	8:H:143:GLU:HB3	2.13	0.49
24:H:402:3PE:H2A1	9:I:70:LEU:HD11	1.94	0.49
9:I:154:TYR:CD1	9:I:154:TYR:N	2.81	0.49
14:T:93:ILE:HG23	14:T:108:LEU:HD11	1.95	0.49
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.49
2:B:144:ALA:O	2:B:145:LEU:C	2.55	0.49
2:B:166:ASN:CB	2:B:190:TYR:HD2	2.24	0.49
2:B:170:TYR:O	2:B:171:TYR:CB	2.60	0.49
4:D:462:ASP:O	4:D:463:ARG:C	2.54	0.49
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.49
5:E:235:GLU:HB2	5:E:236:PRO:HD2	1.93	0.49
7:G:140:GLN:HG3	7:G:141:ASP:N	2.28	0.49
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.49
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
8:H:67:SER:C	8:H:69:SER:N	2.70	0.49
8:H:114:TYR:HB3	8:H:118:TRP:CZ3	2.47	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.49
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.43	0.49
14:T:93:ILE:HD13	14:T:108:LEU:HD22	1.95	0.49
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.93	0.49
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.49
33:q:201:CDL:OB9	33:q:201:CDL:H311	2.12	0.49
3:C:203:LEU:CD2	4:D:123:LEU:HD21	2.32	0.49
4:D:378:LEU:HD21	7:G:129:PRO:HD2	1.95	0.49
7:G:643:ARG:O	7:G:646:LEU:N	2.46	0.49
8:H:64:LEU:HD21	10:P:359:TYR:N	2.28	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.49
10:P:150:ARG:O	10:P:151:ALA:C	2.54	0.49
10:P:205:ASP:OD1	10:P:205:ASP:O	2.30	0.49
19:a:37:ARG:CB	19:a:48:MET:HE2	2.43	0.49
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.49
7:G:572:HIS:HB2	7:G:699:SER:OG	2.13	0.49
8:H:9:LEU:HD11	8:H:86:TRP:HB3	1.93	0.49
8:H:269:THR:O	8:H:273:ILE:HG12	2.12	0.49
17:X:38:LYS:O	17:X:42:GLU:HG3	2.11	0.49
17:X:44:MET:O	17:X:48:TRP:CD1	2.66	0.49
18:Z:114:THR:O	18:Z:114:THR:CG2	2.60	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:226:LYS:O	6:F:227:PRO:C	2.56	0.49
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.49
8:H:136:VAL:O	8:H:140:ILE:HG12	2.13	0.49
8:H:287:HIS:HE1	24:H:402:3PE:N	2.11	0.49
10:P:275:HIS:CE1	10:P:373:LYS:HG2	2.47	0.49
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.94	0.49
16:W:97:ILE:CG1	16:W:98:LYS:N	2.75	0.49
17:X:47:ARG:CZ	17:X:53:PRO:HG3	2.42	0.49
17:X:69:ASN:O	17:X:70:PHE:C	2.56	0.49
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.49
2:B:115:ASP:O	2:B:116:ARG:C	2.55	0.49
3:C:121:ARG:NH2	15:V:114:TRP:HA	2.27	0.49
4:D:274:ASP:H	4:D:325:ASP:HB2	1.78	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
7:G:49:VAL:HG13	7:G:102:ILE:HD13	1.94	0.49
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
9:I:72:MET:CE	22:r:16:SER:HB2	2.43	0.49
9:I:210:LEU:HD23	22:r:39:PRO:O	2.13	0.49
10:P:64:PHE:CZ	10:P:211:ASP:HB3	2.48	0.49
10:P:318:LYS:O	10:P:322:ILE:HG13	2.13	0.49
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.49
17:X:80:GLU:O	17:X:81:PRO:C	2.55	0.49
2:B:222:TYR:O	10:P:137:ARG:NH1	2.45	0.48
3:C:75:VAL:HG22	3:C:85:ILE:HG23	1.94	0.48
3:C:98:PHE:HB2	15:V:94:MET:HE3	1.95	0.48
5:E:77:ALA:C	5:E:80:PRO:HD2	2.38	0.48
7:G:33:GLU:OE2	7:G:40:SER:HA	2.14	0.48
17:X:53:PRO:CD	18:Z:116:TRP:CD1	2.96	0.48
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.48
22:r:32:ALA:HB1	22:r:36:GLN:HE21	1.78	0.48
4:D:203:MET:HE2	4:D:258:VAL:CG1	2.43	0.48
4:D:260:GLU:OE2	9:I:68:ARG:HG2	2.13	0.48
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.93	0.48
7:G:240:ALA:HA	9:I:117:LYS:NZ	2.28	0.48
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.48
9:I:79:ARG:CZ	22:r:20:LEU:HD22	2.43	0.48
10:P:197:GLU:HB3	10:P:259:VAL:HG23	1.93	0.48
10:P:318:LYS:HA	10:P:321:ARG:HH12	1.78	0.48
10:P:375:VAL:C	10:P:377:TYR:H	2.19	0.48
22:r:45:PRO:O	22:r:46:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:PHE:HD2	2:B:141:MET:HE3	1.77	0.48
2:B:95:PHE:CE2	2:B:145:LEU:HA	2.48	0.48
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.48
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.29	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
7:G:617:ARG:NH1	16:W:129:HIS:HA	2.25	0.48
8:H:182:ALA:HB1	24:H:402:3PE:H2I2	1.95	0.48
10:P:328:MET:HE1	10:P:377:TYR:C	2.39	0.48
11:Q:111:LEU:HA	12:R:47:ARG:NH1	2.29	0.48
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.95	0.48
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.48	0.48
21:q:48:TYR:OH	21:q:83:PRO:HD2	2.13	0.48
21:q:64:TYR:CD2	21:q:81:MET:HB2	2.48	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.95	0.48
6:F:50:ASP:CG	6:F:52:ARG:HB2	2.38	0.48
6:F:117:ALA:HB1	6:F:131:MET:SD	2.53	0.48
6:F:170:GLN:HB3	23:s:48:LEU:HD22	1.95	0.48
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.48
7:G:614:GLY:CA	10:P:41:ILE:HG21	2.43	0.48
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.48
10:P:315:THR:HB	10:P:318:LYS:H	1.78	0.48
16:W:87:ILE:O	16:W:91:MET:HG3	2.12	0.48
18:Z:97:ILE:HG13	18:Z:98:MET:HE3	1.95	0.48
21:q:85:GLU:HG2	21:q:98:PRO:HB3	1.94	0.48
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.48	0.48
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.75	0.48
4:D:199:PRO:HG3	4:D:262:LEU:HD11	1.95	0.48
5:E:142:ARG:HG3	5:E:182:ALA:CB	2.44	0.48
5:E:147:ILE:O	5:E:151:LEU:HD13	2.14	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
8:H:26:LYS:HB3	19:a:5:ILE:HG22	1.94	0.48
8:H:53:MET:HB3	8:H:57:MET:HE3	1.96	0.48
10:P:375:VAL:C	10:P:377:TYR:N	2.69	0.48
14:T:104:PHE:CD1	14:T:110:LEU:CB	2.94	0.48
16:W:46:VAL:N	16:W:47:PRO:HD2	2.29	0.48
3:C:67:ILE:CD1	15:V:47:TYR:HD2	2.24	0.48
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.26	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
8:H:142:TYR:HE1	8:H:285:LEU:CD2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:170:LEU:HG	10:P:171:ASN:N	2.28	0.48
16:W:120:ASP:OD1	16:W:121:PHE:N	2.46	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
2:B:68:ARG:NH1	2:B:70:ARG:HB3	2.28	0.48
6:F:102:MET:CG	6:F:149:MET:HB2	2.44	0.48
6:F:278:ILE:HG22	6:F:354:VAL:HB	1.94	0.48
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.48
12:R:46:VAL:HA	12:R:49:VAL:HG23	1.96	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.95	0.48
5:E:153:ARG:NH2	5:E:154:LYS:HE2	2.29	0.48
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.14	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.48
9:I:54:THR:HA	20:b:13:TRP:HE1	1.79	0.48
10:P:272:LEU:HG	10:P:375:VAL:CG2	2.26	0.48
10:P:278:LYS:HB3	10:P:288:PHE:CE2	2.49	0.48
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.48
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.48
13:S:50:ASN:O	13:S:51:LEU:C	2.57	0.48
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.29	0.48
15:V:12:VAL:CG1	15:V:13:GLY:H	2.23	0.48
18:Z:58:ARG:NH2	20:b:46:ASN:HA	2.29	0.48
22:r:25:GLN:H	22:r:25:GLN:CD	2.21	0.48
2:B:154:GLU:HB3	8:H:59:GLU:CB	2.44	0.48
6:F:261:TRP:CE2	6:F:265:PHE:CE2	3.02	0.48
6:F:261:TRP:CE2	6:F:265:PHE:HE2	2.31	0.48
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.44	0.48
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.48
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.96	0.48
7:G:612:PRO:HG2	16:W:129:HIS:CD2	2.48	0.48
12:R:60:ALA:O	12:R:61:ILE:C	2.56	0.48
16:W:42:TRP:O	16:W:46:VAL:HG23	2.14	0.48
17:X:38:LYS:HD2	17:X:38:LYS:HA	1.67	0.48
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.43	0.48
18:Z:129:THR:HB	18:Z:132:GLU:CG	2.43	0.48
2:B:170:TYR:O	2:B:171:TYR:HB2	2.14	0.48
4:D:82:LEU:HD22	4:D:101:LEU:HD11	1.95	0.48
5:E:190:ASN:HB3	5:E:215:PRO:HB3	1.96	0.48
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.43	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.48
8:H:225:MET:SD	28:H:401:UQ9:H20B	2.54	0.48
14:T:134:ASP:O	14:T:138:LEU:HG	2.14	0.48
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.48
21:q:56:PHE:O	21:q:59:HIS:CD2	2.67	0.48
2:B:95:PHE:HB3	2:B:97:LEU:HD13	1.95	0.47
2:B:112:TYR:CE1	9:I:84:ILE:HD11	2.48	0.47
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.47
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.47
8:H:17:MET:SD	8:H:225:MET:HA	2.54	0.47
9:I:89:GLU:OE1	21:q:58:ARG:HD2	2.13	0.47
9:I:105:ARG:HH12	12:R:58:ASN:HB2	1.78	0.47
18:Z:58:ARG:HH21	20:b:46:ASN:HA	1.78	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.47
22:r:7:VAL:HG13	22:r:8:ILE:N	2.28	0.47
4:D:185:MET:SD	4:D:204:PHE:HZ	2.37	0.47
6:F:61:ASP:O	6:F:140:GLU:OE1	2.33	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.47
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.47
7:G:341:ILE:HG13	7:G:545:LEU:HD11	1.95	0.47
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.47
10:P:150:ARG:NE	10:P:190:GLU:HG2	2.27	0.47
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.39	0.47
18:Z:125:TYR:HA	18:Z:128:ARG:HB2	1.95	0.47
22:r:54:TYR:HA	22:r:57:ARG:HG2	1.96	0.47
23:s:55:PHE:O	23:s:56:ARG:C	2.57	0.47
1:A:106:TRP:HZ3	20:b:19:LEU:HD21	1.78	0.47
2:B:97:LEU:HD21	2:B:141:MET:HG2	1.96	0.47
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.78	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.47
7:G:638:THR:O	7:G:639:LEU:C	2.56	0.47
9:I:188:GLU:OE2	12:R:33:HIS:NE2	2.47	0.47
10:P:81:ILE:HD11	12:R:46:VAL:HG11	1.96	0.47
10:P:335:LEU:O	10:P:336:GLU:HB2	2.14	0.47
11:Q:129:SER:HB2	15:V:116:ILE:HD12	1.97	0.47
3:C:203:LEU:HD21	4:D:123:LEU:HD23	1.93	0.47
4:D:85:GLY:O	4:D:89:PRO:HD3	2.14	0.47
5:E:45:GLU:H	5:E:45:GLU:CD	2.21	0.47
6:F:37:ASP:HA	6:F:40:ARG:HD2	1.94	0.47
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
8:H:292:ASN:O	20:b:18:VAL:HG11	2.14	0.47
9:I:35:THR:CG2	22:r:107:SER:HA	2.44	0.47
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.02	0.47
9:I:123:CYS:SG	25:I:302:SF4:S3	3.12	0.47
10:P:276:LEU:O	10:P:280:ILE:HG13	2.15	0.47
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.13	0.47
16:W:46:VAL:O	16:W:50:VAL:HG23	2.14	0.47
16:W:94:GLN:HG3	16:W:98:LYS:NZ	2.29	0.47
4:D:240:LEU:HG	4:D:244:ILE:HD11	1.96	0.47
4:D:300:TRP:HE1	4:D:302:LEU:HD21	1.80	0.47
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.47
5:E:109:MET:HE2	7:G:196:GLY:HA3	1.96	0.47
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.96	0.47
9:I:107:PRO:HG3	21:q:106:ARG:NH1	2.29	0.47
10:P:311:GLU:O	10:P:312:PRO:C	2.57	0.47
17:X:39:THR:CG2	17:X:40:ASN:N	2.77	0.47
17:X:80:GLU:HB3	17:X:81:PRO:HD3	1.96	0.47
2:B:75:VAL:HG13	2:B:218:LEU:HB3	1.95	0.47
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:217:GLU:CD	6:F:224:ARG:HH22	2.23	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
8:H:3:PHE:O	8:H:4:ILE:C	2.58	0.47
9:I:116:CYS:O	9:I:117:LYS:HB2	2.12	0.47
13:S:27:SER:H	13:S:34:ARG:HH22	1.62	0.47
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.49	0.47
17:X:25:LEU:O	17:X:29:ALA:N	2.48	0.47
2:B:98:ALA:HB3	2:B:135:GLY:HA2	1.96	0.47
2:B:174:SER:HA	3:C:203:LEU:CD2	2.45	0.47
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.79	0.47
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.47
3:C:203:LEU:CD2	4:D:123:LEU:CD2	2.87	0.47
4:D:362:LYS:HG3	22:r:54:TYR:CZ	2.50	0.47
5:E:114:VAL:HG13	5:E:118:TYR:CE2	2.50	0.47
6:F:122:PRO:HG3	6:F:373:PHE:CZ	2.50	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.47
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:394:LYS:HB2	7:G:155:GLU:HG2	1.95	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.93	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:70:LEU:CD2	8:H:121:TRP:HD1	2.27	0.47
10:P:55:VAL:HG12	10:P:123:SER:HA	1.96	0.47
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.96	0.47
10:P:207:PHE:CD2	10:P:241:TYR:HD1	2.33	0.47
10:P:235:THR:O	10:P:236:VAL:C	2.56	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
12:R:38:TYR:OH	12:R:47:ARG:NH2	2.48	0.47
13:S:58:CYS:HB2	13:S:61:VAL:CG1	2.43	0.47
17:X:57:LEU:HD21	17:X:61:LYS:HZ1	1.79	0.47
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.15	0.47
19:a:2:TRP:O	19:a:5:ILE:HG12	2.14	0.47
5:E:153:ARG:HG3	5:E:154:LYS:N	2.28	0.47
6:F:254:ILE:O	6:F:258:GLY:N	2.48	0.47
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.95	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
10:P:76:MET:HE1	10:P:254:LYS:CE	2.45	0.47
10:P:192:ARG:HH21	10:P:200:ILE:HG12	1.80	0.47
10:P:209:ARG:O	10:P:210:GLU:HB2	2.15	0.47
16:W:32:LYS:O	16:W:36:ARG:HG3	2.15	0.47
17:X:137:LEU:HA	20:b:58:ARG:NH2	2.30	0.47
3:C:73:GLN:HG2	15:V:103:LEU:HD21	1.96	0.47
3:C:221:GLU:OE1	16:W:114:GLU:HB2	2.14	0.47
4:D:320:ILE:HD11	9:I:36:TYR:CE2	2.49	0.47
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.45	0.47
5:E:163:THR:HB	5:E:164:PRO:HD2	1.97	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.47
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.47
7:G:593:SER:O	7:G:643:ARG:NH2	2.46	0.47
7:G:642:VAL:O	7:G:645:ARG:HB3	2.14	0.47
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.47
8:H:196:ALA:C	8:H:198:PHE:N	2.70	0.47
10:P:237:LYS:HZ2	10:P:322:ILE:HG23	1.80	0.47
15:V:116:ILE:HG23	15:V:116:ILE:O	2.15	0.47
17:X:134:ASP:O	17:X:135:ARG:C	2.58	0.47
3:C:70:LYS:O	15:V:104:VAL:N	2.47	0.47
6:F:225:LEU:O	6:F:228:PRO:HD2	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.47
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.47
16:W:120:ASP:HB3	16:W:123:SER:HG	1.79	0.47
3:C:66:GLU:O	3:C:69:PRO:HD3	2.14	0.46
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.46
6:F:318:ILE:HG22	6:F:326:LEU:CA	2.45	0.46
6:F:424:ILE:HG13	7:G:76:ARG:HD3	1.97	0.46
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.46
9:I:54:THR:HA	20:b:13:TRP:NE1	2.30	0.46
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.44	0.46
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.46
4:D:139:LEU:HD13	4:D:424:ILE:HG21	1.98	0.46
4:D:142:VAL:HG11	4:D:185:MET:CG	2.44	0.46
5:E:180:VAL:CG1	5:E:181:ASN:N	2.78	0.46
6:F:224:ARG:HD3	11:Q:164:PHE:CE1	2.51	0.46
6:F:233:VAL:CG1	11:Q:164:PHE:HB2	2.43	0.46
6:F:274:LYS:HZ2	6:F:352:ALA:HB3	1.80	0.46
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.46
7:G:165:ILE:O	7:G:213:MET:HA	2.16	0.46
7:G:462:PHE:CD1	7:G:465:VAL:HB	2.50	0.46
8:H:14:LEU:O	8:H:17:MET:HB3	2.15	0.46
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.46
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.46
12:R:38:TYR:CD2	12:R:48:PHE:HE2	2.33	0.46
13:S:40:ARG:HH12	13:S:84:ALA:HB1	1.79	0.46
17:X:82:PHE:HB2	17:X:107:PHE:CE1	2.50	0.46
18:Z:54:ASN:HA	18:Z:57:ARG:HD3	1.96	0.46
4:D:159:LEU:HD22	22:r:60:ARG:HG3	1.97	0.46
4:D:259:GLU:HB3	18:Z:25:LEU:HD21	1.97	0.46
5:E:81:VAL:HG21	5:E:104:LEU:HD21	1.95	0.46
6:F:93:PHE:O	6:F:94:PRO:C	2.58	0.46
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.47	0.46
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.46
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.46
9:I:178:GLU:OE2	21:q:119:ALA:HB2	2.16	0.46
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.50	0.46
19:a:49:GLU:CD	19:a:52:ARG:HH11	2.22	0.46
21:q:117:VAL:HB	21:q:122:GLU:HB3	1.96	0.46
22:r:91:GLU:OE1	22:r:91:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:s:52:LEU:HB3	23:s:56:ARG:HH11	1.81	0.46
1:A:113:TRP:CH2	8:H:287:HIS:CD2	3.02	0.46
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.97	0.46
7:G:75:CYS:SG	26:G:803:FES:S1	3.12	0.46
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.97	0.46
18:Z:69:ILE:HG23	20:b:54:PRO:CD	2.46	0.46
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.46
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.81	0.46
1:A:65:PHE:O	1:A:69:ILE:HG13	2.15	0.46
1:A:104:TYR:CZ	1:A:108:GLN:HG3	2.50	0.46
2:B:202:LEU:HD21	9:I:86:TYR:HB2	1.95	0.46
4:D:278:VAL:O	15:V:12:VAL:HG11	2.15	0.46
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.21	0.46
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.97	0.46
10:P:245:VAL:HA	10:P:265:PHE:CD2	2.49	0.46
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.50	0.46
21:q:137:TRP:CH2	21:q:140:PRO:HD3	2.51	0.46
4:D:292:MET:HA	4:D:329:ARG:HD3	1.97	0.46
4:D:293:LEU:CD2	4:D:300:TRP:HB3	2.46	0.46
6:F:88:ARG:HB2	6:F:247:THR:OG1	2.16	0.46
6:F:330:SER:O	6:F:333:GLU:HG2	2.16	0.46
6:F:394:LYS:HD3	7:G:155:GLU:HB3	1.97	0.46
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.46
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.46
8:H:186:PHE:CZ	8:H:270:PHE:HD1	2.32	0.46
19:a:22:SER:O	19:a:23:THR:C	2.57	0.46
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.28	0.46
4:D:301:ASP:HB2	4:D:318:VAL:HG21	1.98	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
6:F:336:LEU:HD23	6:F:336:LEU:H	1.79	0.46
7:G:648:GLU:HG2	13:S:66:TRP:CZ2	2.50	0.46
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.50	0.46
8:H:292:ASN:HD21	24:H:402:3PE:H122	1.80	0.46
10:P:66:GLY:O	10:P:69:VAL:N	2.49	0.46
10:P:295:LEU:O	10:P:296:PHE:C	2.59	0.46
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.46
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.46
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.46
8:H:17:MET:CE	8:H:225:MET:CG	2.94	0.46
8:H:196:ALA:CB	8:H:274:ARG:HA	2.44	0.46
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:104:CYS:C	12:R:106:TYR:N	2.73	0.46
20:b:28:LEU:O	20:b:32:MET:HG2	2.15	0.46
21:q:59:HIS:HE1	21:q:60:ARG:NE	2.14	0.46
4:D:163:PRO:HG2	4:D:168:GLN:HG2	1.96	0.46
6:F:77:LEU:O	6:F:81:LYS:HG2	2.16	0.46
6:F:87:GLY:H	6:F:92:GLY:CA	2.29	0.46
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.46
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.46
9:I:88:PHE:CE2	21:q:30:ALA:HA	2.51	0.46
10:P:288:PHE:CZ	10:P:290:PRO:HB3	2.51	0.46
10:P:331:ASP:O	10:P:332:LEU:C	2.59	0.46
12:R:72:VAL:HG21	12:R:77:ILE:CD1	2.46	0.46
13:S:27:SER:O	13:S:34:ARG:NH2	2.48	0.46
14:T:100:VAL:O	14:T:142:GLN:HB2	2.15	0.46
16:W:50:VAL:HA	16:W:55:LEU:HD12	1.97	0.46
2:B:104:MET:HB2	2:B:104:MET:HE3	1.61	0.46
4:D:137:ASP:O	4:D:223:HIS:CE1	2.68	0.46
4:D:356:ILE:HD11	4:D:357:LYS:HE3	1.98	0.46
6:F:261:TRP:CD2	6:F:265:PHE:HE2	2.34	0.46
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.46
10:P:261:LYS:HB2	10:P:263:PHE:CE1	2.51	0.46
17:X:46:CYS:HB3	17:X:56:CYS:SG	2.56	0.46
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.97	0.45
3:C:186:ILE:HD12	4:D:429:PHE:CZ	2.52	0.45
6:F:45:LEU:O	6:F:46:TYR:HB2	2.16	0.45
6:F:120:GLY:O	6:F:121:GLU:C	2.59	0.45
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.45
9:I:93:LEU:O	21:q:93:MET:CG	2.63	0.45
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.45
15:V:22:GLU:O	15:V:26:ILE:HG12	2.16	0.45
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.45
17:X:28:ALA:HB2	17:X:82:PHE:CZ	2.52	0.45
17:X:35:GLN:HG3	17:X:70:PHE:HE1	1.80	0.45
17:X:54:ARG:NH2	18:Z:116:TRP:HB2	2.31	0.45
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.98	0.45
3:C:85:ILE:HD11	3:C:140:ILE:HD11	1.98	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.97	0.45
5:E:55:THR:O	5:E:56:PRO:C	2.59	0.45
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.45
6:F:270:ASN:HD21	6:F:340:ASP:N	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:43:VAL:HB	7:G:47:THR:HG21	1.99	0.45
7:G:106:SER:O	7:G:107:GLU:C	2.57	0.45
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
16:W:71:MET:C	16:W:73:ASN:N	2.70	0.45
19:a:58:ASN:HB2	19:a:61:TYR:CE2	2.51	0.45
3:C:70:LYS:O	15:V:103:LEU:HA	2.16	0.45
4:D:250:ASN:HA	22:r:23:LYS:HE3	1.98	0.45
7:G:301:ARG:HA	7:G:572:HIS:CD2	2.51	0.45
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.97	0.45
7:G:649:VAL:HA	13:S:20:ARG:NE	2.31	0.45
8:H:88:PRO:CG	8:H:105:ILE:HD11	2.47	0.45
10:P:259:VAL:H	10:P:261:LYS:HG2	1.82	0.45
12:R:51:ARG:HD2	21:q:125:VAL:CG1	2.46	0.45
13:S:51:LEU:CD1	13:S:95:LEU:HD12	2.46	0.45
14:T:144:ILE:O	14:T:148:ILE:HG12	2.15	0.45
15:V:50:GLN:HE22	22:r:93:LYS:HG3	1.80	0.45
16:W:83:ASP:O	16:W:87:ILE:HG12	2.17	0.45
17:X:94:MET:O	17:X:95:GLN:C	2.59	0.45
21:q:68:MET:O	21:q:69:ASN:C	2.57	0.45
22:r:20:LEU:HD12	22:r:21:GLN:N	2.31	0.45
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.45
2:B:90:LEU:O	2:B:92:PRO:HD3	2.16	0.45
2:B:166:ASN:O	2:B:166:ASN:CG	2.59	0.45
4:D:362:LYS:O	4:D:384:LEU:HD21	2.17	0.45
6:F:50:ASP:OD2	6:F:52:ARG:HB2	2.15	0.45
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.45
10:P:157:LYS:O	10:P:160:GLY:N	2.49	0.45
17:X:5:VAL:CG1	17:X:7:LEU:HG	2.46	0.45
17:X:137:LEU:O	17:X:138:PRO:C	2.58	0.45
18:Z:36:PHE:O	18:Z:40:ILE:HG12	2.16	0.45
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.31	0.45
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.45
6:F:47:GLY:O	6:F:48:ARG:HB2	2.17	0.45
6:F:48:ARG:HA	6:F:48:ARG:NH1	2.29	0.45
6:F:61:ASP:O	6:F:256:ARG:NH2	2.50	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.31	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
8:H:312:ALA:HB2	20:b:41:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:203:ALA:CB	21:q:88:ARG:NH1	2.80	0.45
10:P:156:SER:HB2	10:P:161:VAL:CG2	2.47	0.45
10:P:170:LEU:HD12	10:P:171:ASN:H	1.81	0.45
10:P:333:PRO:HB2	10:P:337:ASP:CB	2.36	0.45
15:V:99:PRO:HD2	15:V:100:TRP:CE3	2.51	0.45
17:X:78:CYS:SG	17:X:114:LYS:HD2	2.56	0.45
18:Z:70:ALA:O	18:Z:73:PRO:HD2	2.16	0.45
1:A:65:PHE:CZ	8:H:294:LEU:HD21	2.49	0.45
3:C:124:ARG:HD2	11:Q:140:LYS:HZ1	1.82	0.45
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.98	0.45
5:E:222:PHE:H	5:E:225:GLU:CD	2.23	0.45
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.98	0.45
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.45
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.51	0.45
9:I:155:CYS:SG	25:I:302:SF4:S2	3.14	0.45
12:R:101:THR:HG22	12:R:112:LYS:HB2	1.99	0.45
21:q:44:TYR:CE1	21:q:68:MET:HE3	2.51	0.45
1:A:73:LEU:N	1:A:74:PRO:HD2	2.31	0.45
3:C:217:ARG:HH12	16:W:112:GLU:CB	2.27	0.45
4:D:174:PHE:O	4:D:178:THR:HG23	2.17	0.45
5:E:58:ASN:O	5:E:62:ILE:HG12	2.16	0.45
5:E:73:HIS:ND1	6:F:236:PHE:CD1	2.85	0.45
5:E:176:LEU:HD13	5:E:186:GLN:HB2	1.98	0.45
5:E:182:ALA:O	5:E:183:PRO:C	2.59	0.45
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.45
7:G:283:GLU:O	7:G:283:GLU:CG	2.51	0.45
7:G:639:LEU:O	7:G:640:ASP:C	2.58	0.45
8:H:205:SER:OG	8:H:213:VAL:HG21	2.17	0.45
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.52	0.45
9:I:188:GLU:OE1	12:R:56:ASN:CB	2.65	0.45
17:X:40:ASN:O	17:X:41:LYS:C	2.58	0.45
17:X:131:VAL:N	20:b:59:ASP:OD1	2.49	0.45
18:Z:66:GLU:HA	18:Z:69:ILE:CG1	2.46	0.45
18:Z:68:ARG:O	18:Z:69:ILE:C	2.60	0.45
20:b:19:LEU:HD22	24:b:201:3PE:H221	1.98	0.45
20:b:45:ILE:N	20:b:80:TRP:HH2	2.14	0.45
21:q:44:TYR:CD1	21:q:68:MET:HG3	2.52	0.45
21:q:68:MET:HG2	21:q:115:PHE:HE2	1.82	0.45
33:q:201:CDL:H341	33:q:201:CDL:H171	1.99	0.45
22:r:50:SER:O	22:r:51:ASN:C	2.58	0.45
2:B:100:CYS:CB	2:B:134:ALA:HB1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:THR:O	2:B:200:ALA:HB3	2.16	0.45
4:D:460:GLU:O	4:D:463:ARG:HG2	2.16	0.45
5:E:87:ARG:NH2	6:F:163:TYR:CD1	2.85	0.45
5:E:192:TYR:OH	5:E:213:PRO:HD2	2.16	0.45
6:F:72:GLY:O	6:F:76:ILE:HG13	2.17	0.45
6:F:106:SER:HB2	6:F:111:LYS:HZ2	1.81	0.45
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.45
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.45
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.45
7:G:341:ILE:HD12	7:G:555:ILE:CG1	2.47	0.45
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.45
13:S:40:ARG:HD2	13:S:88:THR:OG1	2.16	0.45
14:T:100:VAL:O	14:T:141:PRO:HD2	2.17	0.45
16:W:23:ILE:CD1	16:W:84:LEU:HD21	2.47	0.45
21:q:86:TRP:CD2	21:q:98:PRO:HG2	2.52	0.45
22:r:54:TYR:CE2	22:r:58:ASP:HB3	2.51	0.45
1:A:102:LEU:HD11	1:A:106:TRP:HE1	1.82	0.45
2:B:95:PHE:CD2	2:B:141:MET:HE3	2.52	0.45
4:D:179:ARG:HH22	4:D:303:ARG:HD3	1.82	0.45
4:D:194:ILE:HD12	4:D:268:TRP:CZ3	2.51	0.45
4:D:243:ASP:OD2	22:r:31:ILE:HG13	2.16	0.45
6:F:75:TRP:O	6:F:79:GLU:HG2	2.17	0.45
6:F:292:MET:O	6:F:293:SER:HB2	2.17	0.45
7:G:36:VAL:HG22	7:G:102:ILE:HD12	1.98	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
8:H:30:TYR:CE1	19:a:1:MET:C	2.95	0.45
10:P:218:ALA:HB2	10:P:280:ILE:CG2	2.47	0.45
16:W:67:ARG:HD2	16:W:71:MET:SD	2.57	0.45
2:B:97:LEU:HB2	2:B:134:ALA:O	2.17	0.45
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.45
4:D:201:PHE:HB2	8:H:32:GLN:HB3	1.98	0.45
5:E:243:GLY:O	6:F:257:ARG:HD2	2.17	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
7:G:160:VAL:O	7:G:174:THR:HG22	2.17	0.45
7:G:621:LYS:HZ3	16:W:131:PRO:HD3	1.81	0.45
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.45
8:H:61:MET:CE	8:H:216:ALA:H	2.30	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.45
9:I:67:ILE:HG13	29:I:301:PC1:H231	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.45
13:S:24:CYS:SG	13:S:61:VAL:O	2.75	0.45
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.45
14:T:123:GLU:HG2	14:T:130:ILE:CD1	2.47	0.45
16:W:97:ILE:HG13	16:W:98:LYS:H	1.78	0.45
19:a:1:MET:HG3	33:q:201:CDL:HB21	1.99	0.45
6:F:227:PRO:HB3	7:G:95:PRO:HD2	1.98	0.44
6:F:270:ASN:HD22	6:F:338:ASP:CB	2.29	0.44
6:F:273:THR:HA	6:F:292:MET:H	1.82	0.44
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.44
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.44
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.44
7:G:544:MET:HE3	7:G:565:PHE:CE2	2.42	0.44
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.47	0.44
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.47	0.44
8:H:196:ALA:O	8:H:198:PHE:N	2.51	0.44
10:P:225:ALA:HB1	10:P:291:TYR:CD1	2.52	0.44
12:R:70:ASN:HB2	12:R:111:PHE:HD2	1.81	0.44
17:X:58:LYS:O	17:X:59:GLU:C	2.58	0.44
23:s:52:LEU:O	23:s:56:ARG:HG2	2.18	0.44
3:C:98:PHE:HE1	15:V:44:TYR:CD1	2.34	0.44
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.50	0.44
5:E:62:ILE:O	5:E:66:VAL:HG23	2.17	0.44
5:E:226:PRO:HB2	5:E:229:GLY:O	2.16	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
7:G:643:ARG:HA	7:G:646:LEU:HD12	1.98	0.44
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.44
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.44
8:H:307:LEU:HD11	18:Z:47:TYR:CD1	2.52	0.44
9:I:184:LEU:HD23	11:Q:114:TRP:CH2	2.51	0.44
10:P:220:TYR:HA	10:P:223:PHE:CD2	2.51	0.44
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.44
15:V:56:LEU:O	15:V:57:ASP:C	2.61	0.44
16:W:45:GLU:O	16:W:46:VAL:C	2.58	0.44
21:q:4:VAL:HA	21:q:7:LEU:HD12	1.99	0.44
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.44
2:B:153:PRO:HB3	8:H:58:LYS:HD3	1.98	0.44
2:B:155:PRO:HD3	8:H:59:GLU:CG	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.44
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.44
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.98	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:17:MET:HE1	8:H:225:MET:CB	2.42	0.44
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.81	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.44
10:P:55:VAL:HA	10:P:79:GLN:O	2.18	0.44
10:P:82:ILE:HD12	10:P:105:PHE:CE1	2.52	0.44
10:P:238:GLN:HB3	10:P:326:ASP:OD2	2.17	0.44
13:S:42:VAL:O	13:S:46:LYS:HG3	2.18	0.44
19:a:37:ARG:HB2	19:a:48:MET:HE2	1.99	0.44
21:q:3:LEU:HD12	21:q:6:VAL:CG2	2.48	0.44
2:B:114:MET:HE3	2:B:119:VAL:HG12	1.97	0.44
4:D:158:LEU:O	4:D:392:PRO:HG2	2.18	0.44
5:E:62:ILE:HG23	5:E:81:VAL:HG22	2.00	0.44
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.44
7:G:68:ARG:O	7:G:189:ILE:HD11	2.17	0.44
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.44
8:H:303:TRP:CZ3	20:b:28:LEU:HG	2.52	0.44
10:P:358:THR:O	10:P:359:TYR:C	2.60	0.44
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.44
18:Z:69:ILE:CG2	20:b:54:PRO:CD	2.96	0.44
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.16	0.44
2:B:170:TYR:O	2:B:171:TYR:CD2	2.71	0.44
4:D:97:LEU:CG	4:D:99:LEU:CD2	2.57	0.44
4:D:97:LEU:HD23	4:D:99:LEU:HD21	1.85	0.44
4:D:159:LEU:O	4:D:161:ILE:HG23	2.17	0.44
4:D:301:ASP:OD2	4:D:318:VAL:HG22	2.16	0.44
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.44
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.44
8:H:184:MET:SD	8:H:296:LEU:HD23	2.58	0.44
10:P:59:PHE:CD1	10:P:83:PRO:HG2	2.52	0.44
10:P:245:VAL:HA	10:P:265:PHE:HD2	1.82	0.44
10:P:298:TYR:O	10:P:299:SER:C	2.61	0.44
10:P:315:THR:O	10:P:316:LYS:C	2.58	0.44
12:R:40:GLU:HG3	12:R:41:LYS:HG2	2.00	0.44
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.44
2:B:223:ARG:C	10:P:138:ASN:HD21	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.44
5:E:181:ASN:OD1	5:E:221:ARG:HD2	2.18	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
6:F:383:THR:HG23	7:G:120:LEU:HD23	1.98	0.44
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.44
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.44
10:P:168:SER:O	10:P:202:ARG:HA	2.17	0.44
10:P:327:VAL:HG22	10:P:328:MET:N	2.32	0.44
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.44
3:C:55:LYS:HE2	3:C:55:LYS:HB3	1.83	0.44
4:D:121:GLU:OE2	4:D:463:ARG:HD2	2.18	0.44
5:E:231:THR:CG2	6:F:303:HIS:HA	2.47	0.44
6:F:231:ALA:O	6:F:239:PRO:HA	2.18	0.44
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.99	0.44
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.27	0.44
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.44
10:P:130:ILE:N	10:P:130:ILE:HD12	2.33	0.44
21:q:55:PHE:HD1	21:q:55:PHE:H	1.65	0.44
21:q:92:CYS:O	22:r:34:ARG:HG3	2.18	0.44
1:A:112:GLU:O	1:A:113:TRP:C	2.58	0.44
2:B:81:LEU:HD11	29:q:202:PC1:H361	2.00	0.44
2:B:91:TRP:O	2:B:129:ASP:N	2.49	0.44
2:B:98:ALA:HA	4:D:116:LEU:HD21	1.99	0.44
2:B:138:THR:HG21	4:D:116:LEU:HA	2.00	0.44
2:B:170:TYR:OH	4:D:131:GLN:O	2.36	0.44
2:B:194:CYS:CB	2:B:195:PRO:HD3	2.42	0.44
4:D:390:GLN:OE1	7:G:145:MET:HE1	2.18	0.44
6:F:379:CYS:SG	25:F:502:SF4:S2	3.16	0.44
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.44
7:G:466:LEU:HD13	7:G:500:ILE:CG1	2.48	0.44
7:G:541:PRO:HB2	7:G:561:PRO:CG	2.46	0.44
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.44
13:S:16:LEU:HD13	13:S:69:TYR:CE1	2.52	0.44
14:T:141:PRO:O	14:T:144:ILE:HB	2.18	0.44
16:W:71:MET:O	16:W:72:LYS:C	2.59	0.44
17:X:140:ASN:HD21	17:X:144:SER:N	2.16	0.44
20:b:59:ASP:OD1	20:b:59:ASP:N	2.49	0.44
2:B:97:LEU:HD23	2:B:136:THR:O	2.18	0.44
4:D:93:GLY:HA3	4:D:458:PHE:HD2	1.83	0.44
4:D:142:VAL:HG11	4:D:185:MET:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:384:LEU:HD23	7:G:144:MET:HE1	2.00	0.44
5:E:180:VAL:HG11	5:E:224:CYS:CB	2.48	0.44
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.98	0.44
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.44
8:H:55:LEU:O	8:H:58:LYS:HB3	2.18	0.44
8:H:134:ARG:NH1	8:H:204:GLU:HG3	2.31	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.44
20:b:15:LYS:O	20:b:15:LYS:HG3	2.18	0.44
20:b:38:TYR:O	20:b:39:THR:C	2.59	0.44
1:A:63:LEU:O	1:A:64:LEU:C	2.61	0.43
1:A:95:VAL:HG11	8:H:302:MET:CG	2.48	0.43
1:A:109:LYS:HD2	1:A:112:GLU:HB2	2.00	0.43
2:B:153:PRO:CB	8:H:58:LYS:HD3	2.48	0.43
3:C:124:ARG:HH12	3:C:125:PHE:HZ	1.56	0.43
3:C:203:LEU:CD1	4:D:123:LEU:CD2	2.85	0.43
4:D:97:LEU:HD21	4:D:99:LEU:CD2	2.42	0.43
4:D:152:SER:HA	4:D:229:PRO:HA	2.00	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.43
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.43
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.43
7:G:593:SER:OG	7:G:639:LEU:HD22	2.17	0.43
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.52	0.43
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.43
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.48	0.43
9:I:79:ARG:NE	22:r:20:LEU:HD22	2.33	0.43
10:P:209:ARG:CA	10:P:352:VAL:HG22	2.47	0.43
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.43
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.43
14:T:140:CYS:SG	14:T:143:GLU:CB	3.03	0.43
17:X:37:ASP:OD2	20:b:70:PRO:HD2	2.17	0.43
21:q:23:LEU:HD11	21:q:33:ILE:HD13	1.99	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
4:D:133:LEU:O	4:D:134:PRO:C	2.60	0.43
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.43
4:D:303:ARG:CG	4:D:401:GLU:HB3	2.48	0.43
5:E:242:PHE:O	6:F:257:ARG:NH1	2.50	0.43
6:F:126:LYS:O	6:F:129:GLU:HG2	2.18	0.43
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.17	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.43
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.43
13:S:30:SER:O	13:S:31:GLN:C	2.59	0.43
3:C:70:LYS:HG2	15:V:104:VAL:HG23	2.01	0.43
6:F:226:LYS:HD3	6:F:226:LYS:HA	1.84	0.43
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.43
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.43
7:G:450:LYS:CD	7:G:453:GLN:HG3	2.31	0.43
7:G:621:LYS:NZ	16:W:131:PRO:HD3	2.33	0.43
8:H:13:ILE:HD13	8:H:13:ILE:HA	1.87	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
12:R:43:TYR:C	12:R:45:ARG:H	2.27	0.43
13:S:18:GLU:O	13:S:19:ILE:HD13	2.18	0.43
1:A:87:MET:HE3	1:A:87:MET:HB3	1.84	0.43
3:C:97:THR:O	15:V:90:LEU:CD1	2.66	0.43
4:D:304:LYS:HG3	4:D:316:PHE:CZ	2.53	0.43
5:E:117:PHE:HB2	6:F:220:GLN:HE21	1.83	0.43
7:G:36:VAL:O	7:G:39:GLN:HG2	2.19	0.43
11:Q:55:VAL:HG21	16:W:78:ASP:OD1	2.18	0.43
13:S:19:ILE:CD1	13:S:94:VAL:HG11	2.48	0.43
14:T:132:ASP:O	14:T:133:ILE:C	2.60	0.43
17:X:46:CYS:SG	17:X:135:ARG:HD3	2.58	0.43
18:Z:121:ILE:HA	18:Z:124:MET:HE2	1.99	0.43
24:b:201:3PE:H281	24:b:201:3PE:H252	1.72	0.43
1:A:10:ASN:ND2	8:H:84:SER:OG	2.51	0.43
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.43
4:D:198:THR:HG21	8:H:275:ALA:HB1	2.00	0.43
5:E:184:MET:HE3	5:E:184:MET:HB3	1.95	0.43
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.43
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.48	0.43
7:G:401:LEU:HD21	7:G:466:LEU:HD11	2.01	0.43
7:G:557:ARG:HD3	21:q:144:TYR:CZ	2.53	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
24:H:402:3PE:H372	9:I:61:LEU:O	2.18	0.43
10:P:76:MET:HE1	10:P:254:LYS:HE2	2.01	0.43
10:P:170:LEU:O	10:P:171:ASN:CG	2.61	0.43
17:X:120:PRO:HG3	20:b:71:GLN:NE2	2.34	0.43
2:B:93:MET:HE2	2:B:93:MET:HB3	1.83	0.43
2:B:199:GLU:O	2:B:200:ALA:C	2.60	0.43
3:C:73:GLN:HE21	15:V:112:TRP:HE1	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.43
4:D:220:ALA:HB3	4:D:224:ALA:HA	2.00	0.43
4:D:232:VAL:O	4:D:356:ILE:HD12	2.18	0.43
6:F:42:PHE:CD1	6:F:137:LYS:HD2	2.54	0.43
6:F:67:GLU:O	6:F:71:LYS:HG2	2.18	0.43
6:F:257:ARG:CG	6:F:261:TRP:CD2	2.93	0.43
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.43
7:G:141:ASP:O	7:G:145:MET:HG2	2.18	0.43
7:G:339:ALA:O	7:G:545:LEU:HD12	2.18	0.43
8:H:17:MET:HE1	8:H:225:MET:CG	2.48	0.43
8:H:142:TYR:CD2	8:H:289:LEU:HD12	2.53	0.43
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.43
10:P:318:LYS:O	10:P:319:VAL:C	2.58	0.43
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.43
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.43
17:X:26:LYS:HE2	17:X:26:LYS:HB3	1.74	0.43
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.53	0.43
33:q:201:CDL:HB61	33:q:201:CDL:OA9	2.18	0.43
22:r:54:TYR:C	22:r:56:THR:N	2.76	0.43
2:B:99:CYS:HB3	4:D:141:TYR:HB2	2.00	0.43
2:B:112:TYR:OH	9:I:91:GLY:HA3	2.19	0.43
2:B:194:CYS:HB2	9:I:153:ILE:C	2.43	0.43
4:D:129:TYR:CE2	4:D:391:VAL:HG22	2.54	0.43
4:D:240:LEU:CG	4:D:244:ILE:HD11	2.49	0.43
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.46	0.43
5:E:232:SER:HB2	6:F:37:ASP:OD1	2.18	0.43
6:F:46:TYR:O	6:F:48:ARG:HG2	2.19	0.43
6:F:394:LYS:CB	7:G:155:GLU:HG2	2.49	0.43
6:F:398:ARG:HH22	7:G:155:GLU:CD	2.26	0.43
7:G:144:MET:HG3	7:G:144:MET:O	2.17	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.43
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.83	0.43
12:R:104:CYS:C	12:R:106:TYR:H	2.26	0.43
18:Z:111:PHE:CE2	18:Z:117:VAL:HG21	2.52	0.43
19:a:55:SER:O	19:a:56:GLY:C	2.61	0.43
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.43
21:q:79:GLY:O	21:q:82:VAL:HG22	2.19	0.43
1:A:92:PHE:HZ	8:H:306:SER:HB2	1.83	0.43
2:B:95:PHE:CZ	2:B:145:LEU:HD12	2.53	0.43
2:B:167:GLY:HA3	9:I:150:THR:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:51:TRP:HB3	6:F:133:HIS:O	2.17	0.43
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.54	0.43
7:G:360:LYS:HE3	7:G:632:ILE:CB	2.38	0.43
7:G:639:LEU:HD21	7:G:643:ARG:NH2	2.34	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.96	0.43
8:H:257:THR:O	8:H:260:MET:HB3	2.18	0.43
8:H:272:TRP:CZ2	9:I:74:LEU:HB2	2.54	0.43
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.43
10:P:64:PHE:CE1	10:P:209:ARG:O	2.69	0.43
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.43
17:X:69:ASN:O	17:X:73:GLN:HG3	2.19	0.43
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.43
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.43
3:C:70:LYS:HA	15:V:102:PRO:C	2.44	0.43
3:C:224:GLU:OE2	10:P:45:LYS:HD3	2.18	0.43
4:D:268:TRP:CE2	4:D:272:THR:HG21	2.53	0.43
5:E:38:PHE:O	7:G:205:GLN:NE2	2.52	0.43
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.49	0.43
7:G:612:PRO:HG2	16:W:129:HIS:HD2	1.83	0.43
8:H:84:SER:O	8:H:87:VAL:HG23	2.19	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
9:I:113:CYS:SG	25:I:303:SF4:S4	3.17	0.43
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.43
14:T:87:LEU:HA	14:T:87:LEU:HD23	1.72	0.43
16:W:38:LEU:HG	16:W:70:PHE:HZ	1.84	0.43
18:Z:98:MET:HA	18:Z:101:VAL:HG23	2.01	0.43
18:Z:98:MET:HB3	18:Z:104:TRP:CD1	2.53	0.43
2:B:202:LEU:HD21	9:I:86:TYR:HB3	1.99	0.43
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.43
3:C:227:GLN:HE22	9:I:129:THR:HG1	1.67	0.43
4:D:203:MET:HE1	4:D:255:ILE:HA	2.01	0.43
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.19	0.43
5:E:247:GLY:O	6:F:64:LYS:CD	2.67	0.43
6:F:317:VAL:HG22	6:F:356:VAL:HG22	2.00	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
8:H:202:GLU:O	8:H:202:GLU:HG2	2.19	0.43
10:P:275:HIS:CB	10:P:372:ALA:HB1	2.48	0.43
21:q:125:VAL:O	21:q:125:VAL:CG2	2.67	0.43
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
4:D:104:GLU:HB2	8:H:130:PHE:CZ	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:79:LEU:HB2	5:E:80:PRO:HD3	2.01	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
7:G:346:VAL:HG21	7:G:548:LEU:HD21	2.00	0.42
8:H:24:GLU:CD	8:H:195:ARG:HH22	2.27	0.42
8:H:142:TYR:O	8:H:146:MET:HB2	2.19	0.42
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.42
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.42
14:T:93:ILE:CD1	14:T:108:LEU:HD22	2.49	0.42
14:T:99:SER:O	14:T:141:PRO:HG2	2.19	0.42
16:W:55:LEU:CB	16:W:107:MET:HE1	2.38	0.42
22:r:54:TYR:HA	22:r:57:ARG:CG	2.48	0.42
2:B:91:TRP:HH2	28:H:401:UQ9:H10A	1.78	0.42
3:C:64:VAL:HG21	3:C:85:ILE:HD11	2.01	0.42
4:D:267:ILE:HD13	8:H:280:PHE:CE1	2.53	0.42
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.42
6:F:81:LYS:HD3	6:F:96:GLY:HA3	2.02	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
6:F:268:GLU:HG2	6:F:269:ARG:N	2.34	0.42
8:H:223:PHE:O	8:H:226:ALA:HB3	2.19	0.42
9:I:79:ARG:NH2	22:r:20:LEU:HD22	2.34	0.42
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.01	0.42
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.42
13:S:16:LEU:CD1	13:S:19:ILE:HD11	2.47	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.54	0.42
2:B:154:GLU:HB3	8:H:59:GLU:HG3	1.98	0.42
2:B:172:HIS:CE1	2:B:179:ARG:HD3	2.54	0.42
4:D:280:ALA:HB3	15:V:11:LEU:HD23	2.01	0.42
4:D:420:TYR:CD2	15:V:114:TRP:HH2	2.37	0.42
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.40	0.42
6:F:51:TRP:HB2	6:F:133:HIS:O	2.19	0.42
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.42
7:G:356:ASP:O	7:G:360:LYS:HG3	2.19	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
8:H:68:MET:HG3	8:H:68:MET:O	2.19	0.42
29:I:301:PC1:H221	18:Z:35:MET:HE2	2.00	0.42
10:P:235:THR:HG21	10:P:323:HIS:CD2	2.55	0.42
11:Q:52:LEU:HD23	16:W:19:SER:O	2.19	0.42
18:Z:98:MET:HA	18:Z:98:MET:HE2	2.01	0.42
21:q:34:ARG:HD3	21:q:54:GLN:OE1	2.18	0.42
1:A:72:LEU:HB3	8:H:151:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:381:GLN:HG3	7:G:74:ASN:OD1	2.19	0.42
7:G:62:ARG:HD2	7:G:65:TYR:CD2	2.29	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
9:I:135:ARG:NH1	12:R:61:ILE:HG23	2.27	0.42
10:P:316:LYS:O	10:P:320:GLU:HG2	2.19	0.42
12:R:77:ILE:HG12	12:R:78:ALA:N	2.34	0.42
14:T:138:LEU:HD11	14:T:147:TYR:CD2	2.54	0.42
16:W:120:ASP:HB3	16:W:123:SER:OG	2.19	0.42
19:a:17:VAL:O	19:a:18:ILE:C	2.62	0.42
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.42
33:q:201:CDL:H511	22:r:8:ILE:HD11	2.01	0.42
2:B:194:CYS:SG	4:D:138:ARG:NH2	2.87	0.42
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.54	0.42
4:D:207:ARG:O	4:D:211:PHE:CD1	2.69	0.42
5:E:180:VAL:CG1	5:E:181:ASN:H	2.32	0.42
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.34	0.42
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.42
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.93	0.42
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.42
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.42
7:G:360:LYS:HB3	7:G:632:ILE:HB	2.01	0.42
8:H:49:PHE:HB3	29:q:202:PC1:H381	2.02	0.42
9:I:50:MET:CE	20:b:10:LYS:HG2	2.49	0.42
9:I:67:ILE:CG1	29:I:301:PC1:H251	2.38	0.42
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.42
11:Q:51:GLN:HB3	16:W:26:ARG:HH22	1.84	0.42
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.42
13:S:51:LEU:HA	13:S:52:PRO:HD3	1.87	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
3:C:52:VAL:O	3:C:56:GLN:HG3	2.20	0.42
4:D:361:ALA:HB3	7:G:149:ASP:HB3	2.01	0.42
4:D:378:LEU:HD22	7:G:126:LEU:HD13	2.00	0.42
5:E:64:ALA:HA	5:E:67:LYS:HD3	2.02	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
7:G:639:LEU:C	7:G:641:GLN:N	2.77	0.42
7:G:667:GLN:HB3	13:S:42:VAL:HG13	2.01	0.42
8:H:42:PRO:HD2	8:H:45:ILE:CD1	2.49	0.42
8:H:57:MET:O	8:H:58:LYS:C	2.63	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
8:H:277:TYR:CE2	24:H:402:3PE:H281	2.55	0.42
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
10:P:243:ALA:O	10:P:244:ASP:C	2.62	0.42
10:P:259:VAL:N	10:P:261:LYS:HG2	2.33	0.42
14:T:108:LEU:HD23	14:T:108:LEU:C	2.44	0.42
14:T:133:ILE:HG23	14:T:134:ASP:N	2.35	0.42
18:Z:10:MET:HB3	18:Z:10:MET:HE2	1.75	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42
20:b:78:LEU:C	20:b:80:TRP:N	2.77	0.42
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.91	0.42
2:B:70:ARG:HG3	2:B:72:GLU:H	1.85	0.42
2:B:91:TRP:HH2	28:H:401:UQ9:H12	1.84	0.42
2:B:114:MET:HB2	2:B:119:VAL:HB	2.01	0.42
3:C:104:ASN:HD22	22:r:94:ALA:HB1	1.83	0.42
4:D:179:ARG:HG3	4:D:183:HIS:NE2	2.34	0.42
5:E:101:ALA:HA	5:E:106:VAL:HG22	2.01	0.42
5:E:142:ARG:HG3	5:E:182:ALA:HB3	2.01	0.42
7:G:240:ALA:HA	9:I:117:LYS:HZ3	1.85	0.42
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.74	0.42
8:H:186:PHE:CE1	8:H:270:PHE:CD1	2.94	0.42
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.42
17:X:91:TYR:OH	19:a:28:LYS:HE2	2.19	0.42
3:C:85:ILE:CD1	3:C:140:ILE:HD11	2.50	0.42
4:D:398:THR:O	4:D:398:THR:HG23	2.20	0.42
5:E:162:THR:HG22	5:E:163:THR:N	2.34	0.42
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.42
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.42
6:F:384:PRO:HA	7:G:119:PHE:CD2	2.54	0.42
7:G:102:ILE:O	7:G:103:LEU:C	2.60	0.42
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.42
7:G:282:ASN:HB2	7:G:285:TRP:O	2.20	0.42
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.54	0.42
7:G:614:GLY:CA	10:P:41:ILE:CD1	2.88	0.42
8:H:196:ALA:O	8:H:279:ARG:HG2	2.19	0.42
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.01	0.42
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.42
10:P:207:PHE:O	10:P:241:TYR:HA	2.20	0.42
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.42
13:S:23:LEU:O	13:S:57:GLU:HA	2.20	0.42
17:X:10:LEU:H	17:X:10:LEU:HD12	1.84	0.42
17:X:141:PRO:C	17:X:143:HIS:H	2.27	0.42
22:r:54:TYR:HD1	22:r:57:ARG:HG3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:s:53:SER:HA	23:s:56:ARG:HG2	2.02	0.42
3:C:49:ARG:HH21	3:C:54:HIS:CG	2.37	0.42
4:D:280:ALA:HB1	15:V:11:LEU:CG	2.44	0.42
4:D:381:HIS:HE1	9:I:161:ALA:O	2.02	0.42
5:E:110:ARG:HA	5:E:110:ARG:HD3	1.81	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
6:F:217:GLU:OE2	6:F:224:ARG:NH2	2.53	0.42
8:H:23:VAL:HG11	19:a:9:LEU:HD21	2.02	0.42
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
17:X:41:LYS:HD2	20:b:56:PRO:HG3	2.01	0.42
20:b:11:ASN:O	20:b:15:LYS:HG2	2.20	0.42
20:b:69:HIS:HB3	20:b:72:ASP:CG	2.45	0.42
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.51	0.42
1:A:112:GLU:O	1:A:113:TRP:CD1	2.73	0.42
2:B:154:GLU:O	2:B:156:ARG:N	2.52	0.42
3:C:72:VAL:HG23	3:C:72:VAL:O	2.20	0.42
3:C:224:GLU:OE1	11:Q:118:ALA:HB2	2.20	0.42
5:E:62:ILE:HD13	5:E:84:LEU:HD13	2.01	0.42
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.35	0.42
7:G:53:CYS:SG	7:G:102:ILE:HG21	2.60	0.42
7:G:161:GLU:OE2	12:R:96:ASP:N	2.53	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.20	0.42
8:H:43:TYR:CE2	21:q:27:PHE:CZ	3.06	0.42
9:I:183:LEU:HD23	9:I:183:LEU:HA	1.75	0.42
10:P:99:ASP:HB3	10:P:102:GLN:CD	2.45	0.42
14:T:97:LYS:NZ	14:T:108:LEU:N	2.66	0.42
16:W:120:ASP:OD1	16:W:120:ASP:C	2.61	0.42
17:X:41:LYS:O	17:X:42:GLU:C	2.59	0.42
17:X:143:HIS:ND1	18:Z:115:ARG:HA	2.35	0.42
1:A:65:PHE:HE2	8:H:294:LEU:HD21	1.76	0.41
3:C:78:SER:C	3:C:80:LEU:H	2.26	0.41
3:C:232:PHE:CE1	7:G:244:GLU:HG3	2.55	0.41
5:E:114:VAL:O	5:E:118:TYR:HD2	2.02	0.41
5:E:183:PRO:O	5:E:194:ASP:N	2.53	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:544:MET:HE2	7:G:546:PHE:CZ	2.55	0.41
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.41
29:I:301:PC1:H382	29:I:301:PC1:H352	1.88	0.41
10:P:220:TYR:CG	10:P:226:VAL:HG13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:265:PHE:CD1	10:P:334:GLY:HA3	2.55	0.41
12:R:81:GLY:CA	12:R:88:HIS:CD2	3.02	0.41
15:V:37:HIS:O	15:V:38:PHE:C	2.63	0.41
16:W:28:LEU:O	16:W:32:LYS:HG3	2.20	0.41
16:W:53:MET:SD	16:W:106:VAL:HG21	2.60	0.41
16:W:71:MET:O	16:W:74:ALA:N	2.39	0.41
17:X:48:TRP:CZ2	20:b:55:VAL:CG2	2.98	0.41
17:X:142:TYR:O	17:X:143:HIS:C	2.62	0.41
18:Z:7:LYS:HE3	18:Z:7:LYS:HB2	1.90	0.41
19:a:49:GLU:OE2	19:a:49:GLU:HA	2.20	0.41
21:q:47:LYS:HE3	21:q:47:LYS:HB2	1.88	0.41
3:C:160:ILE:HG13	4:D:285:ASN:ND2	2.34	0.41
4:D:149:GLN:NE2	4:D:309:ASP:OD2	2.53	0.41
4:D:159:LEU:CD2	22:r:60:ARG:HG3	2.50	0.41
4:D:266:ARG:HD2	24:H:402:3PE:O22	2.20	0.41
5:E:176:LEU:HB3	5:E:191:TYR:OH	2.20	0.41
6:F:268:GLU:CG	6:F:269:ARG:H	2.32	0.41
6:F:309:GLY:HA3	6:F:313:ASN:HD22	1.85	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:127:ASP:HA	12:R:106:TYR:OH	2.20	0.41
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
8:H:42:PRO:HD2	8:H:45:ILE:HD11	2.02	0.41
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.41
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.41
10:P:242:VAL:HG13	10:P:243:ALA:N	2.35	0.41
10:P:283:MET:SD	10:P:369:THR:HG21	2.60	0.41
14:T:110:LEU:HG	14:T:114:ASP:HB3	1.98	0.41
17:X:132:LYS:HB3	17:X:132:LYS:HE2	1.84	0.41
4:D:184:ILE:HD12	4:D:210:MET:HE1	2.02	0.41
6:F:54:LYS:HG3	6:F:55:GLY:H	1.85	0.41
6:F:418:GLN:NE2	22:r:53:TYR:OH	2.53	0.41
7:G:75:CYS:O	7:G:76:ARG:C	2.63	0.41
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.41
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.41
8:H:142:TYR:CE1	8:H:285:LEU:HD21	2.55	0.41
9:I:130:ILE:HD11	9:I:145:TYR:HE1	1.86	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
10:P:230:SER:O	10:P:231:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:359:TYR:HA	10:P:362:LEU:HG	2.02	0.41
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.55	0.41
18:Z:65:LEU:CB	20:b:50:PRO:O	2.63	0.41
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
2:B:144:ALA:O	2:B:147:LYS:N	2.54	0.41
4:D:179:ARG:CG	4:D:183:HIS:CD2	3.04	0.41
4:D:266:ARG:HH21	9:I:63:TRP:HA	1.85	0.41
4:D:267:ILE:CD1	8:H:280:PHE:CE1	3.03	0.41
5:E:68:ASN:ND2	23:s:56:ARG:NH2	2.68	0.41
5:E:131:ILE:HD13	5:E:151:LEU:HD21	2.02	0.41
6:F:398:ARG:HH21	7:G:155:GLU:HG3	1.85	0.41
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.41
7:G:674:LEU:HD11	13:S:46:LYS:HE2	2.03	0.41
8:H:125:SER:HB2	8:H:128:SER:OG	2.20	0.41
8:H:312:ALA:CB	20:b:41:TYR:HB2	2.51	0.41
9:I:162:CYS:SG	25:I:303:SF4:S2	3.19	0.41
13:S:48:HIS:HE1	13:S:95:LEU:CD2	2.25	0.41
18:Z:142:TRP:C	18:Z:143:TYR:CD2	2.99	0.41
20:b:15:LYS:O	20:b:16:GLU:HB2	2.20	0.41
20:b:49:THR:HA	20:b:50:PRO:HD3	1.89	0.41
1:A:6:VAL:HG11	8:H:87:VAL:HG22	2.01	0.41
5:E:226:PRO:HA	6:F:286:CYS:HB3	2.02	0.41
6:F:303:HIS:O	6:F:304:ALA:HB3	2.20	0.41
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.41
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.41
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.41
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.84	0.41
8:H:7:LEU:HD13	8:H:7:LEU:HA	1.94	0.41
8:H:136:VAL:O	8:H:140:ILE:HG23	2.21	0.41
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.41
10:P:295:LEU:O	10:P:298:TYR:N	2.53	0.41
12:R:44:ARG:O	12:R:47:ARG:HB2	2.21	0.41
12:R:76:ILE:HD11	12:R:92:TYR:CB	2.48	0.41
13:S:36:PHE:HZ	13:S:44:LEU:HD12	1.86	0.41
14:T:133:ILE:HG13	14:T:137:LYS:NZ	2.36	0.41
16:W:23:ILE:CG2	16:W:83:ASP:HB2	2.50	0.41
21:q:110:TRP:HB2	21:q:113:HIS:CE1	2.55	0.41
3:C:232:PHE:HE2	9:I:126:GLN:OE1	2.04	0.41
4:D:211:PHE:O	4:D:212:GLU:C	2.62	0.41
5:E:109:MET:HE1	7:G:198:THR:CG2	2.51	0.41
6:F:69:LEU:CD1	6:F:143:LEU:HD21	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:113:LEU:HD13	6:F:149:MET:SD	2.60	0.41
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.36	0.41
6:F:147:ARG:HD3	6:F:191:TYR:HD2	1.71	0.41
8:H:187:ILE:HG23	8:H:198:PHE:CZ	2.56	0.41
9:I:48:VAL:CG1	9:I:53:ALA:HB2	2.50	0.41
9:I:91:GLY:HA2	9:I:92:PRO:HD3	1.92	0.41
9:I:140:ARG:O	9:I:141:ARG:HG2	2.20	0.41
10:P:88:VAL:HG12	10:P:92:MET:HE2	2.02	0.41
10:P:197:GLU:HB3	10:P:259:VAL:HG22	1.99	0.41
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.41
17:X:17:GLU:HG3	17:X:64:ASN:ND2	2.35	0.41
17:X:21:SER:O	17:X:22:SER:C	2.63	0.41
17:X:53:PRO:O	17:X:54:ARG:C	2.64	0.41
19:a:48:MET:HE3	19:a:48:MET:HB2	1.77	0.41
1:A:93:ILE:HD13	1:A:93:ILE:HA	1.90	0.41
1:A:104:TYR:HA	1:A:107:THR:OG1	2.21	0.41
2:B:166:ASN:HB2	2:B:190:TYR:CD2	2.45	0.41
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.55	0.41
5:E:109:MET:HE2	7:G:196:GLY:CA	2.50	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.41
8:H:14:LEU:HD13	8:H:83:LEU:HD21	2.03	0.41
8:H:17:MET:SD	8:H:225:MET:C	3.04	0.41
16:W:23:ILE:HG21	16:W:83:ASP:HB2	2.02	0.41
16:W:86:VAL:O	16:W:87:ILE:C	2.61	0.41
17:X:20:VAL:CG1	17:X:24:VAL:HB	2.51	0.41
17:X:90:ASP:OD2	19:a:62:VAL:HG11	2.21	0.41
22:r:28:TYR:O	22:r:29:GLN:C	2.62	0.41
22:r:54:TYR:CD1	22:r:57:ARG:HG3	2.56	0.41
2:B:92:PRO:HA	2:B:130:VAL:O	2.20	0.41
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.41
3:C:68:LEU:HD13	3:C:95:THR:HA	2.03	0.41
4:D:154:ALA:HB2	4:D:398:THR:HG22	2.00	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:77:LEU:HD13	6:F:100:SER:HA	2.03	0.41
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.03	0.41
7:G:44:GLU:O	7:G:47:THR:HG23	2.21	0.41
7:G:49:VAL:HB	7:G:91:ALA:HA	2.03	0.41
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
8:H:197:PRO:HD3	8:H:273:ILE:HG22	2.03	0.41
9:I:82:ALA:CA	22:r:26:LEU:HD21	2.50	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
9:I:162:CYS:HB3	9:I:165:ASP:HA	2.02	0.41
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.41
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.21	0.41
10:P:283:MET:HE3	10:P:357:ARG:NH1	2.35	0.41
17:X:120:PRO:HG3	20:b:71:GLN:HE21	1.86	0.41
20:b:23:PHE:HE2	24:b:201:3PE:H252	1.85	0.41
21:q:129:THR:O	21:q:129:THR:CG2	2.67	0.41
1:A:58:VAL:O	1:A:61:THR:N	2.54	0.41
1:A:113:TRP:CH2	8:H:287:HIS:HB2	2.55	0.41
2:B:107:MET:HG2	2:B:114:MET:HB3	2.02	0.41
3:C:97:THR:HG21	15:V:97:TRP:HH2	1.86	0.41
4:D:144:MET:SD	4:D:144:MET:N	2.93	0.41
4:D:216:ARG:NH2	4:D:240:LEU:HA	2.35	0.41
4:D:225:ALA:O	4:D:228:ARG:NE	2.35	0.41
4:D:268:TRP:O	4:D:269:ARG:C	2.63	0.41
4:D:326:CYS:SG	4:D:453:THR:HG21	2.61	0.41
4:D:354:GLY:O	22:r:42:PRO:HG2	2.20	0.41
5:E:157:ILE:HG13	5:E:161:GLU:HB2	2.03	0.41
5:E:167:LEU:HB3	5:E:168:PHE:CD1	2.56	0.41
6:F:69:LEU:HD11	6:F:143:LEU:HG	2.03	0.41
6:F:80:MET:O	6:F:83:SER:HB3	2.21	0.41
6:F:276:PHE:CE2	6:F:290:GLU:HB3	2.56	0.41
7:G:114:GLU:OE2	22:r:53:TYR:CA	2.60	0.41
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.41
7:G:567:VAL:HG23	7:G:567:VAL:O	2.20	0.41
7:G:639:LEU:O	7:G:641:GLN:N	2.54	0.41
8:H:235:ASN:ND2	8:H:270:PHE:CD2	2.73	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
9:I:41:LYS:HD3	22:r:112:TYR:HE2	1.85	0.41
9:I:184:LEU:CD2	11:Q:114:TRP:CH2	3.03	0.41
9:I:211:TYR:CD2	22:r:39:PRO:HG3	2.54	0.41
10:P:49:SER:O	11:Q:107:TRP:HZ2	2.04	0.41
14:T:104:PHE:CE1	14:T:105:MET:HG2	2.56	0.41
17:X:57:LEU:CD2	17:X:61:LYS:HZ1	2.33	0.41
17:X:136:PRO:O	17:X:137:LEU:C	2.63	0.41
18:Z:55:GLN:O	18:Z:59:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:140:PHE:CD1	19:a:45:TRP:HB2	2.54	0.41
20:b:16:GLU:N	20:b:17:PRO:HD3	2.35	0.41
20:b:25:VAL:O	20:b:26:TRP:C	2.64	0.41
21:q:78:ASP:OD1	21:q:78:ASP:O	2.39	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
22:r:32:ALA:HB1	22:r:36:GLN:NE2	2.36	0.41
22:r:41:LEU:N	22:r:41:LEU:HD22	2.35	0.41
3:C:66:GLU:OE1	15:V:47:TYR:CE2	2.74	0.41
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.41
4:D:97:LEU:CD2	4:D:447:VAL:HG11	2.51	0.41
4:D:270:ASN:HB2	8:H:284:GLN:OE1	2.20	0.41
4:D:275:ILE:HG22	4:D:450:ILE:HD11	2.03	0.41
4:D:391:VAL:HG23	4:D:413:SER:OG	2.21	0.41
6:F:66:LYS:NZ	6:F:189:SER:CA	2.79	0.41
7:G:176:CYS:SG	25:G:802:SF4:S1	3.19	0.41
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.41
8:H:11:VAL:O	8:H:15:ILE:HG12	2.21	0.41
9:I:201:ILE:O	9:I:205:ILE:HG12	2.21	0.41
10:P:56:ALA:HA	10:P:125:VAL:O	2.21	0.41
10:P:190:GLU:O	10:P:193:SER:N	2.54	0.41
10:P:275:HIS:NE2	10:P:373:LYS:HG2	2.36	0.41
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.41
15:V:94:MET:SD	15:V:99:PRO:HG3	2.61	0.41
16:W:122:LEU:HG	16:W:126:TYR:CE2	2.56	0.41
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.55	0.40
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.40
7:G:401:LEU:CD1	7:G:462:PHE:CE2	2.88	0.40
8:H:9:LEU:HD23	8:H:91:MET:HE1	2.02	0.40
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.43	0.40
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.40
9:I:75:SER:O	22:r:12:ARG:HG2	2.22	0.40
9:I:149:MET:HE2	9:I:185:TYR:HD2	1.86	0.40
10:P:108:TRP:CZ2	30:P:401:NDP:H2A	2.57	0.40
14:T:93:ILE:HG23	14:T:108:LEU:HD13	2.03	0.40
14:T:93:ILE:HD13	14:T:108:LEU:CD2	2.51	0.40
17:X:25:LEU:HD11	19:a:50:ARG:NH2	2.36	0.40
17:X:45:LEU:HD21	20:b:58:ARG:HE	1.86	0.40
21:q:64:TYR:CD1	21:q:77:VAL:HG11	2.56	0.40
23:s:52:LEU:HD23	23:s:52:LEU:HA	1.93	0.40
2:B:146:ARG:NH2	3:C:211:TYR:CZ	2.89	0.40
3:C:128:VAL:HG22	3:C:143:LYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:170:ILE:CD1	4:D:236:LEU:HD11	2.49	0.40
4:D:253:LEU:HD23	4:D:254:ARG:HH22	1.86	0.40
6:F:76:ILE:O	6:F:80:MET:HG2	2.21	0.40
6:F:169:LEU:O	6:F:173:ILE:N	2.49	0.40
6:F:208:GLU:OE1	6:F:210:THR:N	2.52	0.40
6:F:427:LEU:HB2	27:F:501:FMN:HM71	2.02	0.40
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.40
7:G:302:LEU:N	7:G:571:HIS:O	2.45	0.40
7:G:339:ALA:C	7:G:545:LEU:HD12	2.47	0.40
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.21	0.40
9:I:90:LYS:HG2	21:q:90:LEU:HD21	2.03	0.40
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.40
10:P:105:PHE:C	10:P:106:LEU:HD12	2.47	0.40
12:R:79:CYS:O	12:R:88:HIS:CE1	2.74	0.40
13:S:17:ARG:O	13:S:52:PRO:HD2	2.21	0.40
14:T:110:LEU:HD12	14:T:110:LEU:HA	1.92	0.40
19:a:49:GLU:O	19:a:50:ARG:C	2.62	0.40
23:s:41:ASN:HD21	23:s:43:TYR:HB2	1.87	0.40
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.40
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.40
3:C:241:PHE:HB3	3:C:242:PRO:HD2	2.03	0.40
4:D:274:ASP:N	4:D:325:ASP:HB2	2.37	0.40
4:D:322:SER:OG	4:D:323:ARG:HG3	2.20	0.40
6:F:98:LYS:HA	6:F:101:PHE:HD2	1.87	0.40
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.86	0.40
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.40
7:G:32:ILE:HG22	7:G:33:GLU:N	2.36	0.40
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.40
7:G:379:THR:HG22	7:G:379:THR:O	2.21	0.40
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.40
8:H:64:LEU:CD2	10:P:359:TYR:CB	2.62	0.40
9:I:92:PRO:HB3	21:q:92:CYS:HB2	2.02	0.40
10:P:203:PRO:HG2	30:P:401:NDP:C6N	2.51	0.40
12:R:36:GLN:O	12:R:36:GLN:HG3	2.22	0.40
21:q:8:LYS:HE3	21:q:8:LYS:HB2	1.84	0.40
1:A:67:LEU:O	1:A:70:ALA:HB3	2.21	0.40
2:B:98:ALA:O	4:D:141:TYR:CE2	2.75	0.40
4:D:161:ILE:HG21	4:D:363:VAL:HG21	2.03	0.40
4:D:320:ILE:HD11	9:I:38:TYR:CE1	2.57	0.40
6:F:53:LEU:O	6:F:54:LYS:C	2.62	0.40
6:F:177:TYR:O	6:F:178:GLU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:F:501:FMN:H9	27:F:501:FMN:HI1	1.91	0.40
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.40
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.40
9:I:105:ARG:HH12	12:R:58:ASN:CB	2.35	0.40
10:P:80:VAL:HB	10:P:103:LEU:HD22	2.04	0.40
10:P:138:ASN:OD1	10:P:138:ASN:N	2.55	0.40
14:T:105:MET:SD	14:T:115:GLN:HB2	2.61	0.40
15:V:114:TRP:O	15:V:116:ILE:HG22	2.21	0.40
16:W:27:ASP:O	16:W:28:LEU:C	2.64	0.40
17:X:121:ASP:OD1	17:X:122:LEU:N	2.54	0.40
17:X:122:LEU:HD21	20:b:81:LEU:CD2	2.46	0.40
20:b:11:ASN:CG	20:b:15:LYS:HE3	2.46	0.40
2:B:141:MET:O	2:B:141:MET:HG3	2.21	0.40
4:D:182:ASN:O	4:D:185:MET:HB3	2.22	0.40
4:D:261:MET:HE3	4:D:261:MET:HB3	1.74	0.40
5:E:140:MET:O	5:E:143:ASP:N	2.53	0.40
5:E:192:TYR:CD2	5:E:203:ILE:HD13	2.57	0.40
6:F:167:SER:OG	23:s:40:TYR:CZ	2.73	0.40
6:F:227:PRO:HB3	7:G:95:PRO:CD	2.52	0.40
8:H:155:LEU:O	8:H:315:PRO:HG3	2.22	0.40
8:H:295:PRO:HG3	24:b:201:3PE:H382	2.03	0.40
10:P:99:ASP:CG	10:P:100:LEU:H	2.29	0.40
10:P:265:PHE:CD1	10:P:265:PHE:N	2.87	0.40
10:P:336:GLU:N	10:P:340:VAL:O	2.55	0.40
15:V:50:GLN:NE2	22:r:93:LYS:HG3	2.37	0.40
18:Z:104:TRP:O	18:Z:105:LYS:C	2.65	0.40
21:q:44:TYR:HE1	21:q:69:ASN:OD1	2.05	0.40
21:q:64:TYR:CE2	21:q:82:VAL:HG13	2.56	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	87/115 (76%)	83 (95%)	4 (5%)	0	100	100
2	B	155/224 (69%)	146 (94%)	7 (4%)	2 (1%)	9	39
3	C	196/263 (74%)	186 (95%)	10 (5%)	0	100	100
4	D	377/463 (81%)	362 (96%)	15 (4%)	0	100	100
5	E	208/248 (84%)	203 (98%)	5 (2%)	0	100	100
6	F	424/464 (91%)	407 (96%)	17 (4%)	0	100	100
7	G	685/727 (94%)	633 (92%)	52 (8%)	0	100	100
8	H	304/318 (96%)	290 (95%)	13 (4%)	1 (0%)	36	65
9	I	176/212 (83%)	175 (99%)	1 (1%)	0	100	100
10	P	337/377 (89%)	308 (91%)	28 (8%)	1 (0%)	36	65
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	78 (96%)	3 (4%)	0	100	100
13	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
14	T	73/156 (47%)	69 (94%)	4 (6%)	0	100	100
15	V	110/116 (95%)	106 (96%)	4 (4%)	0	100	100
16	W	112/131 (86%)	110 (98%)	2 (2%)	0	100	100
17	X	140/172 (81%)	129 (92%)	11 (8%)	0	100	100
18	Z	137/144 (95%)	133 (97%)	4 (3%)	0	100	100
19	a	65/70 (93%)	62 (95%)	3 (5%)	0	100	100
20	b	77/84 (92%)	71 (92%)	6 (8%)	0	100	100
21	q	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
22	r	91/113 (80%)	81 (89%)	9 (10%)	1 (1%)	11	43
23	s	20/104 (19%)	20 (100%)	0	0	100	100
All	All	4193/5036 (83%)	3978 (95%)	210 (5%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
10	P	329	PRO
2	B	171	TYR
22	r	39	PRO

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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	83/104 (80%)	83 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	73	77
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	328/395 (83%)	326 (99%)	2 (1%)	78	79
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	80
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	273/280 (98%)	273 (100%)	0	100	100
9	I	152/178 (85%)	152 (100%)	0	100	100
10	P	296/325 (91%)	294 (99%)	2 (1%)	76	78
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68	75
12	R	70/96 (73%)	69 (99%)	1 (1%)	59	71
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	71
14	T	69/135 (51%)	69 (100%)	0	100	100
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	129 (100%)	0	100	100
18	Z	120/123 (98%)	119 (99%)	1 (1%)	73	77
19	a	57/60 (95%)	57 (100%)	0	100	100
20	b	70/73 (96%)	70 (100%)	0	100	100
21	q	129/131 (98%)	129 (100%)	0	100	100
22	r	85/96 (88%)	84 (99%)	1 (1%)	63	73
23	s	22/95 (23%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3685/4292 (86%)	3673 (100%)	12 (0%)	84	83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	170	TYR
4	D	127	LYS
4	D	142	VAL
5	E	124	LYS
7	G	271	MET
10	P	242	VAL
10	P	316	LYS
11	Q	96	LYS
12	R	76	ILE
13	S	68	ARG
18	Z	6	VAL
22	r	92	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	108	GLN
2	B	83	ASN
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	92	HIS
4	D	112	HIS
4	D	117	HIS
4	D	147	ASN
4	D	160	ASN
4	D	168	GLN
4	D	182	ASN

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Mol	Chain	Res	Type
4	D	270	ASN
4	D	381	HIS
4	D	454	GLN
5	E	68	ASN
5	E	122	ASN
5	E	132	GLN
5	E	245	GLN
6	F	44	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	281	HIS
6	F	303	HIS
6	F	313	ASN
6	F	346	GLN
6	F	393	ASN
6	F	418	GLN
6	F	436	GLN
7	G	74	ASN
7	G	140	GLN
7	G	205	GLN
7	G	406	ASN
7	G	495	ASN
7	G	498	GLN
7	G	571	HIS
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	169	GLN
8	H	194	ASN
8	H	212	ASN
8	H	258	ASN
8	H	287	HIS
10	P	43	HIS
10	P	79	GLN
10	P	102	GLN
10	P	166	HIS
10	P	216	HIS

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Mol	Chain	Res	Type
10	P	251	ASN
10	P	269	ASN
10	P	275	HIS
10	P	323	HIS
10	P	341	GLN
10	P	356	HIS
11	Q	51	GLN
11	Q	88	GLN
12	R	58	ASN
13	S	25	GLN
13	S	48	HIS
15	V	41	HIS
16	W	54	GLN
16	W	94	GLN
16	W	105	HIS
17	X	35	GLN
17	X	77	HIS
17	X	140	ASN
18	Z	135	ASN
19	a	31	ASN
21	q	31	ASN
21	q	52	ASN
21	q	59	HIS
21	q	87	HIS
21	q	91	HIS
21	q	113	HIS
21	q	116	ASN
22	r	21	GLN
22	r	29	GLN
22	r	52	ASN
22	r	110	GLN
23	s	59	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
27	FMN	F	501	-	33,33,33	1.39	5 (15%)	48,50,50	1.23	7 (14%)
25	SF4	I	303	9	0,12,12	-	-	-	-	-
30	NDP	P	401	-	49,52,52	1.21	5 (10%)	66,80,80	1.67	11 (16%)
26	FES	E	301	5	0,4,4	-	-	-	-	-
32	EHZ	W	201	-	27,31,37	1.73	5 (18%)	37,41,47	1.55	6 (16%)
29	PC1	q	202	-	34,34,53	1.14	2 (5%)	40,42,61	1.20	4 (10%)
24	3PE	A	401	-	45,45,50	1.11	5 (11%)	48,50,55	1.27	3 (6%)
24	3PE	H	402	-	45,45,50	0.95	2 (4%)	48,50,55	1.12	2 (4%)
25	SF4	B	301	2	0,12,12	-	-	-	-	-
33	CDL	q	201	-	56,56,99	1.19	4 (7%)	62,68,111	1.26	6 (9%)
28	UQ9	H	401	-	35,35,58	0.80	2 (5%)	42,45,73	0.63	0
24	3PE	b	201	-	45,45,50	0.97	2 (4%)	48,50,55	1.10	3 (6%)
25	SF4	G	802	7	0,12,12	-	-	-	-	-
26	FES	G	803	7	0,4,4	-	-	-	-	-
25	SF4	I	302	9	0,12,12	-	-	-	-	-
25	SF4	F	502	6	0,12,12	-	-	-	-	-
29	PC1	I	301	-	46,46,53	0.99	2 (4%)	52,54,61	1.10	3 (5%)
25	SF4	G	801	7	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	FMN	F	501	-	-	0/18/18/18	0/3/3/3
25	SF4	I	303	9	-	-	0/6/5/5
30	NDP	P	401	-	-	2/34/77/77	0/5/5/5
25	SF4	F	502	6	-	-	0/6/5/5
26	FES	E	301	5	-	-	0/1/1/1
32	EHZ	W	201	-	-	12/39/39/45	-
29	PC1	q	202	-	-	14/38/38/57	-
24	3PE	A	401	-	-	18/49/49/54	-
24	3PE	H	402	-	-	13/49/49/54	-
25	SF4	B	301	2	-	-	0/6/5/5
28	UQ9	H	401	-	-	12/30/54/81	0/1/1/1
24	3PE	b	201	-	-	10/49/49/54	-
25	SF4	G	802	7	-	-	0/6/5/5
26	FES	G	803	7	-	-	0/1/1/1
25	SF4	I	302	9	-	-	0/6/5/5
33	CDL	q	201	-	-	15/67/67/110	-
29	PC1	I	301	-	-	10/50/50/57	-
25	SF4	G	801	7	-	-	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	5.19	1.45	1.33
32	W	201	EHZ	C12-N1	5.03	1.44	1.33
27	F	501	FMN	C9A-C5A	4.80	1.49	1.41
24	b	201	3PE	O31-C31	4.28	1.45	1.33
30	P	401	NDP	C5A-C4A	4.25	1.46	1.39
33	q	201	CDL	OB8-CB7	4.16	1.45	1.33
29	I	301	PC1	O31-C31	4.14	1.45	1.33
24	H	402	3PE	O21-C21	4.11	1.45	1.34
24	H	402	3PE	O31-C31	4.11	1.45	1.33
33	q	201	CDL	OA8-CA7	4.10	1.45	1.33
29	q	202	PC1	O31-C31	4.09	1.45	1.33
29	q	202	PC1	O21-C21	4.02	1.45	1.34
24	b	201	3PE	O21-C21	4.02	1.45	1.34
29	I	301	PC1	O21-C21	4.01	1.45	1.34
33	q	201	CDL	OA6-CA5	4.00	1.45	1.34
33	q	201	CDL	OB6-CB5	3.99	1.45	1.34
24	A	401	3PE	O21-C21	3.24	1.43	1.34
30	P	401	NDP	C6N-C5N	3.21	1.39	1.33
27	F	501	FMN	C8-C7	2.99	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	401	3PE	O31-C31	2.95	1.42	1.33
27	F	501	FMN	C4-N3	-2.63	1.34	1.38
30	P	401	NDP	C5A-C6A	2.60	1.48	1.41
28	H	401	UQ9	C3-C2	-2.54	1.41	1.48
28	H	401	UQ9	C4-C5	-2.50	1.41	1.48
30	P	401	NDP	C8A-N7A	2.42	1.36	1.31
32	W	201	EHZ	O4-C15	-2.42	1.18	1.23
30	P	401	NDP	C5A-N7A	-2.39	1.34	1.39
32	W	201	EHZ	O3-C12	-2.38	1.18	1.23
27	F	501	FMN	C4A-N5	2.18	1.35	1.30
32	W	201	EHZ	C9-S1	2.17	1.81	1.76
27	F	501	FMN	C5A-N5	-2.13	1.35	1.39
24	A	401	3PE	P-O12	-2.11	1.45	1.55
24	A	401	3PE	O21-C2	-2.08	1.41	1.46
24	A	401	3PE	O31-C3	-2.01	1.40	1.45

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	P	401	NDP	C5A-C4A-N3A	-6.14	118.74	126.75
32	W	201	EHZ	C8-C9-S1	6.06	121.13	113.63
30	P	401	NDP	N3A-C4A-N9A	4.75	134.91	127.08
24	A	401	3PE	O21-C21-C22	4.71	121.65	111.50
33	q	201	CDL	OA6-CA5-C11	4.38	120.94	111.50
24	H	402	3PE	O21-C21-C22	4.37	120.91	111.50
29	I	301	PC1	O21-C21-C22	4.33	120.84	111.50
24	b	201	3PE	O21-C21-C22	4.19	120.53	111.50
29	q	202	PC1	O21-C21-C22	4.06	120.26	111.50
30	P	401	NDP	PN-O3-PA	-3.90	119.43	132.83
30	P	401	NDP	C2A-N3A-C4A	3.82	120.78	111.75
33	q	201	CDL	OB6-CB5-C51	3.60	119.25	111.50
30	P	401	NDP	C4A-C5A-N7A	-3.29	106.62	110.62
29	q	202	PC1	O31-C31-C32	3.06	121.52	111.91
30	P	401	NDP	N3A-C2A-N1A	-3.02	123.88	128.60
29	I	301	PC1	O31-C31-C32	2.86	120.88	111.91
29	I	301	PC1	C2-O21-C21	-2.83	110.83	117.79
30	P	401	NDP	C5A-N7A-C8A	2.78	107.46	103.51
24	A	401	3PE	O31-C31-C32	2.78	120.63	111.91
27	F	501	FMN	C4-C4A-N5	2.74	122.13	118.23
33	q	201	CDL	OB8-CB7-C71	2.70	120.39	111.91
30	P	401	NDP	C4A-N9A-C8A	2.67	108.63	105.73
33	q	201	CDL	OA8-CA7-C31	2.64	120.21	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	W	201	EHZ	C10-S1-C9	2.64	110.08	101.87
24	b	201	3PE	C2-O21-C21	-2.62	111.35	117.79
24	b	201	3PE	O31-C31-C32	2.55	119.90	111.91
27	F	501	FMN	C4A-C10-N1	-2.54	118.83	124.73
24	H	402	3PE	O31-C31-C32	2.52	119.82	111.91
32	W	201	EHZ	C13-C12-N1	2.45	120.54	116.42
32	W	201	EHZ	C14-N2-C15	-2.44	118.23	122.59
33	q	201	CDL	CA4-OA6-CA5	-2.44	111.79	117.79
32	W	201	EHZ	O2-C9-S1	-2.35	119.57	122.61
29	q	202	PC1	C2-O21-C21	-2.34	112.03	117.79
33	q	201	CDL	CB4-OB6-CB5	-2.30	112.14	117.79
24	A	401	3PE	O12-P-O14	-2.25	101.11	112.24
27	F	501	FMN	O2-C2-N1	-2.24	118.12	121.83
30	P	401	NDP	C6A-C5A-N7A	2.19	136.11	132.02
27	F	501	FMN	O4-C4-C4A	-2.19	120.80	126.60
27	F	501	FMN	C4A-C10-N10	2.18	119.66	116.48
30	P	401	NDP	N9A-C8A-N7A	-2.17	110.94	113.91
29	q	202	PC1	O31-C31-O32	-2.13	118.23	123.59
27	F	501	FMN	C10-N1-C2	2.09	121.08	116.90
30	P	401	NDP	C3D-C2D-C1D	2.08	105.38	101.43
27	F	501	FMN	C4A-C4-N3	2.02	118.31	113.19
32	W	201	EHZ	C16-C15-N2	2.00	120.56	116.58

There are no chirality outliers.

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	401	3PE	O22-C21-O21-C2
24	H	402	3PE	C1-O11-P-O12
24	b	201	3PE	C1-O11-P-O14
24	b	201	3PE	O22-C21-O21-C2
28	H	401	UQ9	C6-C7-C8-C9
29	I	301	PC1	C11-O13-P-O12
29	I	301	PC1	C11-O13-P-O14
29	I	301	PC1	C11-O13-P-O11
29	q	202	PC1	C11-O13-P-O14
29	q	202	PC1	C1-O11-P-O12
29	q	202	PC1	C1-O11-P-O14
29	q	202	PC1	C1-O11-P-O13
32	W	201	EHZ	O1-C7-C8-C9
32	W	201	EHZ	C6-C7-C8-C9
32	W	201	EHZ	C16-C17-C20-O6

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Mol	Chain	Res	Type	Atoms
32	W	201	EHZ	O2-C9-S1-C10
32	W	201	EHZ	C8-C9-S1-C10
33	q	201	CDL	CA3-OA5-PA1-OA3
33	q	201	CDL	CA3-OA5-PA1-OA4
24	b	201	3PE	C32-C31-O31-C3
24	H	402	3PE	O32-C31-O31-C3
24	b	201	3PE	O32-C31-O31-C3
24	A	401	3PE	C22-C21-O21-C2
24	b	201	3PE	C22-C21-O21-C2
24	H	402	3PE	C32-C31-O31-C3
29	I	301	PC1	C32-C31-O31-C3
29	I	301	PC1	O32-C31-O31-C3
28	H	401	UQ9	C25-C24-C26-C27
28	H	401	UQ9	C20-C19-C21-C22
28	H	401	UQ9	C15-C14-C16-C17
28	H	401	UQ9	C12-C11-C9-C10
28	H	401	UQ9	C23-C24-C26-C27
28	H	401	UQ9	C18-C19-C21-C22
28	H	401	UQ9	C13-C14-C16-C17
28	H	401	UQ9	C12-C11-C9-C8
24	A	401	3PE	C32-C31-O31-C3
29	q	202	PC1	C2-C1-O11-P
24	H	402	3PE	C21-C22-C23-C24
24	A	401	3PE	O32-C31-O31-C3
33	q	201	CDL	C12-C13-C14-C15
24	H	402	3PE	C1-O11-P-O13
29	q	202	PC1	C11-O13-P-O11
33	q	201	CDL	CA3-OA5-PA1-OA2
32	W	201	EHZ	C18-C17-C20-O6
32	W	201	EHZ	C19-C17-C20-O6
24	A	401	3PE	C3-C2-O21-C21
24	A	401	3PE	O13-C11-C12-N
24	H	402	3PE	C35-C36-C37-C38
24	H	402	3PE	O22-C21-O21-C2
24	H	402	3PE	C22-C21-O21-C2
32	W	201	EHZ	C3-C4-C5-C6
33	q	201	CDL	C11-CA5-OA6-CA4
24	A	401	3PE	C27-C28-C29-C2A
32	W	201	EHZ	C5-C6-C7-O1
24	A	401	3PE	O21-C2-C3-O31
32	W	201	EHZ	C5-C6-C7-C8
33	q	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
29	q	202	PC1	C32-C31-O31-C3
30	P	401	NDP	O4D-C1D-N1N-C6N
24	H	402	3PE	C22-C23-C24-C25
24	A	401	3PE	C37-C38-C39-C3A
33	q	201	CDL	OB6-CB4-CB6-OB8
33	q	201	CDL	OA7-CA5-OA6-CA4
29	I	301	PC1	C11-C12-N-C15
24	A	401	3PE	C2B-C2C-C2D-C2E
33	q	201	CDL	OA9-CA7-OA8-CA6
33	q	201	CDL	CB3-CB4-CB6-OB8
29	q	202	PC1	O32-C31-O31-C3
29	I	301	PC1	C11-C12-N-C13
29	q	202	PC1	C32-C33-C34-C35
24	A	401	3PE	C22-C23-C24-C25
24	b	201	3PE	C1-O11-P-O13
29	I	301	PC1	C1-O11-P-O13
33	q	201	CDL	CA4-CA3-OA5-PA1
24	b	201	3PE	C1-O11-P-O12
29	q	202	PC1	C11-O13-P-O12
32	W	201	EHZ	C2-C3-C4-C5
29	q	202	PC1	O13-C11-C12-N
33	q	201	CDL	C1-CB2-OB2-PB2
32	W	201	EHZ	O4-C15-C16-O5
29	I	301	PC1	C11-C12-N-C14
24	A	401	3PE	O11-C1-C2-O21
33	q	201	CDL	CB2-OB2-PB2-OB5
24	A	401	3PE	C1-C2-C3-O31
24	A	401	3PE	C25-C26-C27-C28
30	P	401	NDP	PN-O3-PA-O2A
33	q	201	CDL	C1-CA2-OA2-PA1
29	q	202	PC1	O11-C1-C2-C3
24	H	402	3PE	C24-C25-C26-C27
28	H	401	UQ9	C5-C4-O4-C4M
24	b	201	3PE	C25-C26-C27-C28
24	A	401	3PE	C21-C22-C23-C24
24	H	402	3PE	C2D-C2E-C2F-C2G
29	q	202	PC1	C34-C35-C36-C37
24	b	201	3PE	C2B-C2C-C2D-C2E
24	A	401	3PE	C39-C3A-C3B-C3C
29	q	202	PC1	C11-C12-N-C15
28	H	401	UQ9	C3-C4-O4-C4M
24	H	402	3PE	C23-C24-C25-C26

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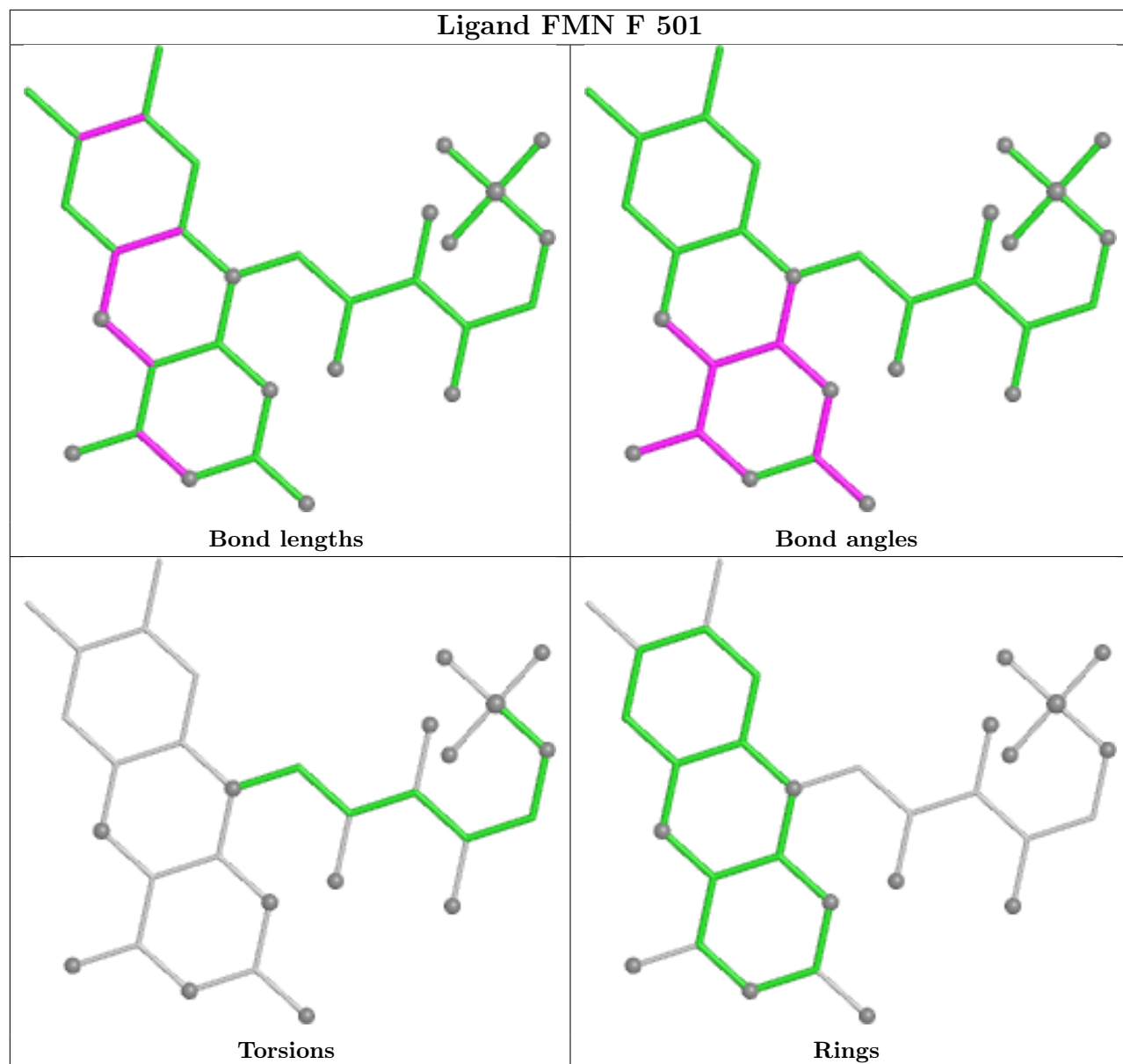
Mol	Chain	Res	Type	Atoms
24	A	401	3PE	C1-O11-P-O14
28	H	401	UQ9	C16-C17-C18-C19
24	A	401	3PE	O11-C1-C2-C3
24	H	402	3PE	O31-C31-C32-C33
24	b	201	3PE	C37-C38-C39-C3A
33	q	201	CDL	C18-C19-C20-C21
29	I	301	PC1	C2C-C2D-C2E-C2F

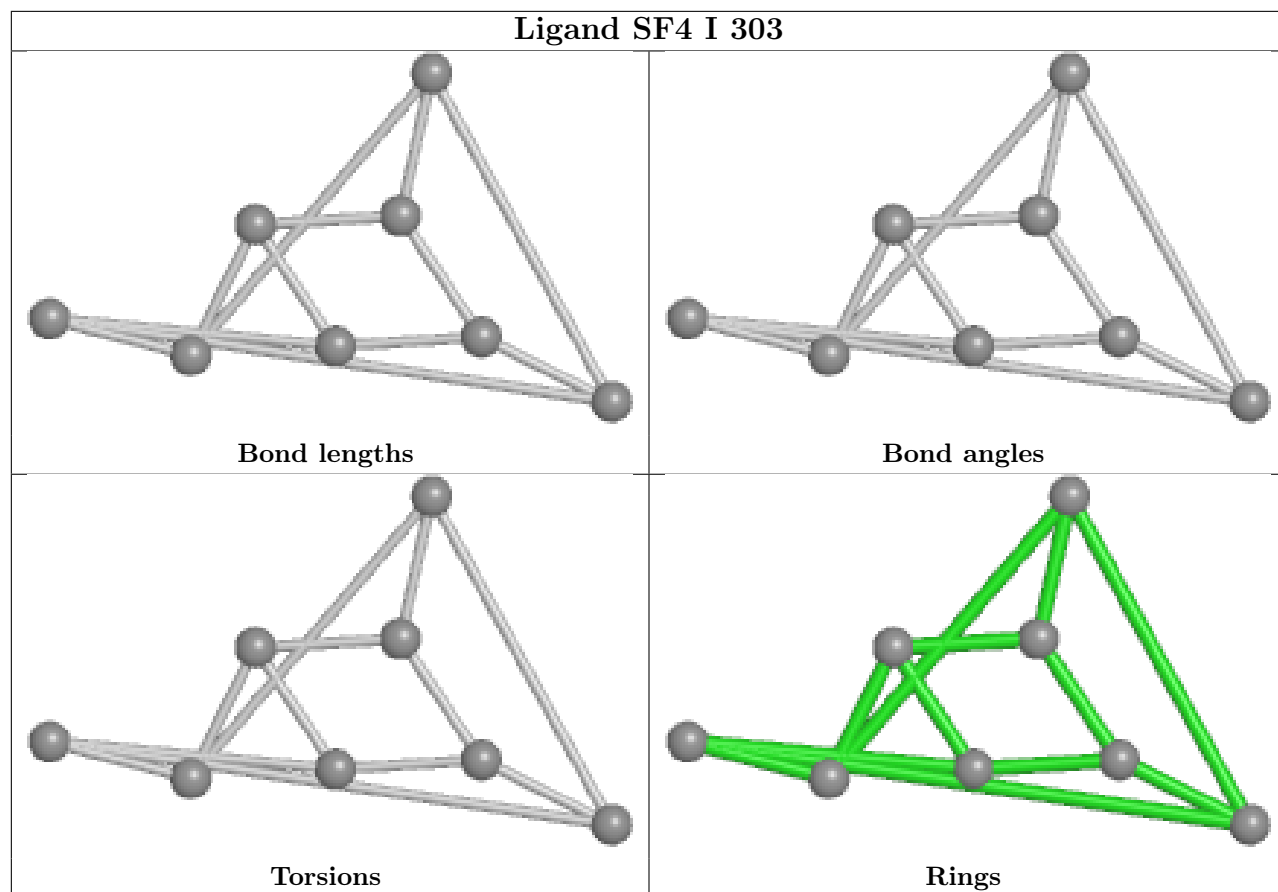
There are no ring outliers.

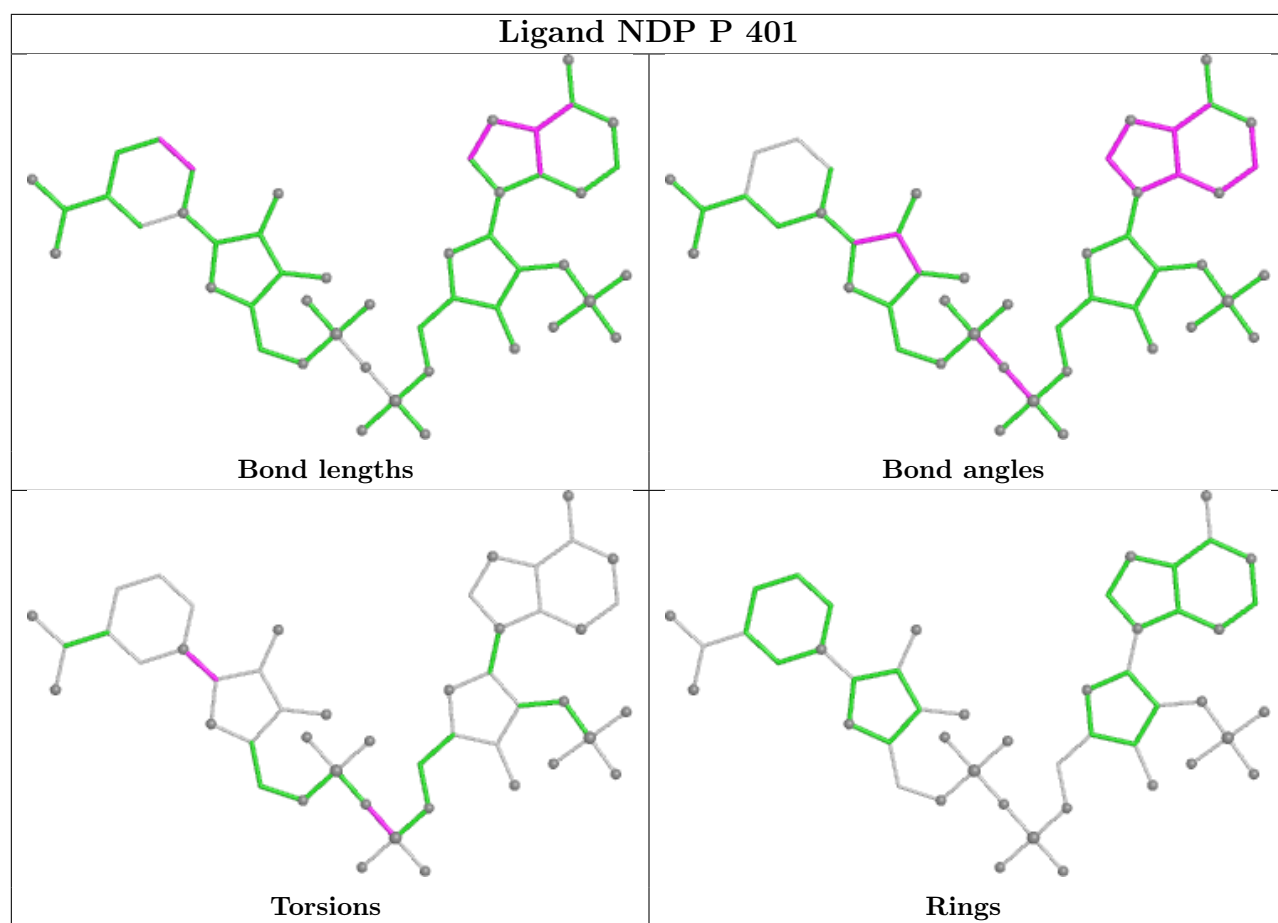
16 monomers are involved in 109 short contacts:

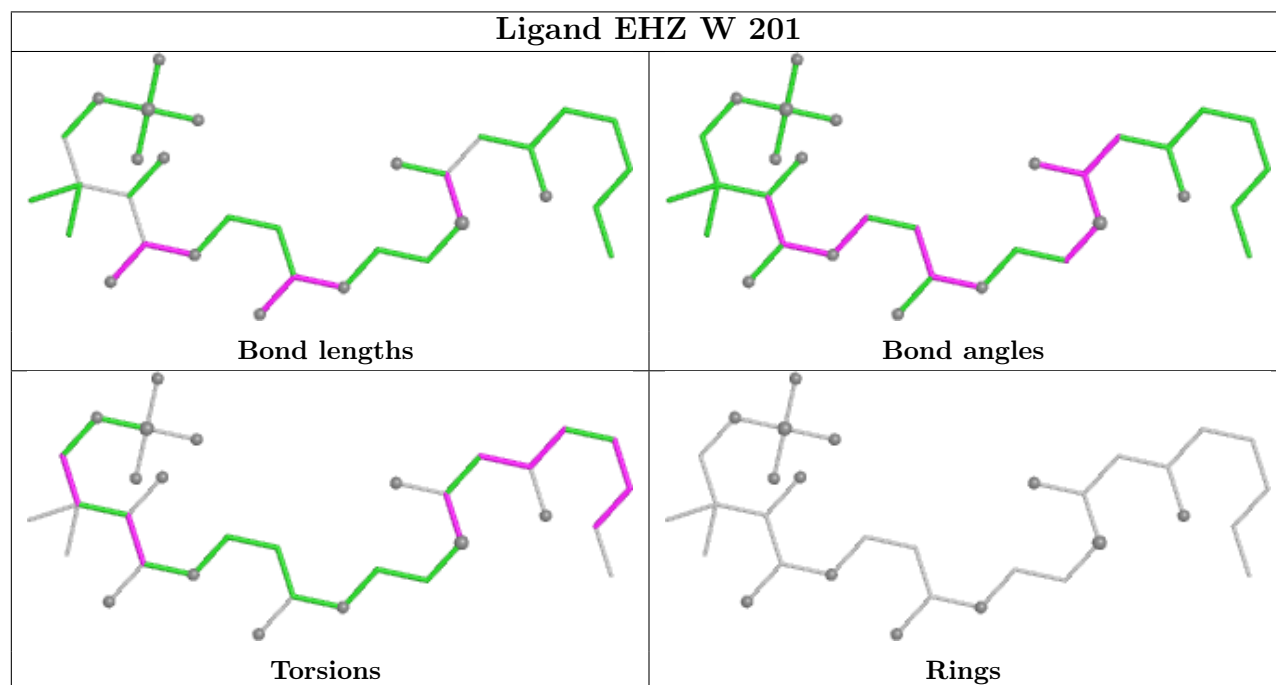
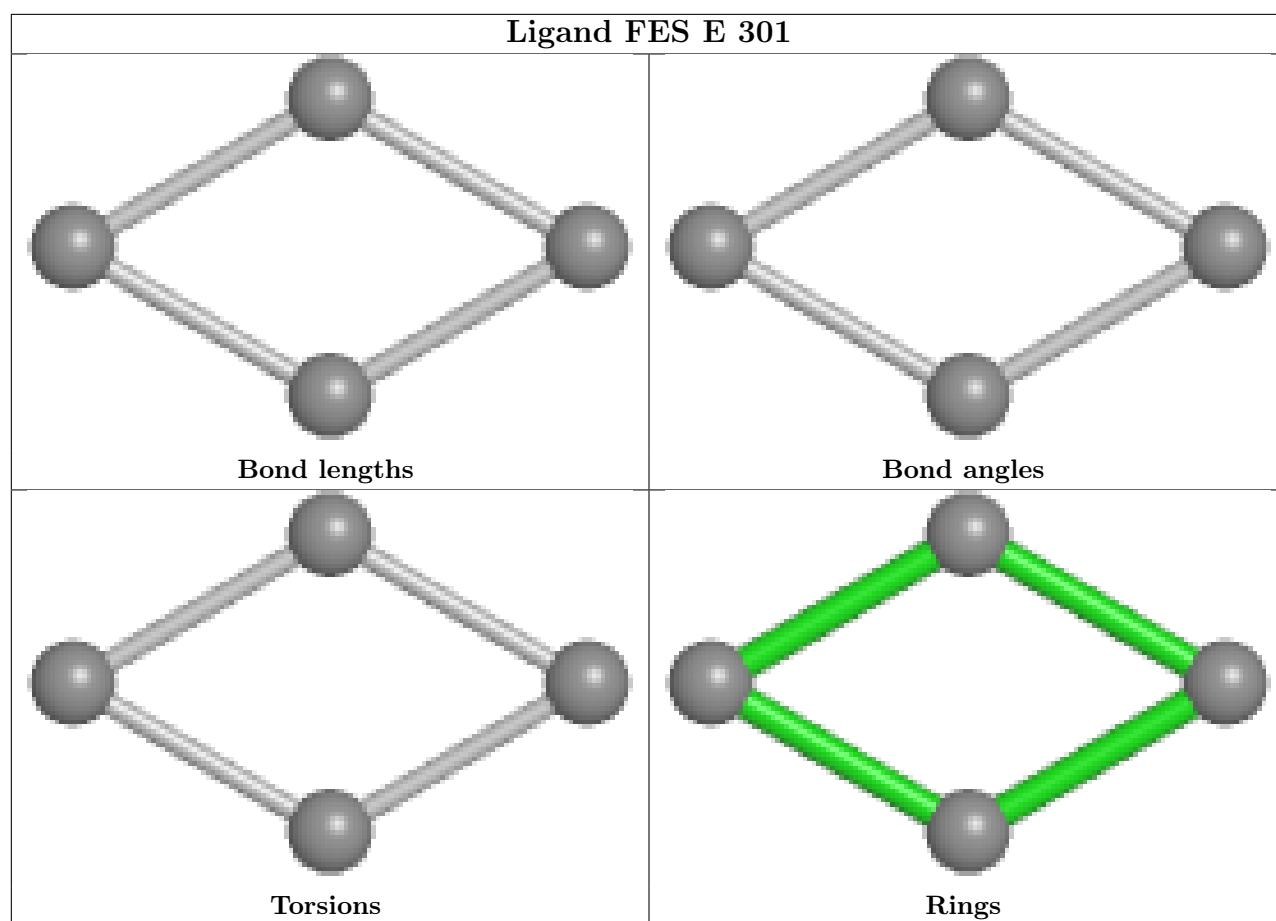
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	F	501	FMN	3	0
25	I	303	SF4	6	0
30	P	401	NDP	2	0
26	E	301	FES	3	0
29	q	202	PC1	6	0
24	A	401	3PE	3	0
24	H	402	3PE	10	0
25	B	301	SF4	2	0
33	q	201	CDL	8	0
28	H	401	UQ9	16	0
24	b	201	3PE	13	0
25	G	802	SF4	3	0
26	G	803	FES	6	0
25	I	302	SF4	9	0
25	F	502	SF4	9	0
29	I	301	PC1	10	0

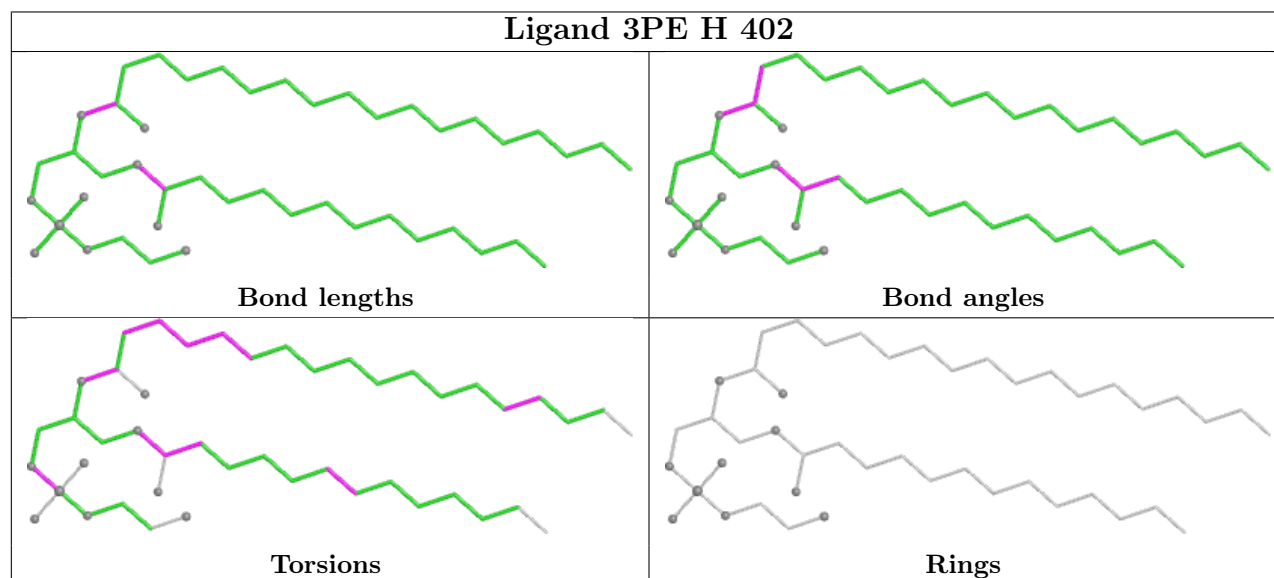
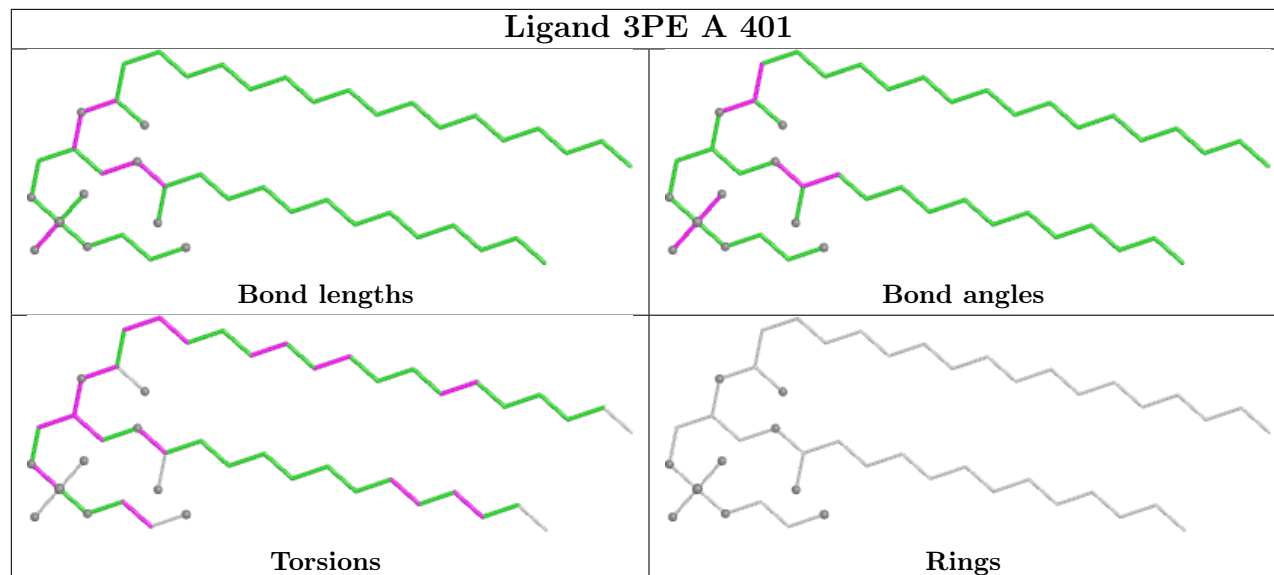
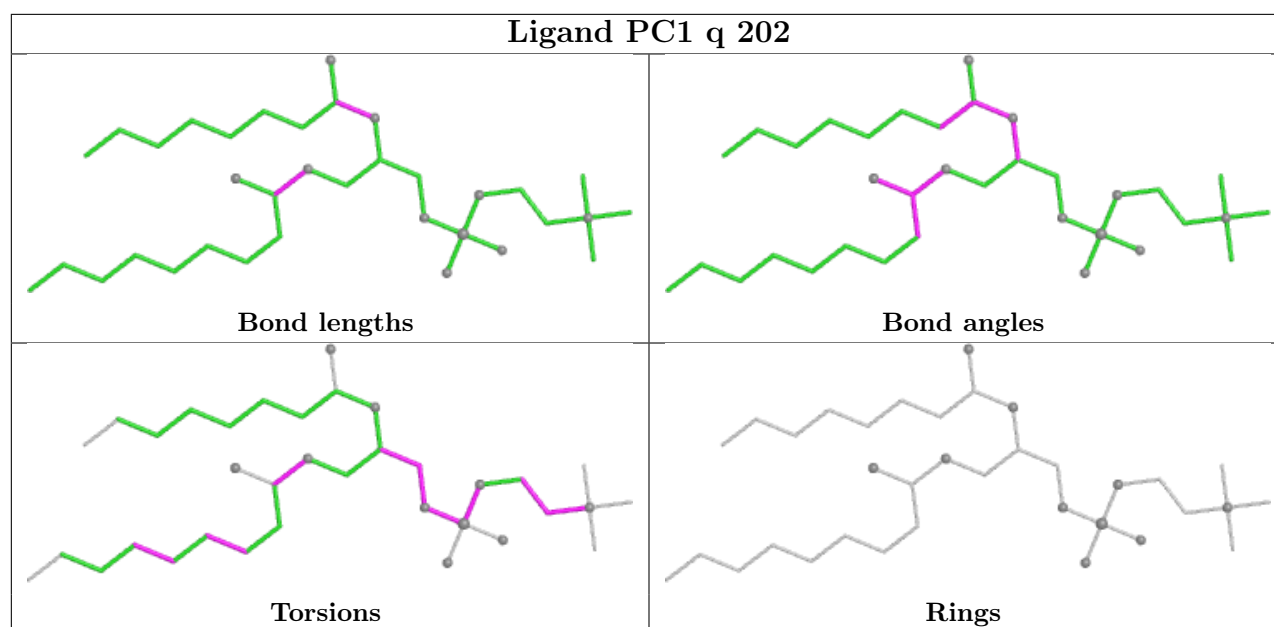
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

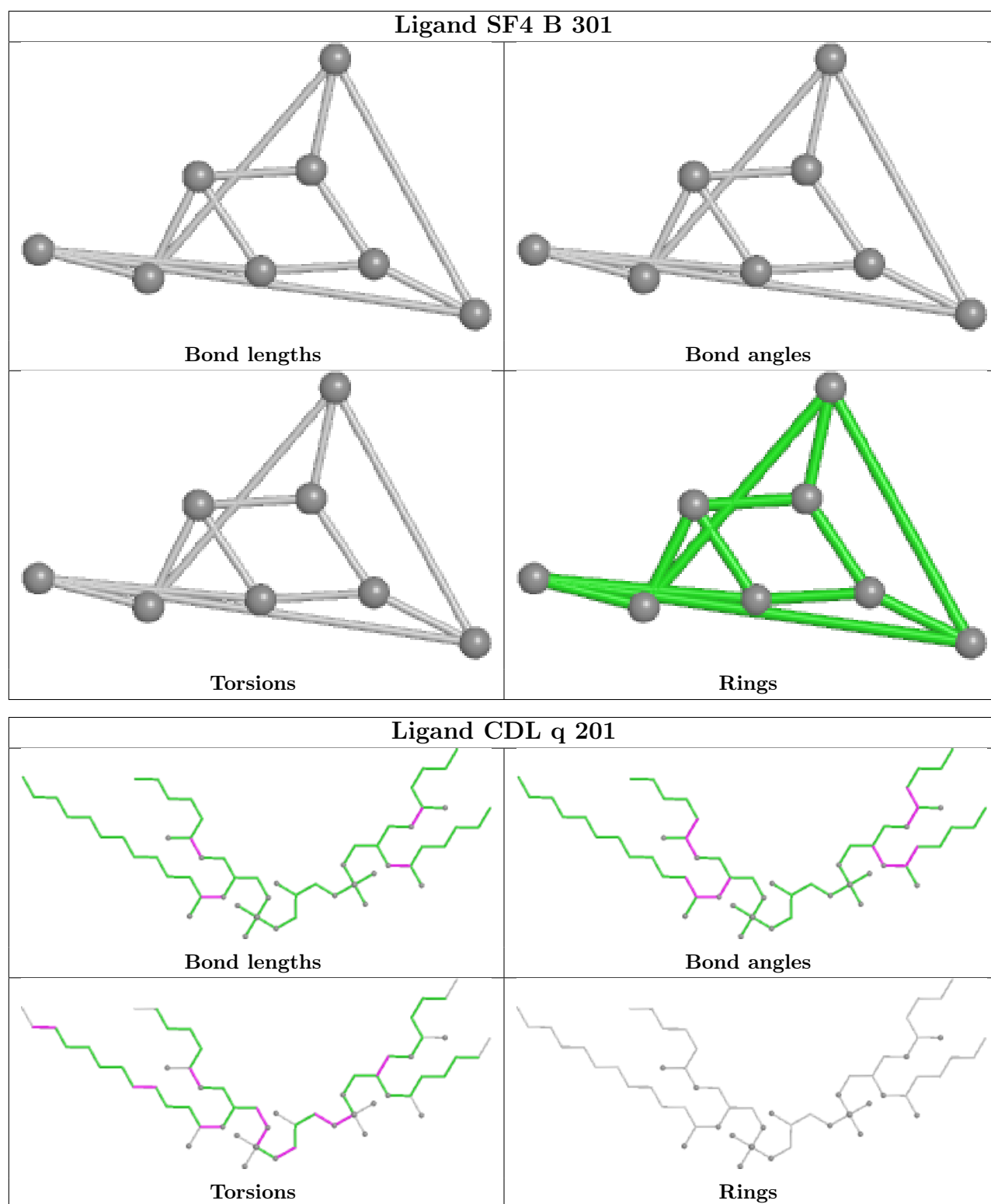


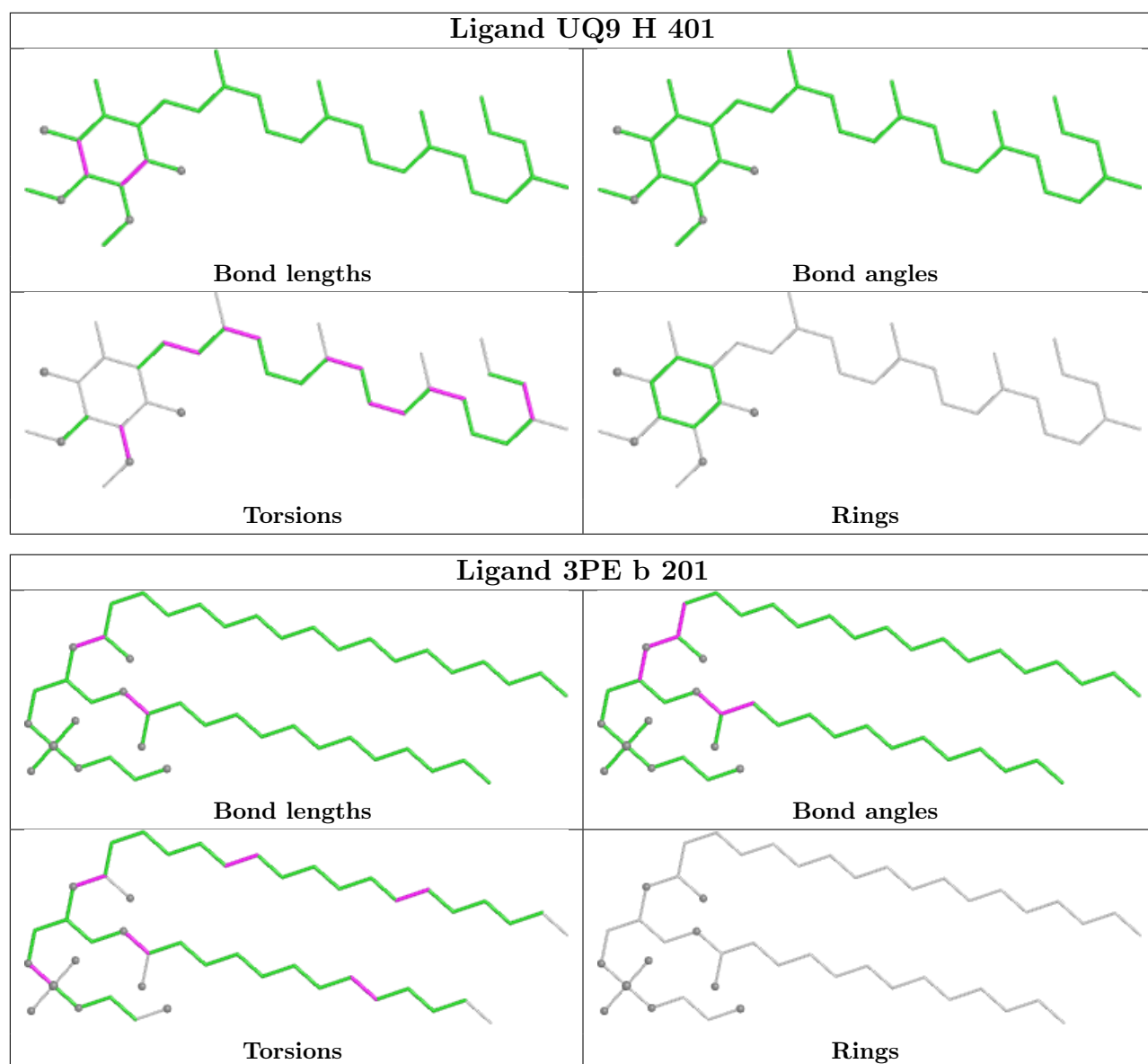


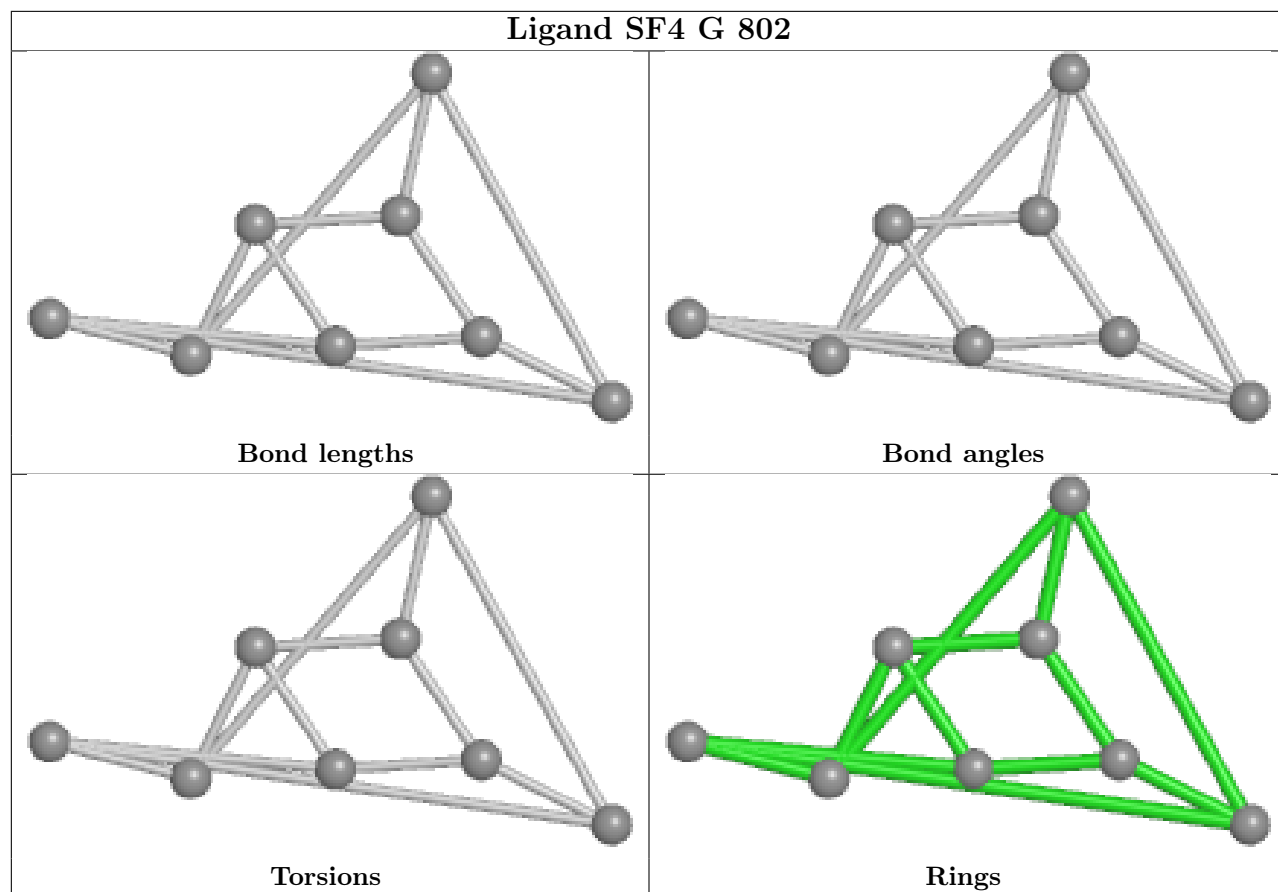


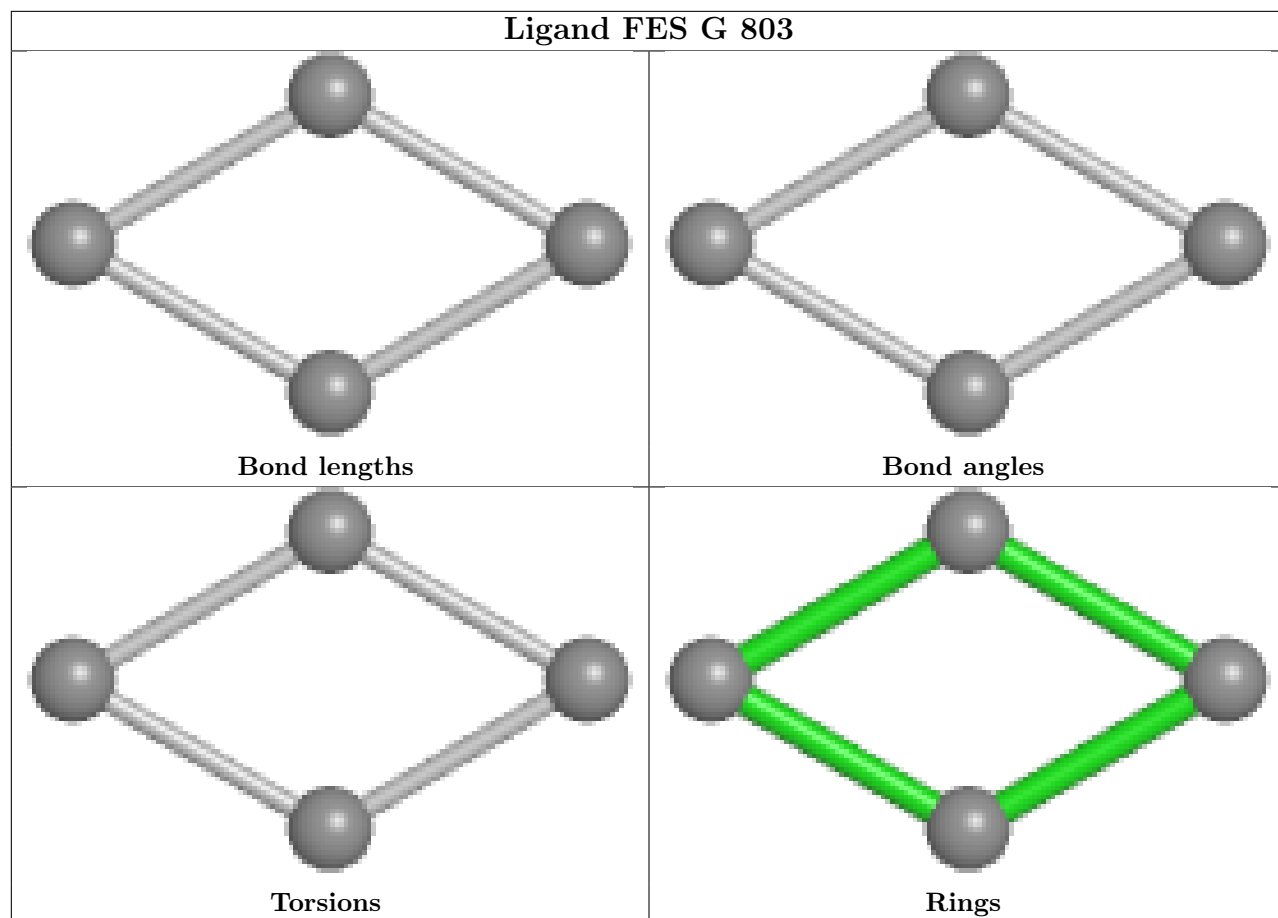




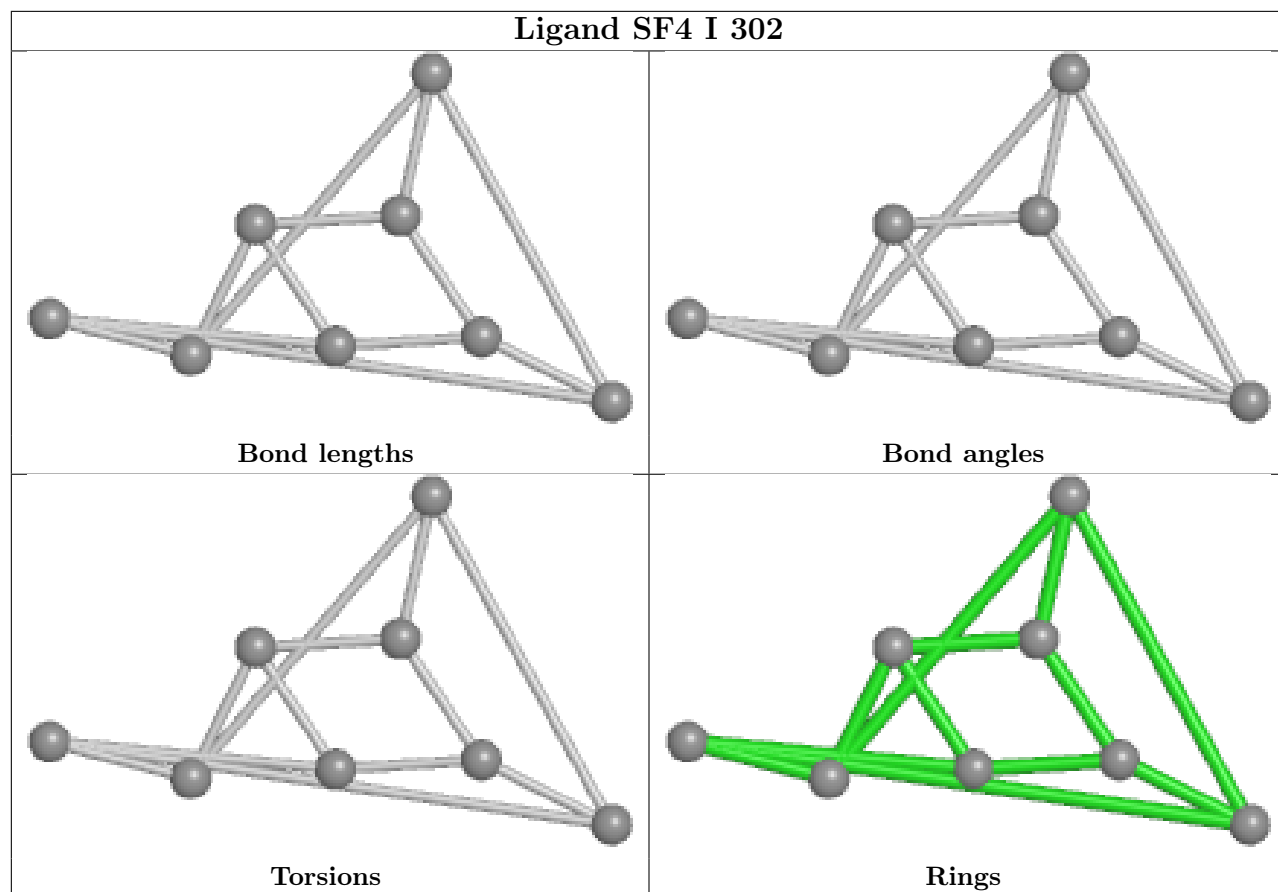




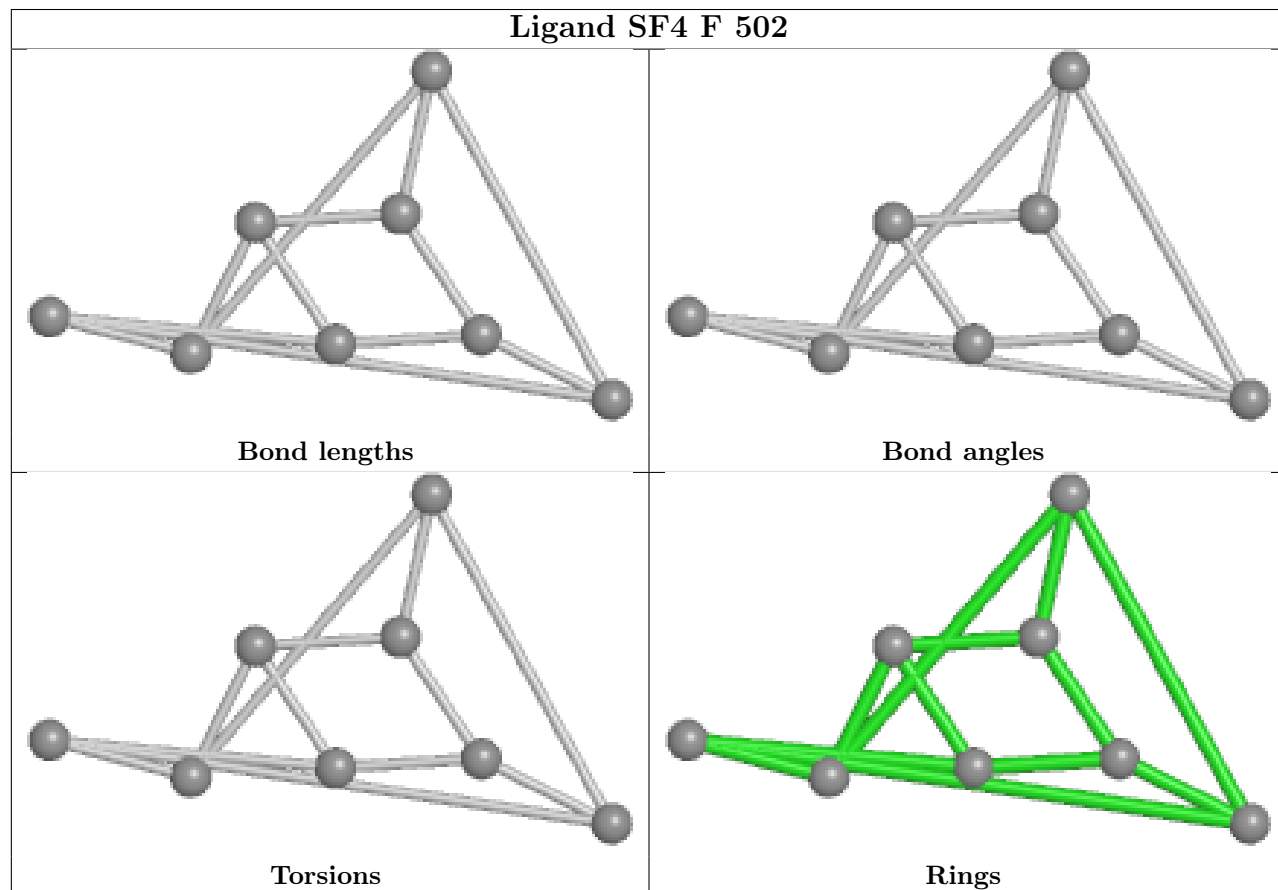


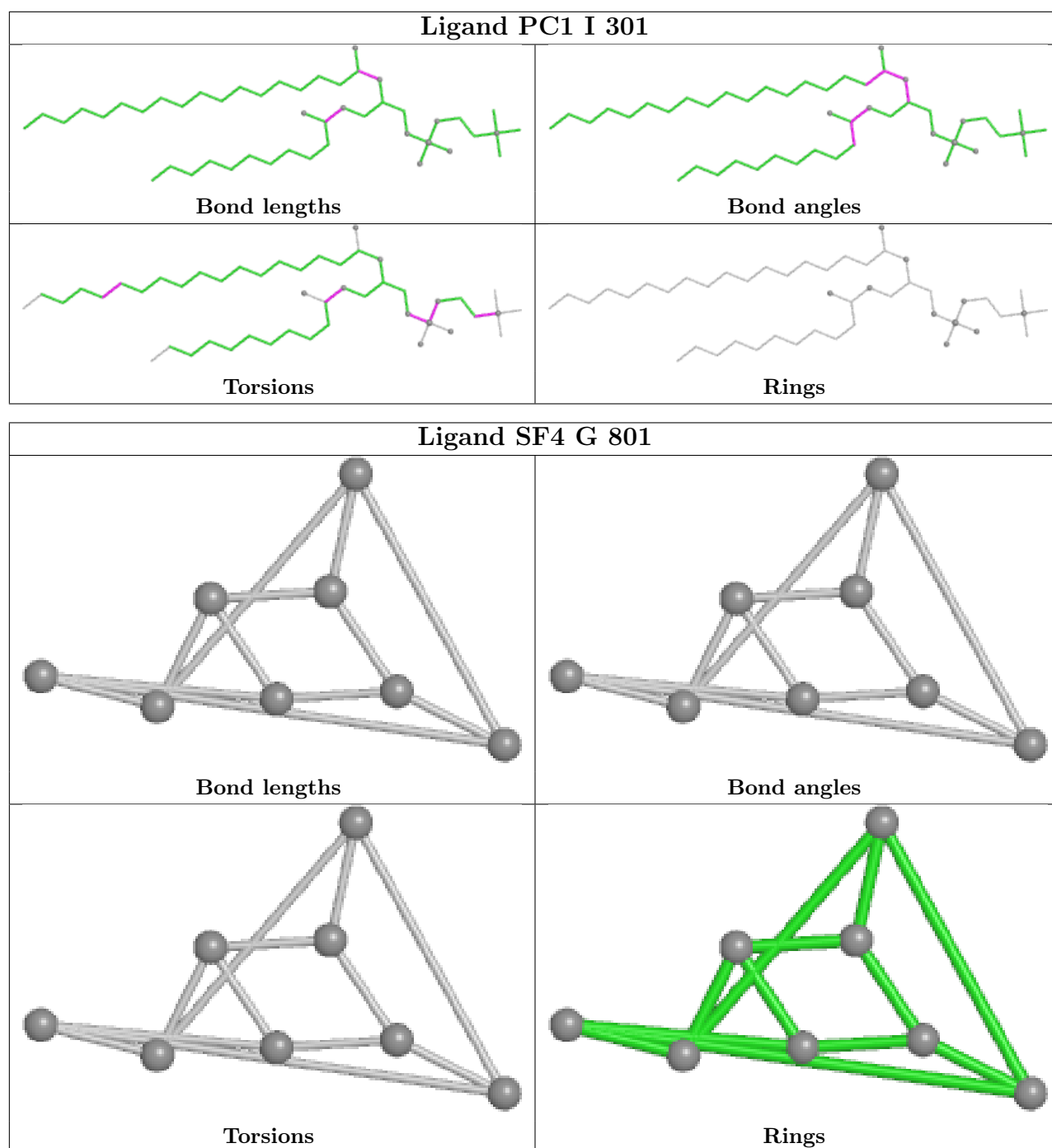


Ligand SF4 I 302



Ligand SF4 F 502





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.

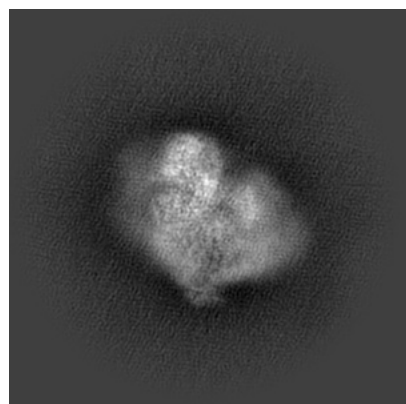
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38508. These allow visual inspection of the internal detail of the map and identification of artifacts.

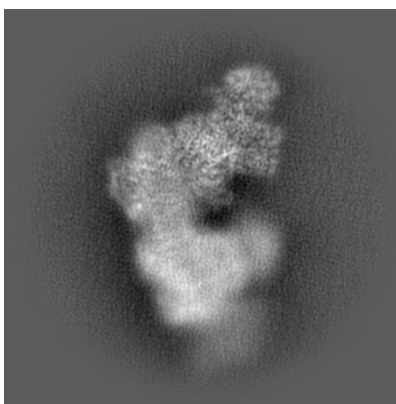
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

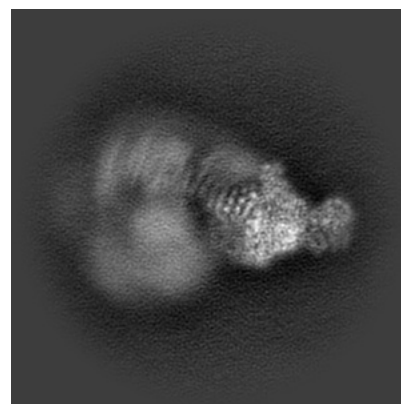
6.1.1 Primary map



X

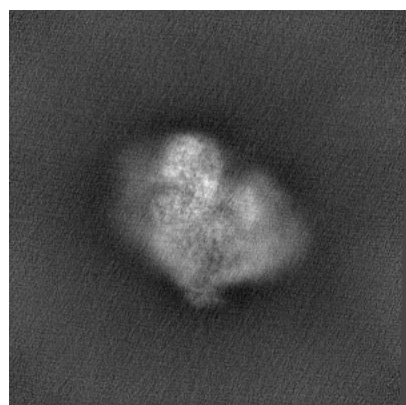


Y

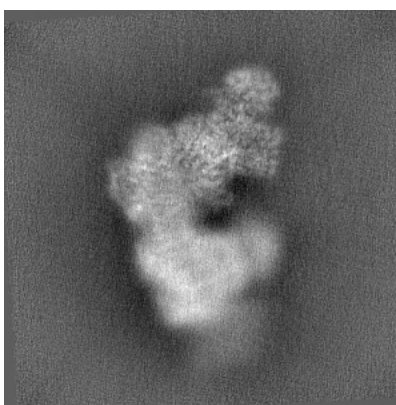


Z

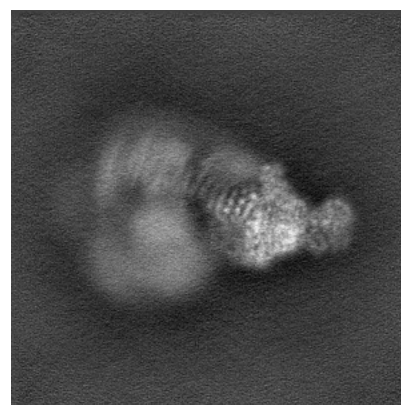
6.1.2 Raw map



X



Y

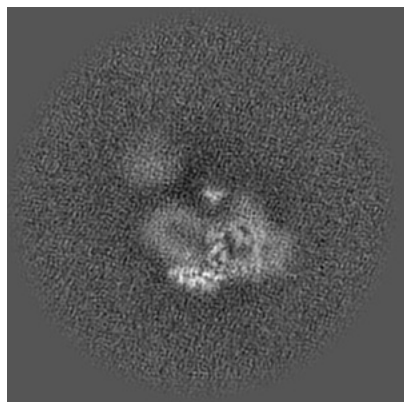


Z

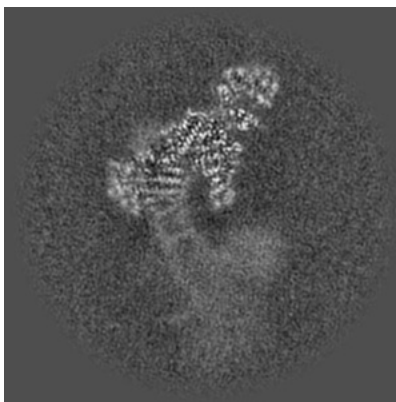
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

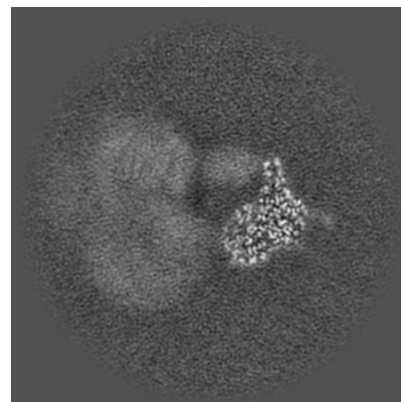
6.2.1 Primary map



X Index: 192

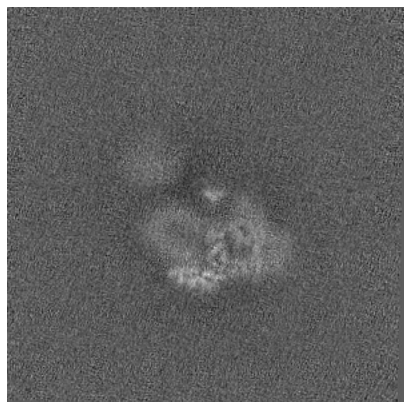


Y Index: 192

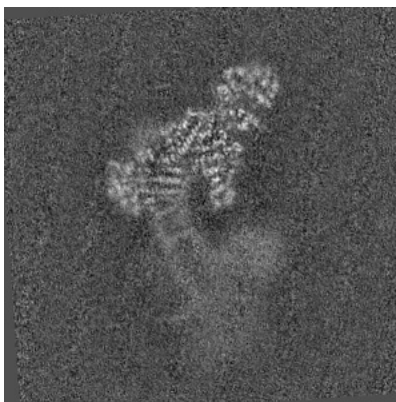


Z Index: 192

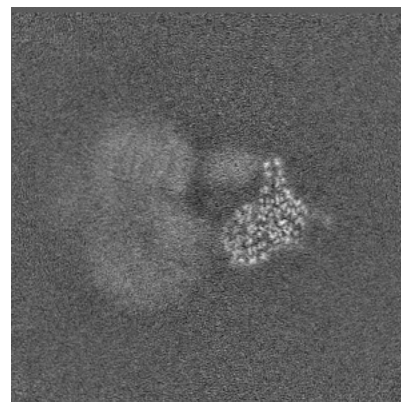
6.2.2 Raw map



X Index: 192



Y Index: 192

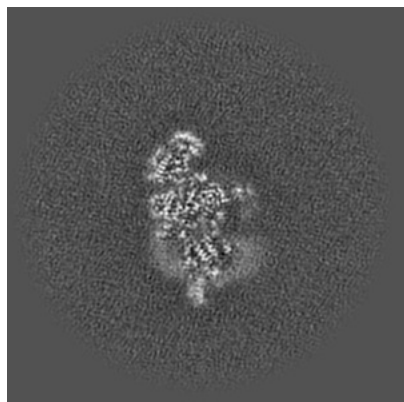


Z Index: 192

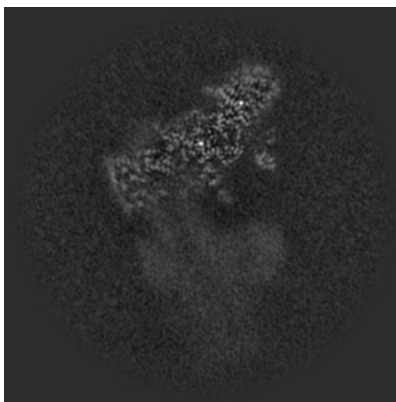
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

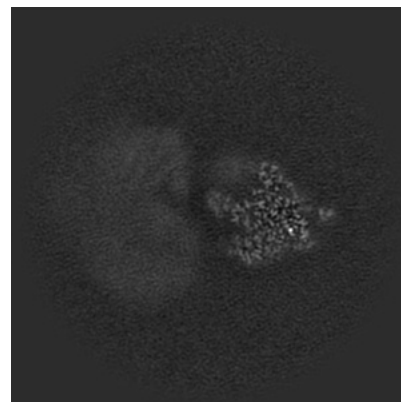
6.3.1 Primary map



X Index: 238

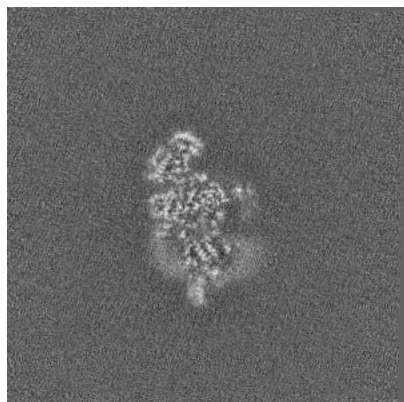


Y Index: 180

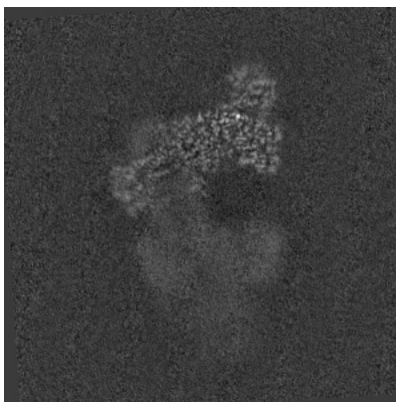


Z Index: 202

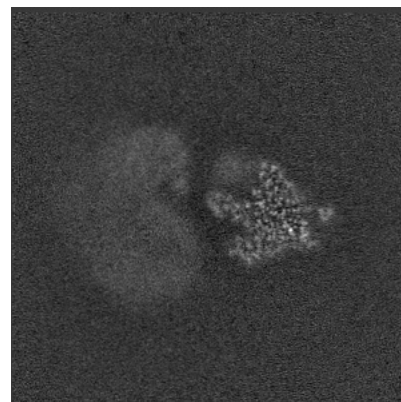
6.3.2 Raw map



X Index: 238



Y Index: 172

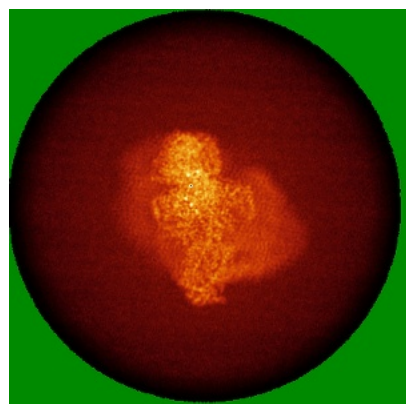


Z Index: 203

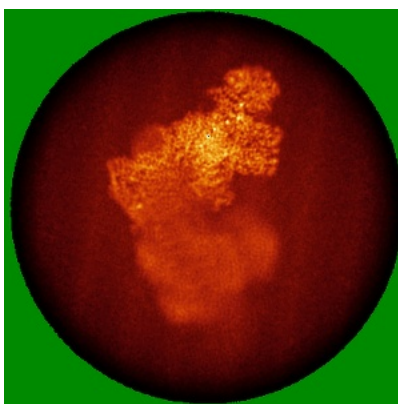
The images above show the largest variance slices of the map in three orthogonal directions.

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

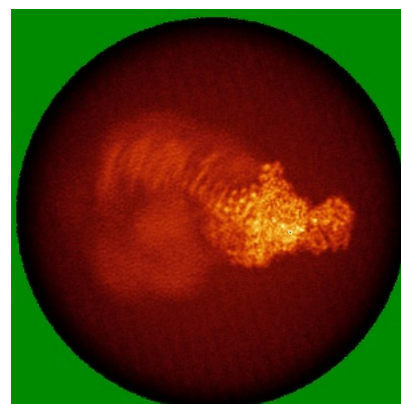
6.4.1 Primary map



X

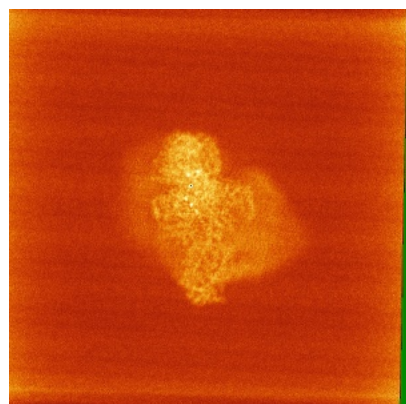


Y

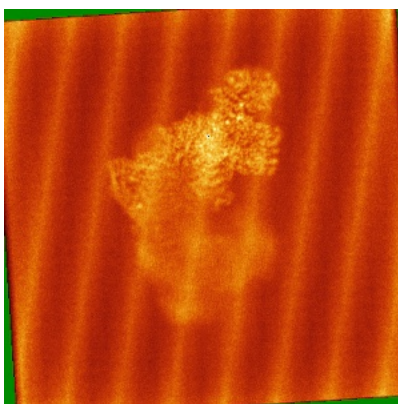


Z

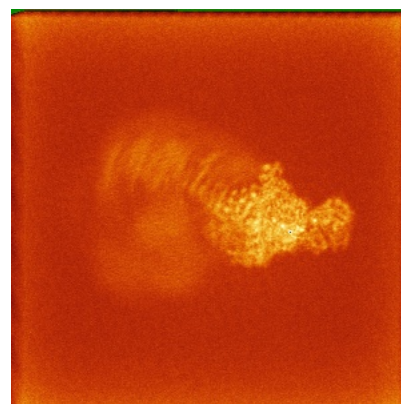
6.4.2 Raw map



X



Y

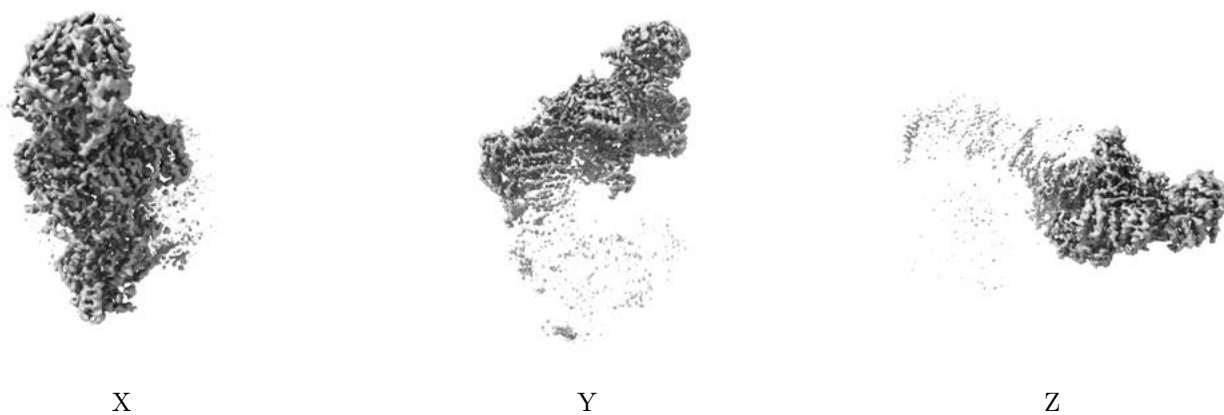


Z

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.

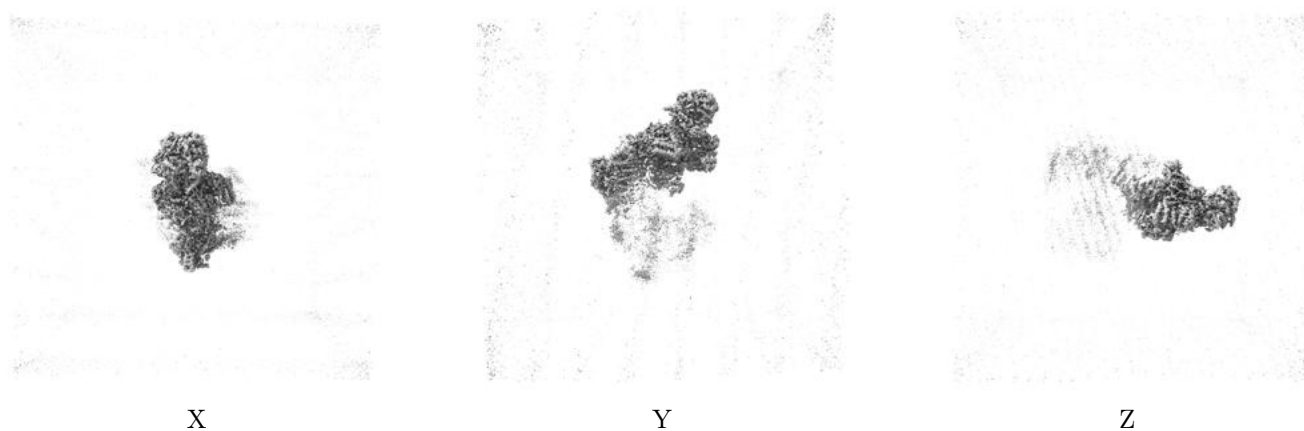
6.5 Orthogonal surface views [i](#)

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.

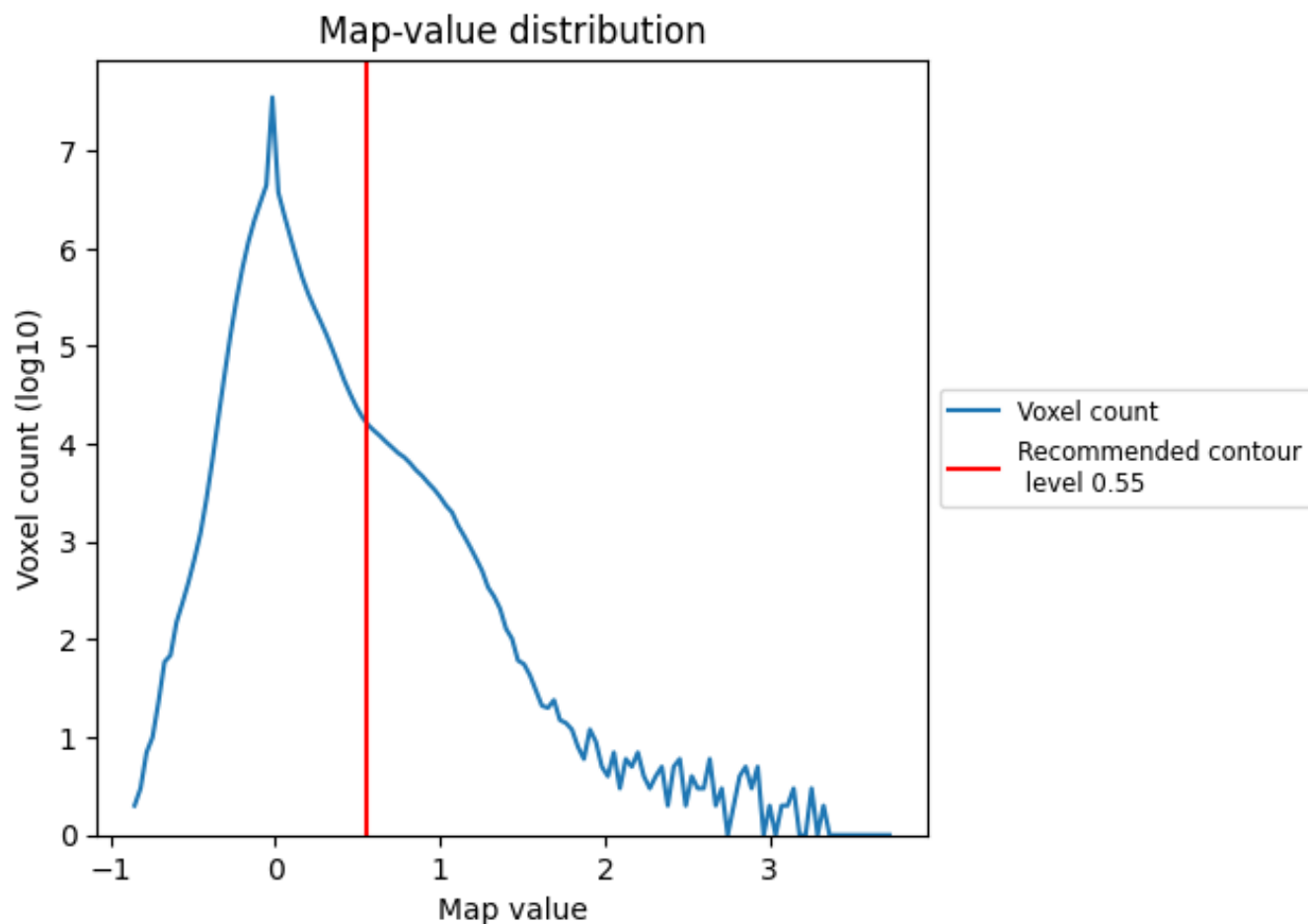
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

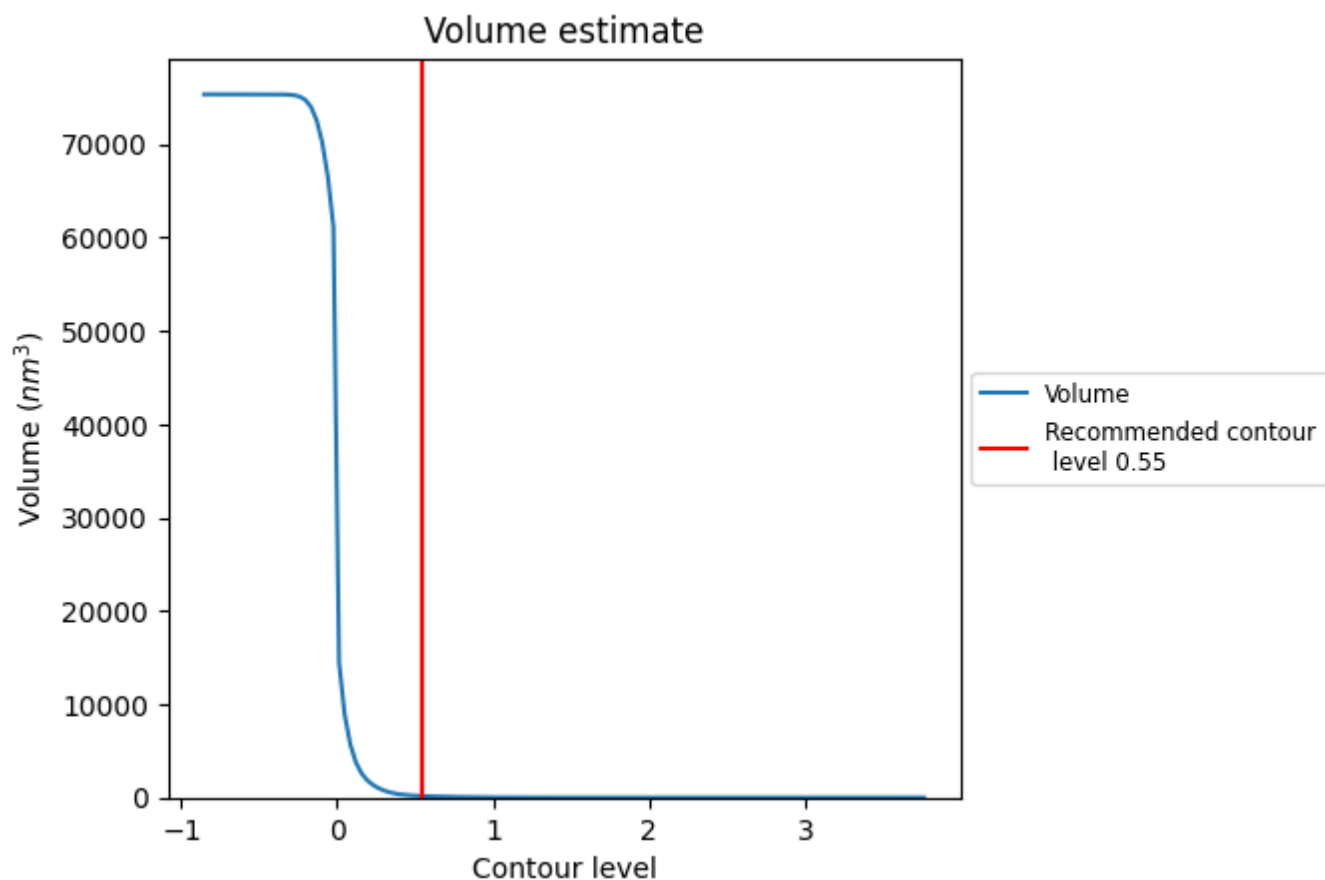
This section contains the results of statistical analysis of the map.

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.

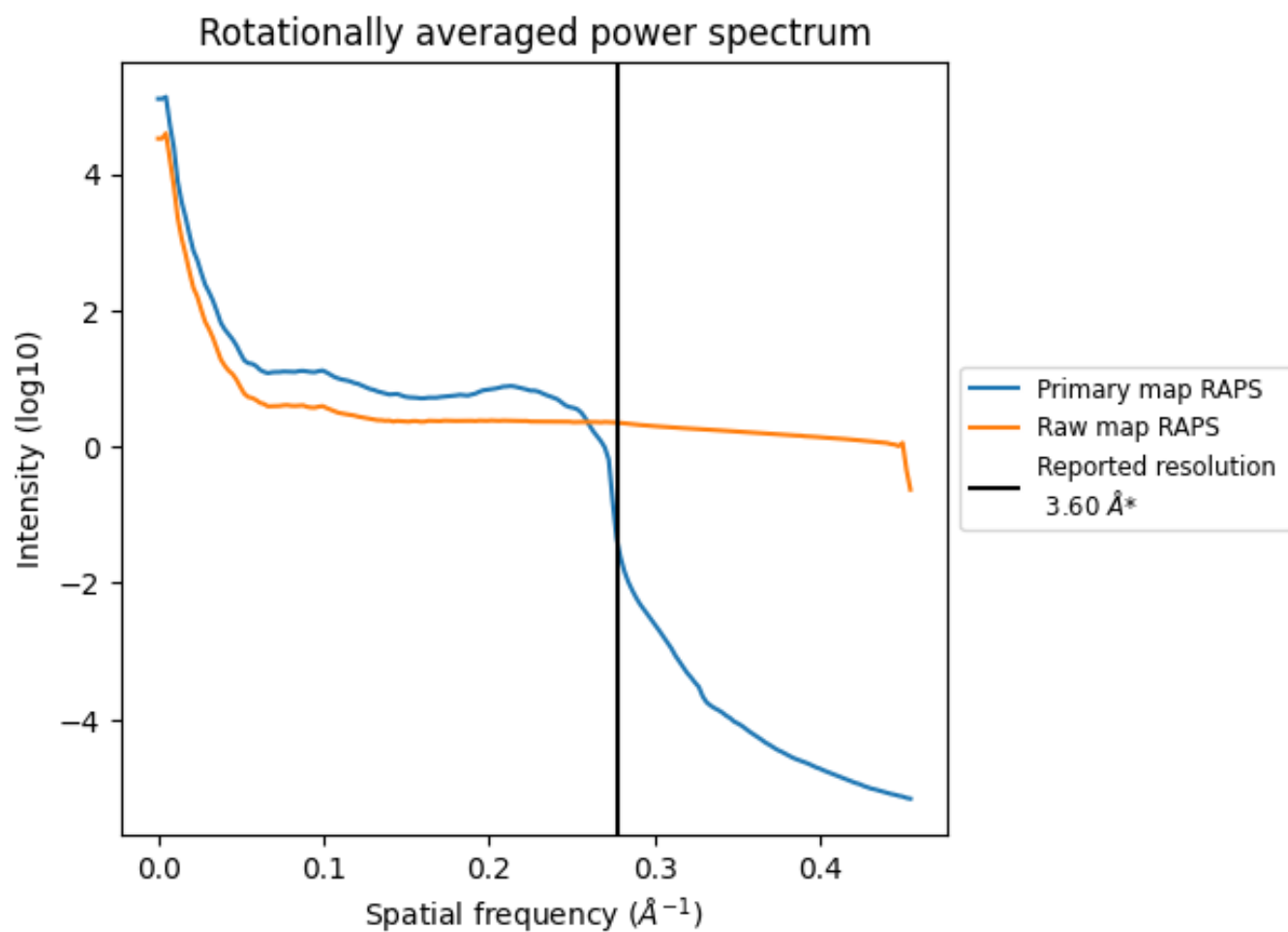
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm³; this corresponds to an approximate mass of 145 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 ⓘ

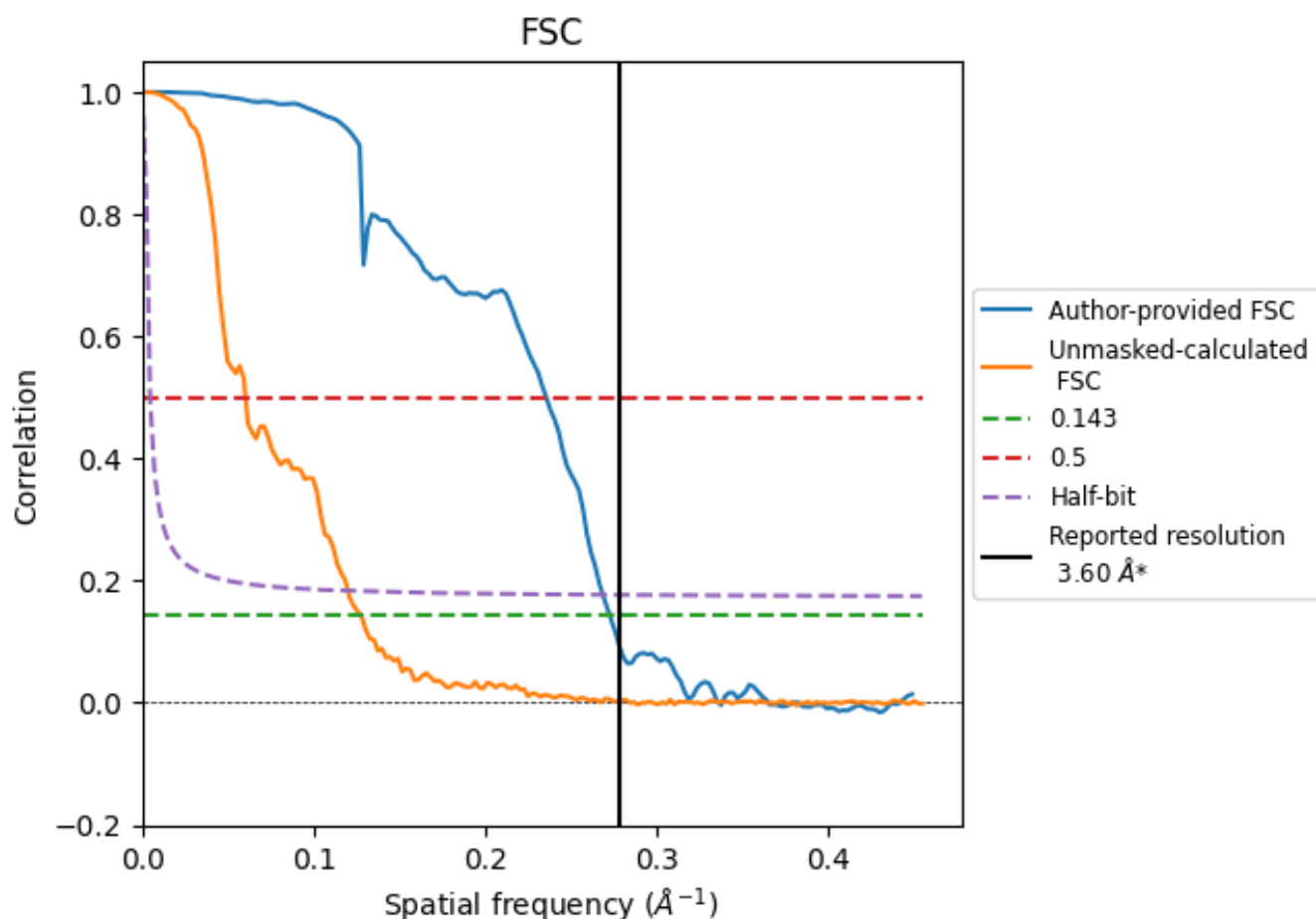


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

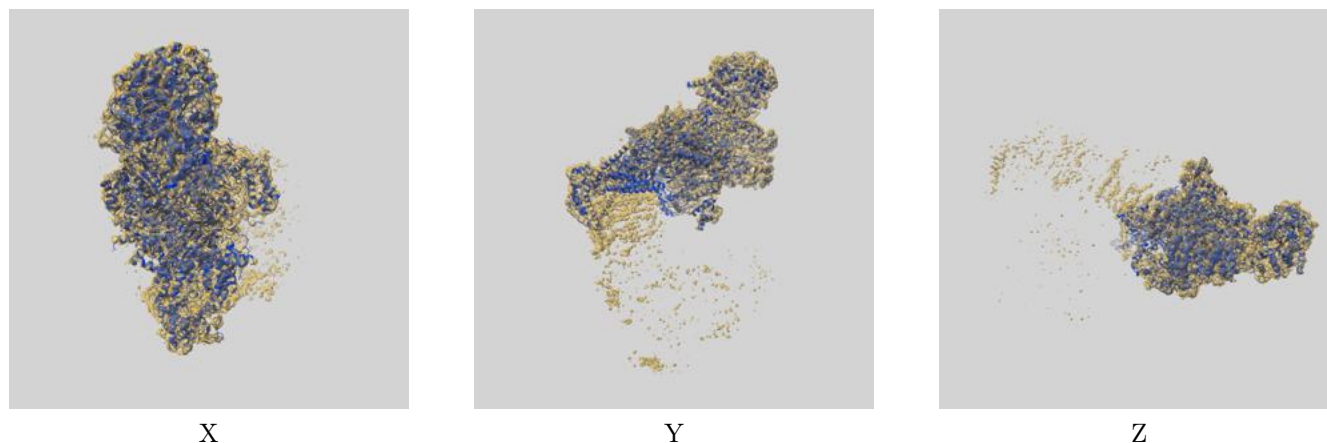
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.67	4.25	3.72
Unmasked-calculated*	7.86	16.61	8.34

*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 7.86 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

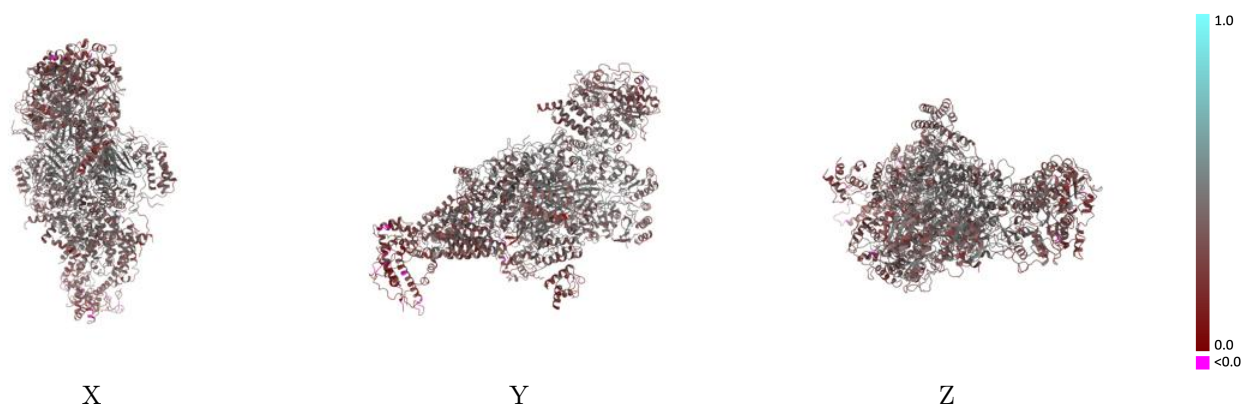
This section contains information regarding the fit between EMDB map EMD-38508 and PDB model 8XNN. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



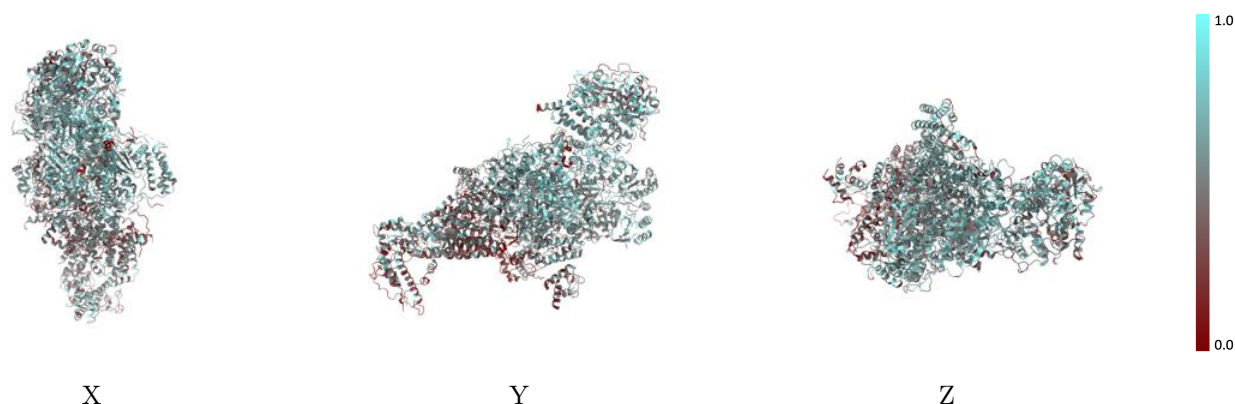
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



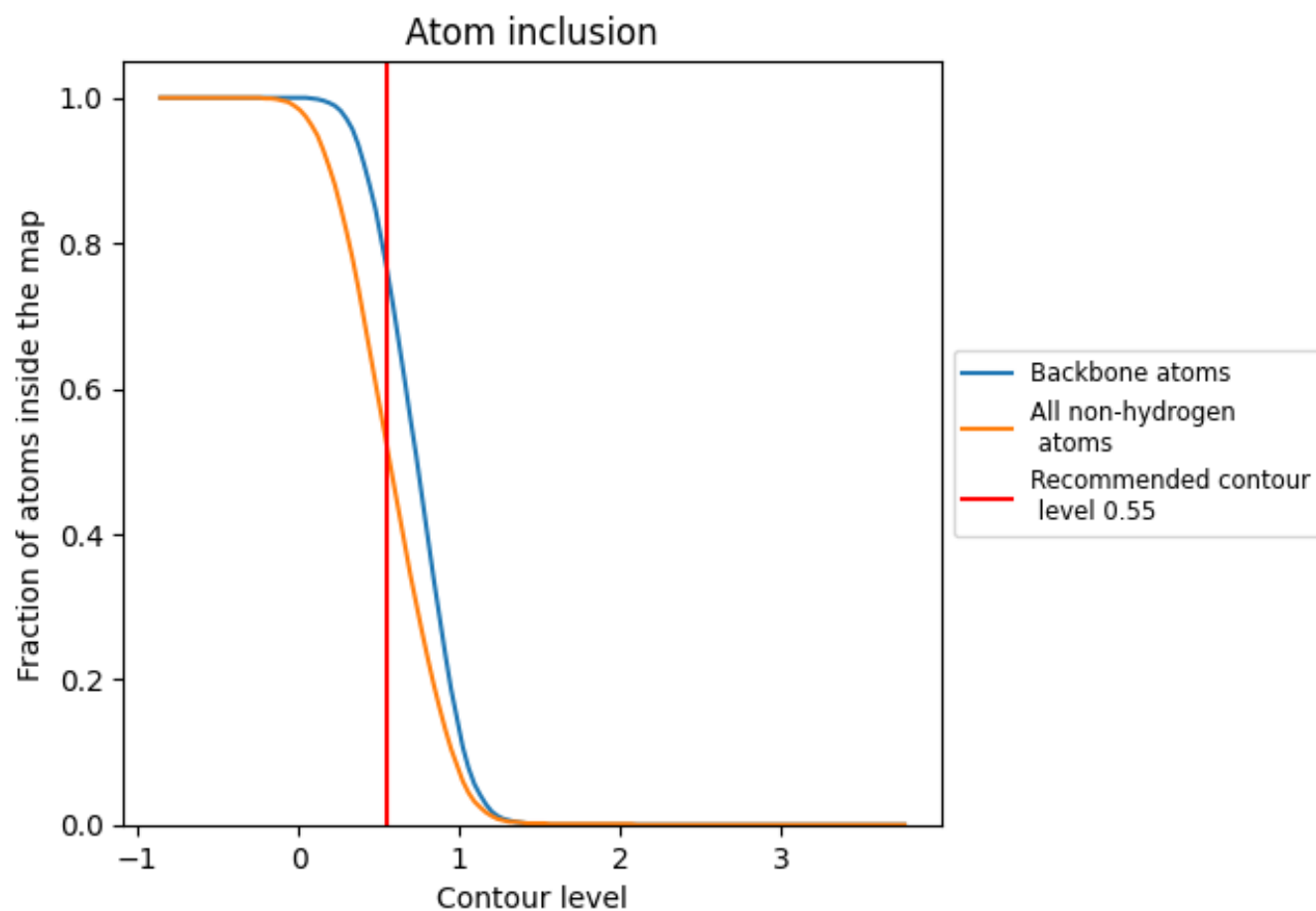
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 77% of all backbone atoms, 52% 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	 0.5220	 0.3700
A	 0.2710	 0.3220
B	 0.5740	 0.4130
C	 0.6190	 0.4350
D	 0.5940	 0.4220
E	 0.5220	 0.3380
F	 0.5770	 0.3540
G	 0.6160	 0.4070
H	 0.4340	 0.3840
I	 0.5980	 0.4160
P	 0.4250	 0.3350
Q	 0.5130	 0.4100
R	 0.4840	 0.3850
S	 0.6220	 0.3700
T	 0.3820	 0.2760
V	 0.5870	 0.3570
W	 0.4980	 0.3720
X	 0.4300	 0.2200
Z	 0.4340	 0.2810
a	 0.5010	 0.3100
b	 0.3890	 0.2730
q	 0.4560	 0.3860
r	 0.3760	 0.3730
s	 0.3460	 0.2780

