



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 05:06 PM JST

PDB ID : 8IBE / pdb_00008ibe
EMDB ID : EMD-35341
Title : Respiratory complex Peripheral Arm of CI, focus-refined map of type II, Wild type mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

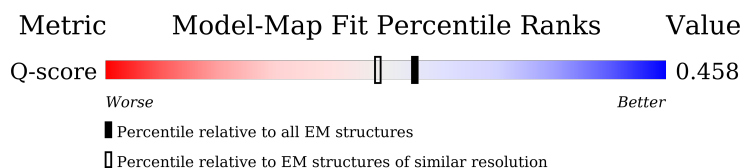
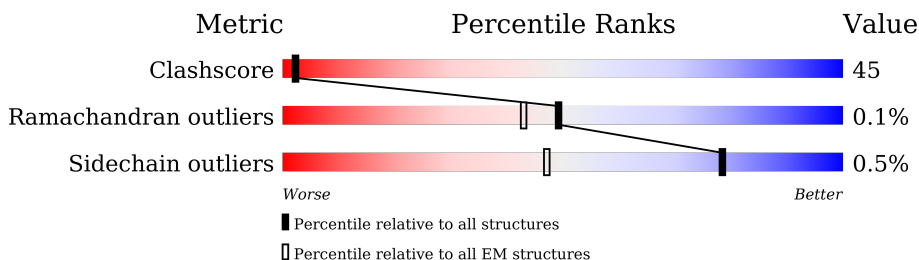
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	
2	B	224	
3	C	263	
4	D	463	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	UQ1	B	302	-	-	X	-
28	FES	E	301	-	-	X	-
28	FES	G	803	-	-	X	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 34255 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	98	Total	C	N	O	S	0	0
			799	552	112	130	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1241	793	222	212	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
			1643	1061	279	300	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	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	317	Total	C	N	O	S	0	0
			2532	1702	383	425	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	172	Total	C	N	O	S	0	0
			1380	869	237	262	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	116	Total	C	N	O	S	0	0
			940	598	161	177	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	138	Total	C	N	O	S	0	0
			1145	736	203	198	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	80	Total	C	N	O	S	0	0
			628	414	99	111	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	123	Total	C	N	O	S	0	0
			1025	658	181	182	4		

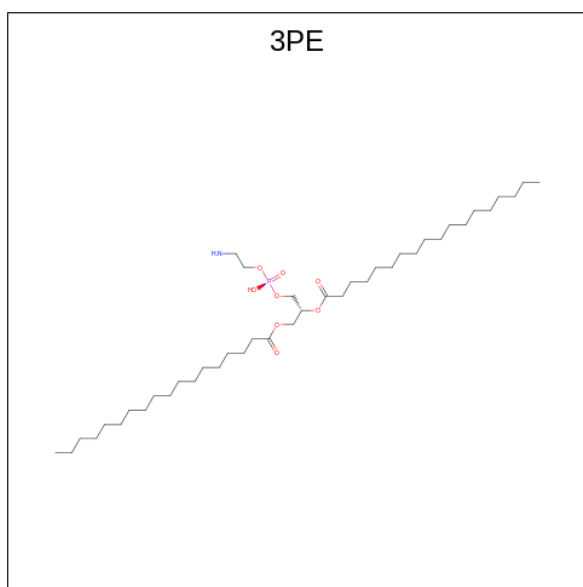
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	84	Total	C	N	O	S	0	0
			686	435	128	121	2		

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

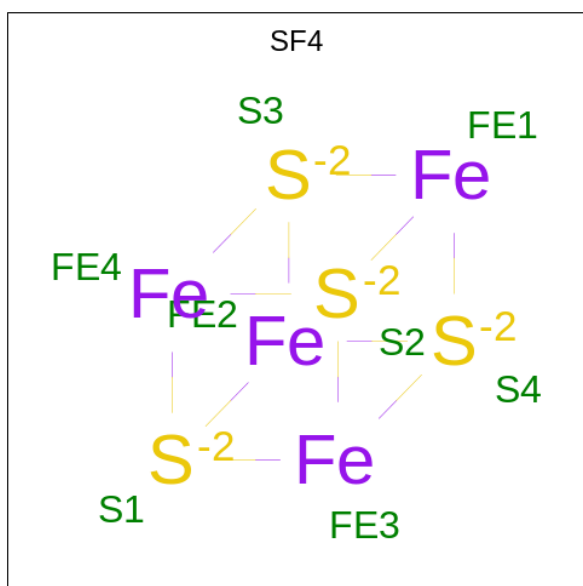
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	23	Total	C	N	O	0	0
			193	126	30	37		

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



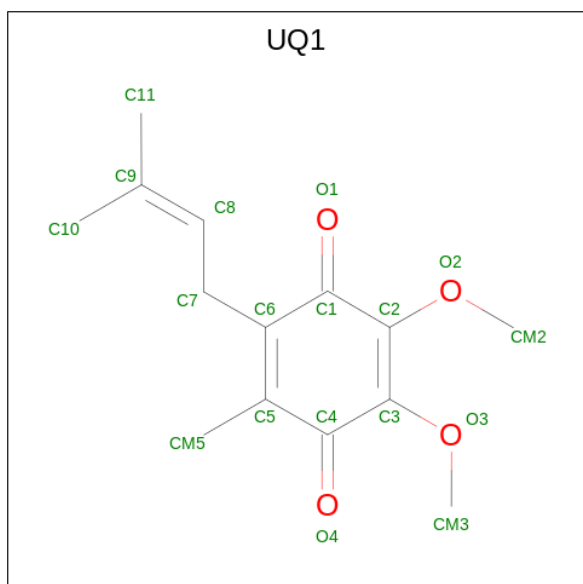
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
24	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
24	I	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



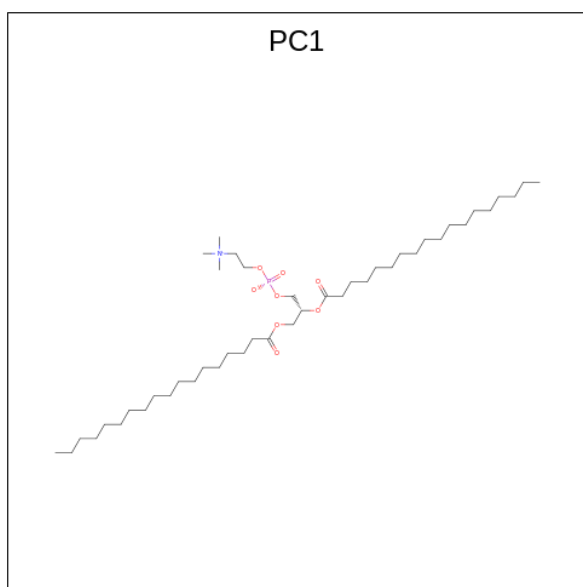
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	Fe	S	0
			8	4	4	
25	F	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



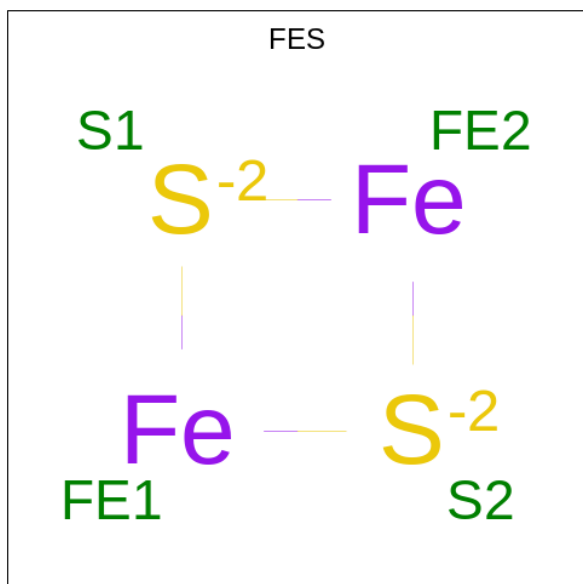
Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total	C	O	0
			18	14	4	

- Molecule 27 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
27	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
27	B	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 28 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



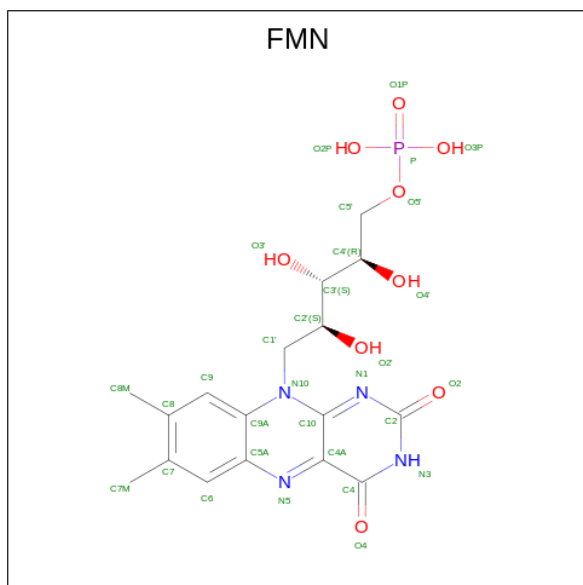
Mol	Chain	Residues	Atoms			AltConf
28	E	1	Total	Fe	S	0
			4	2	2	

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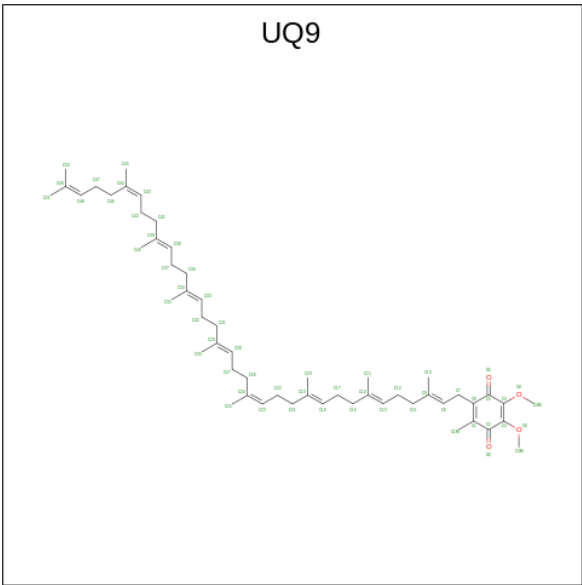
Mol	Chain	Residues	Atoms			AltConf
28	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 29 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



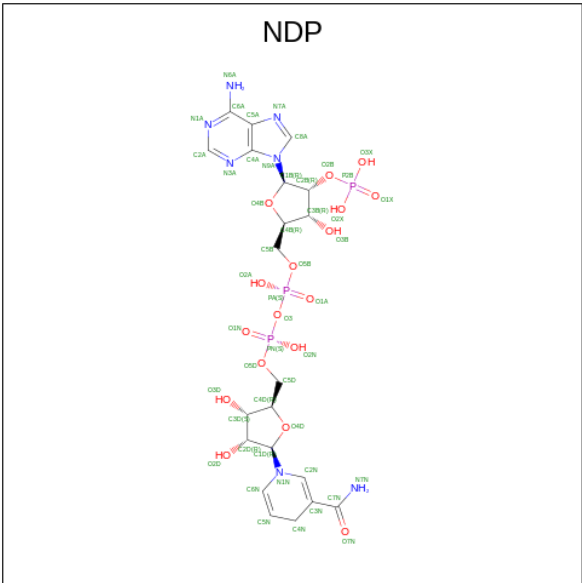
Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 30 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
30	H	1	Total	C	O		0
			35	31	4		

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



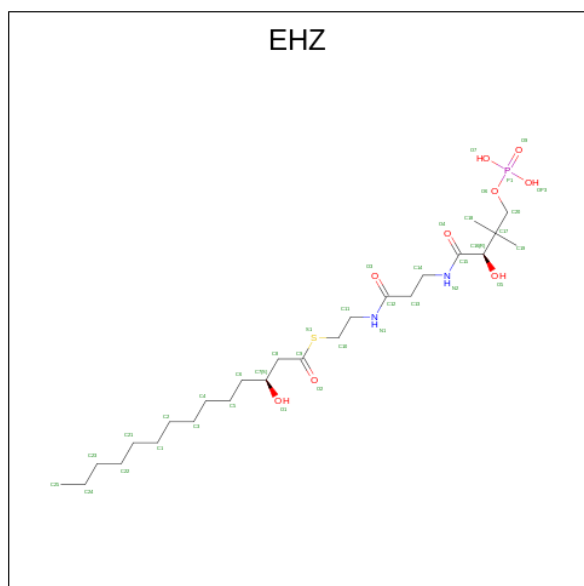
Mol	Chain	Residues	Atoms					AltConf
31	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

depositor).

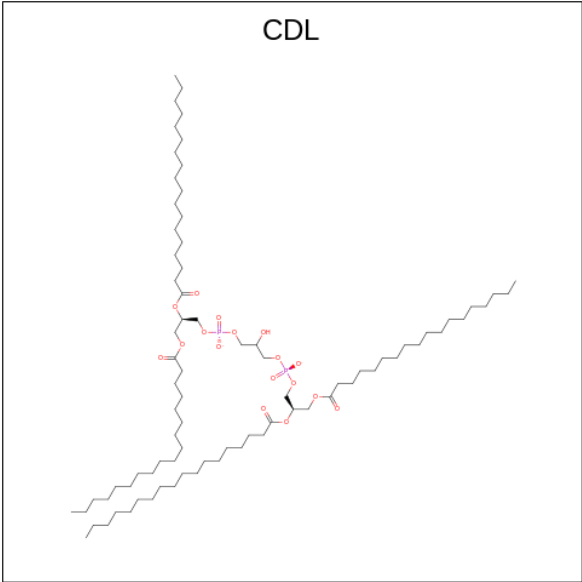
Mol	Chain	Residues	Atoms		AltConf
32	R	1	Total	Zn	0
			1	1	

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

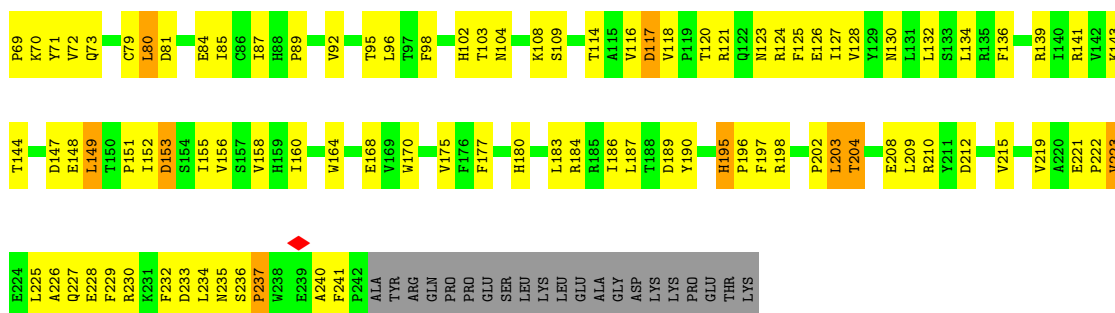


Mol	Chain	Residues	Atoms						AltConf
33	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

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

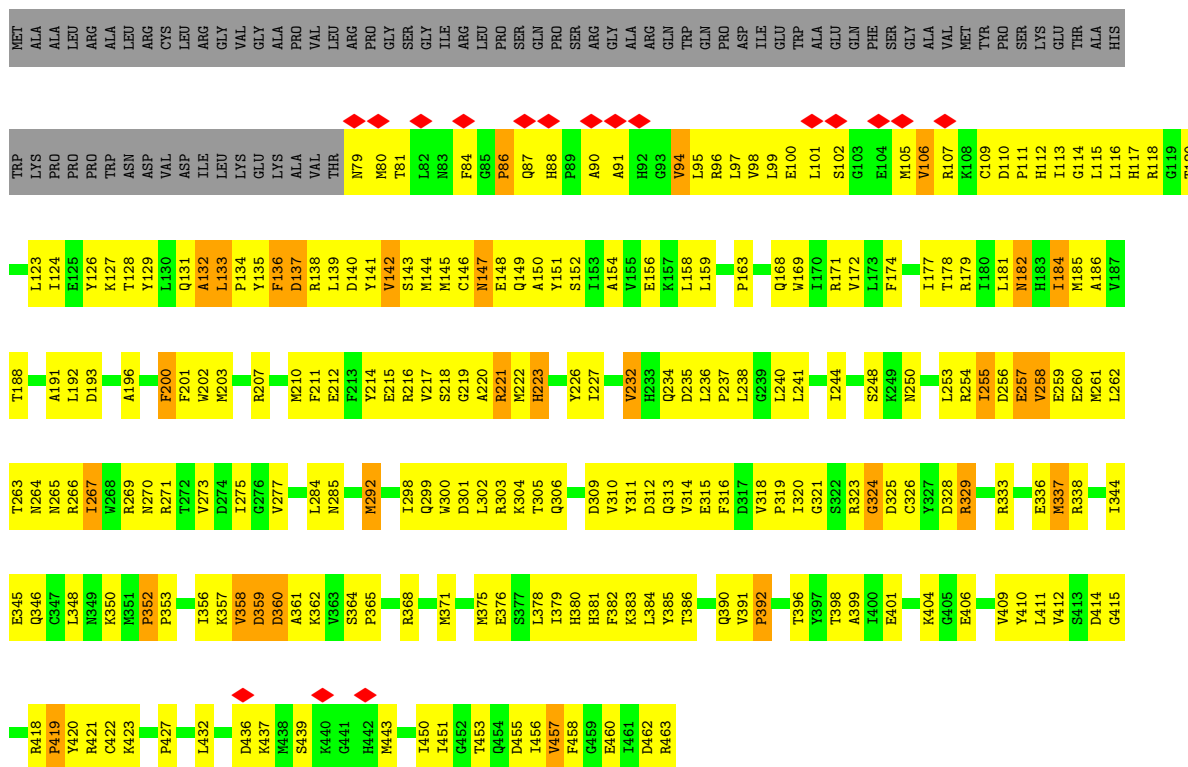


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
34	a	1	57	38	17	2	0



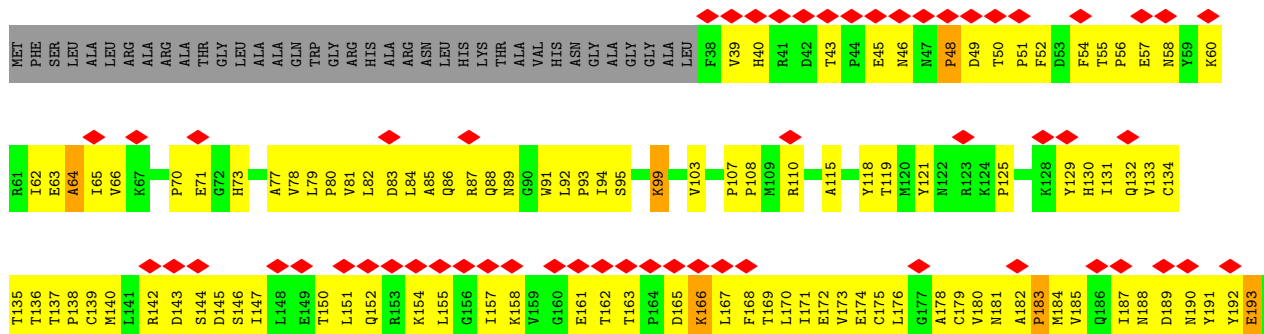
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 32% 44% 6% 17%



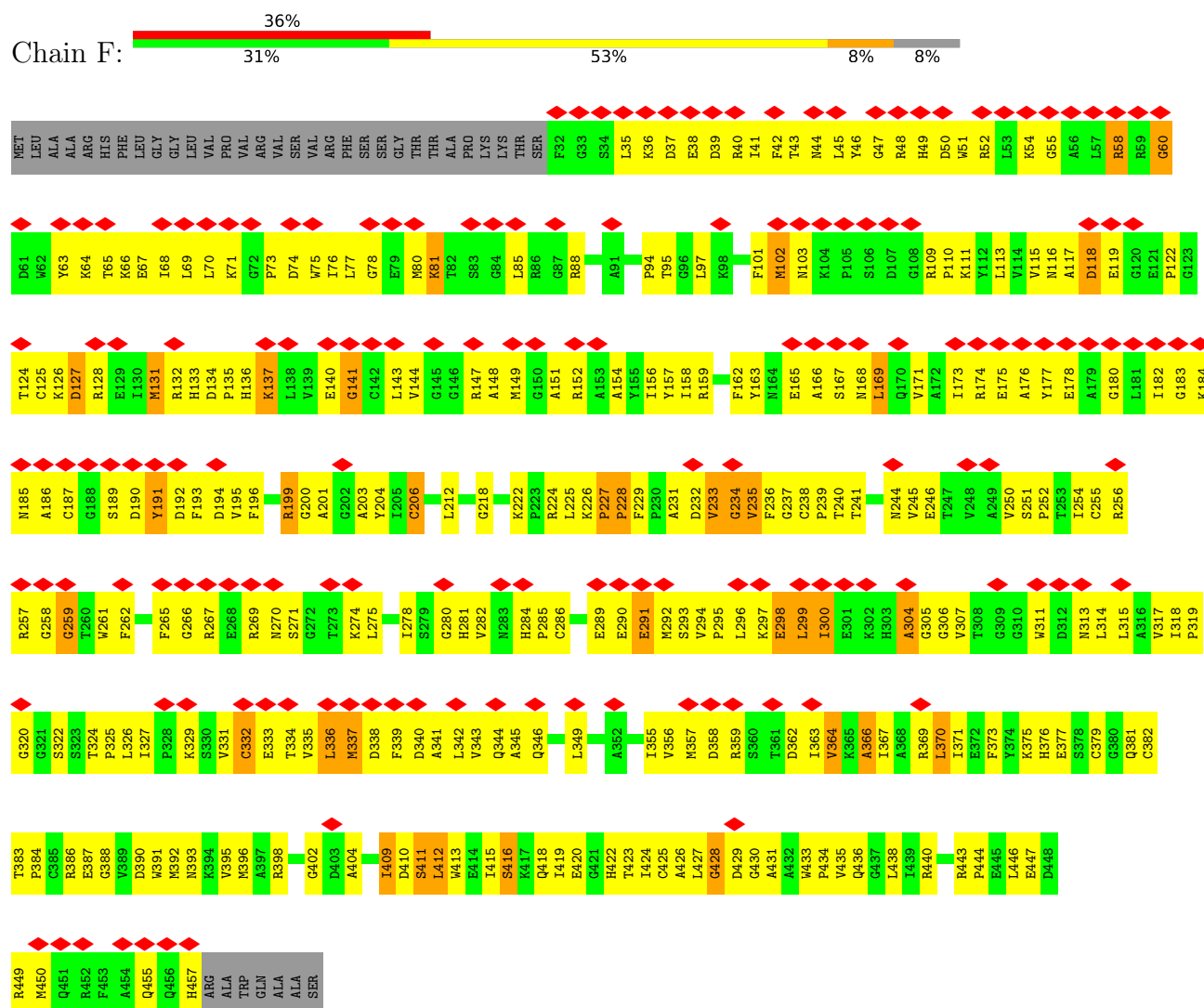
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 40% 27% 53% 15%

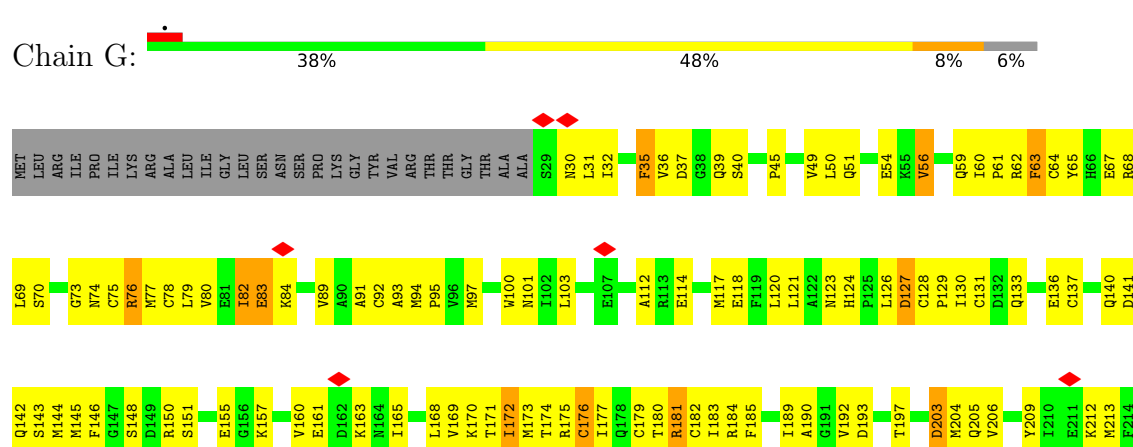


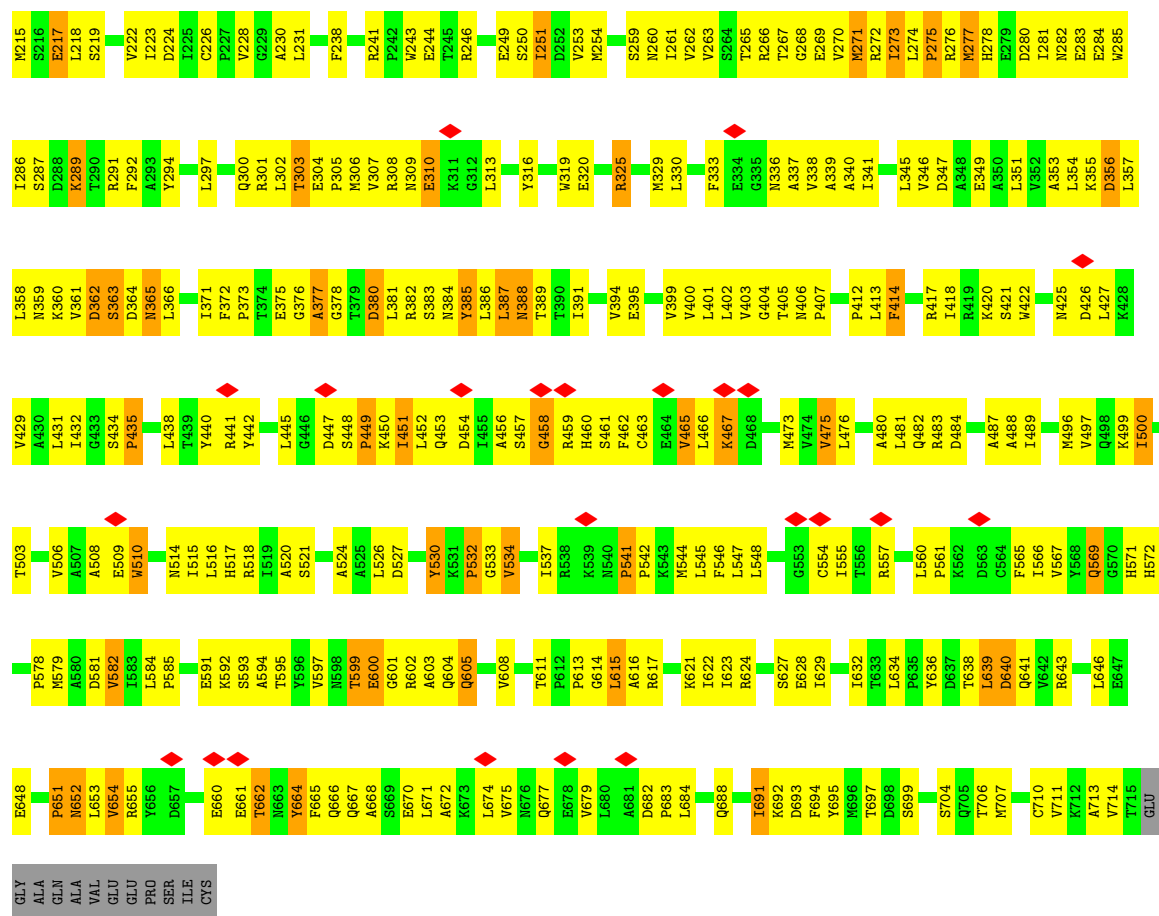


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

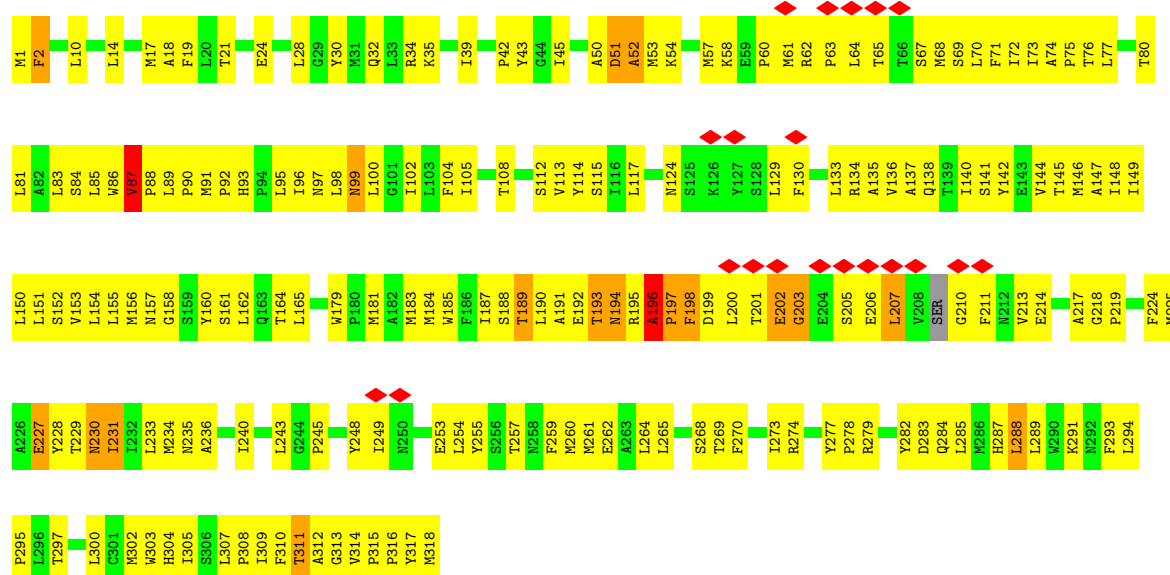


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

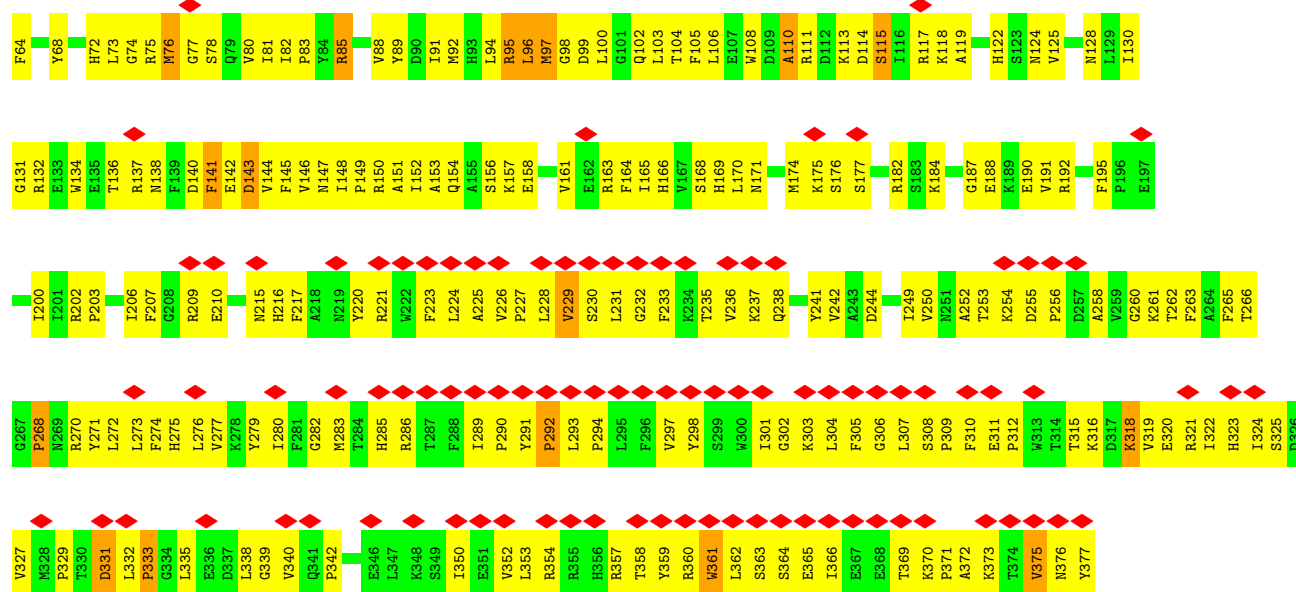




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



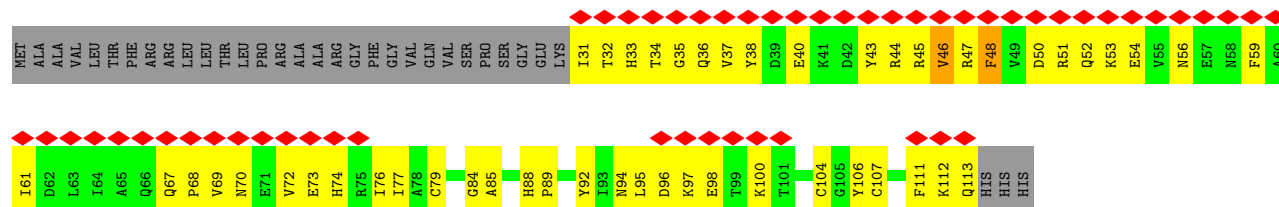
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



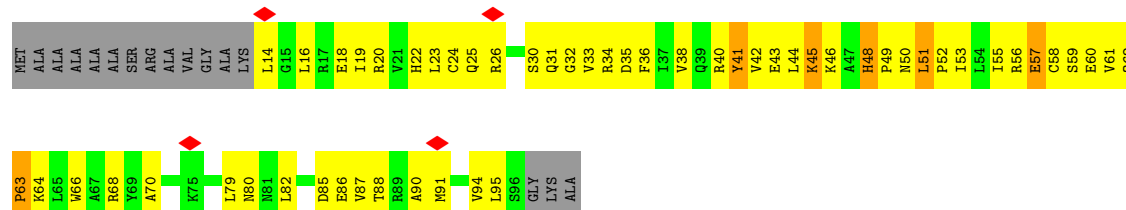
- [illegible]



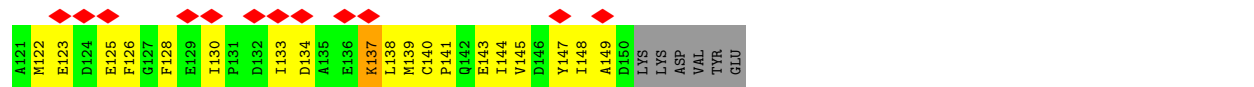
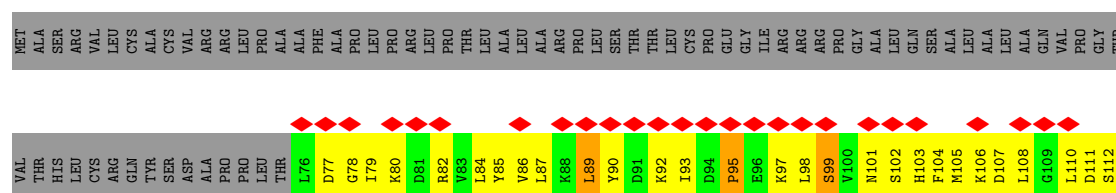
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



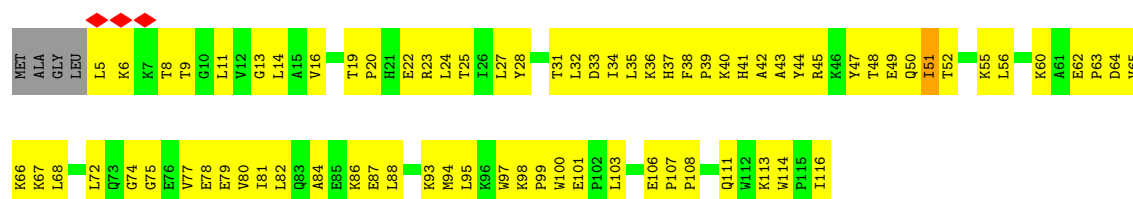
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



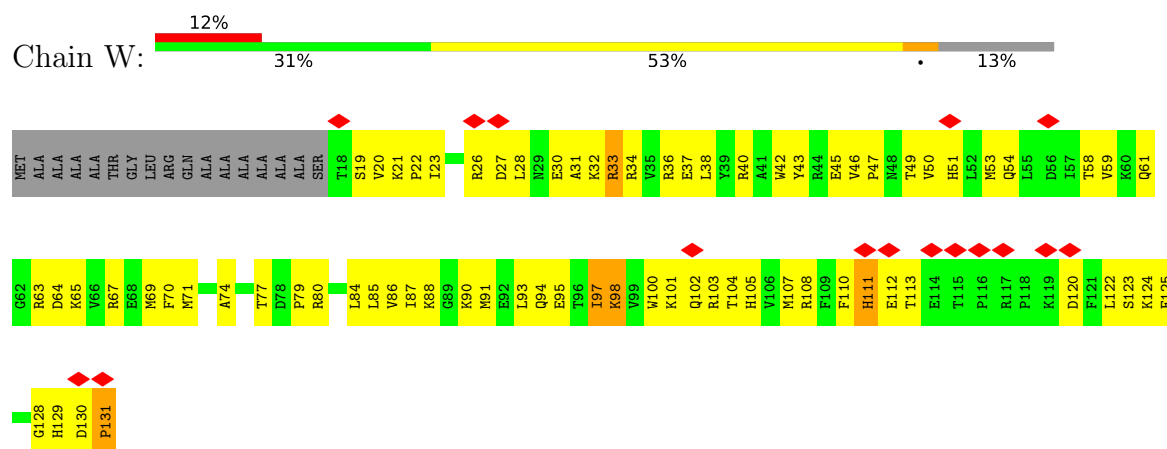
- Molecule 14: Acyl carrier protein, mitochondrial



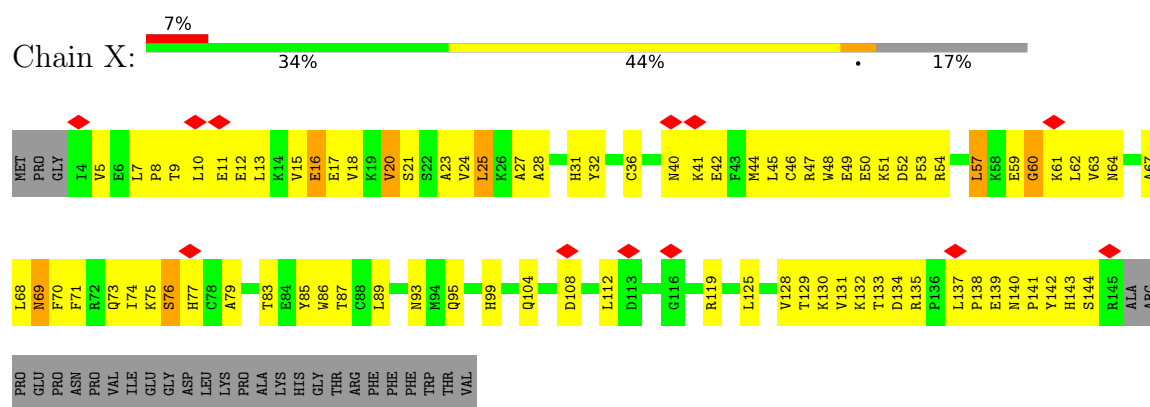
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



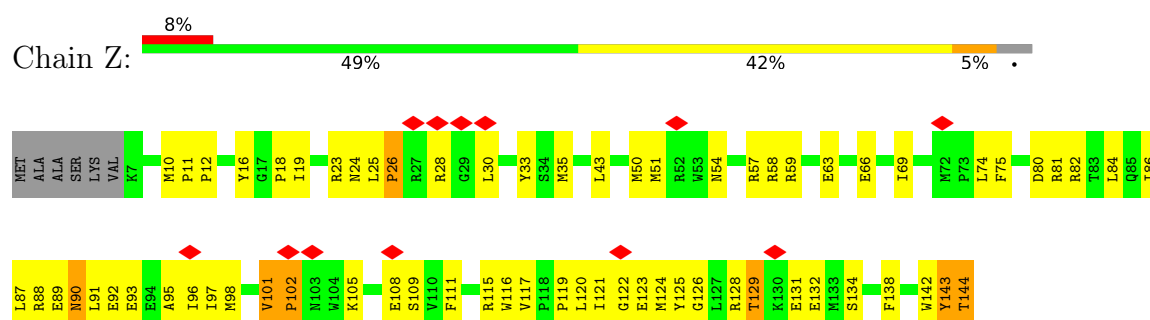
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



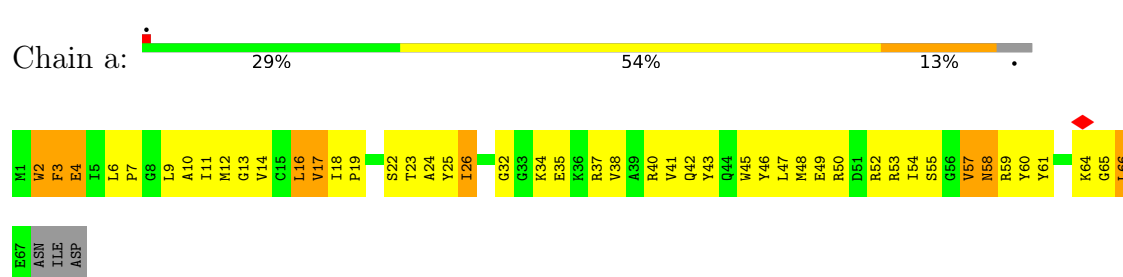
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



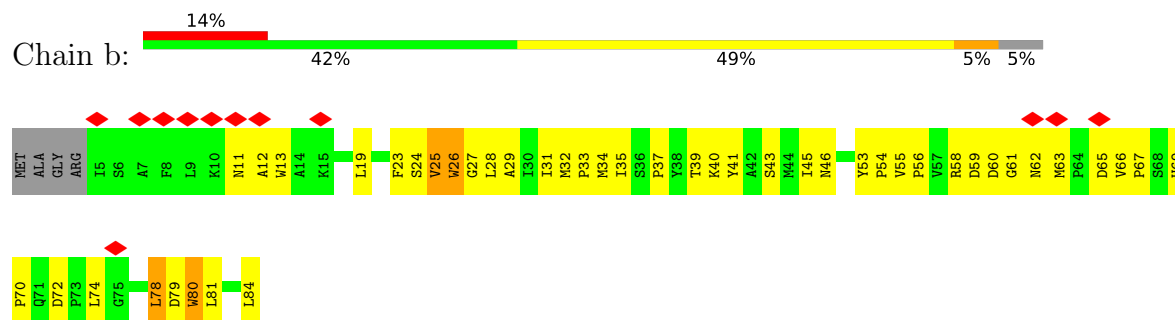
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



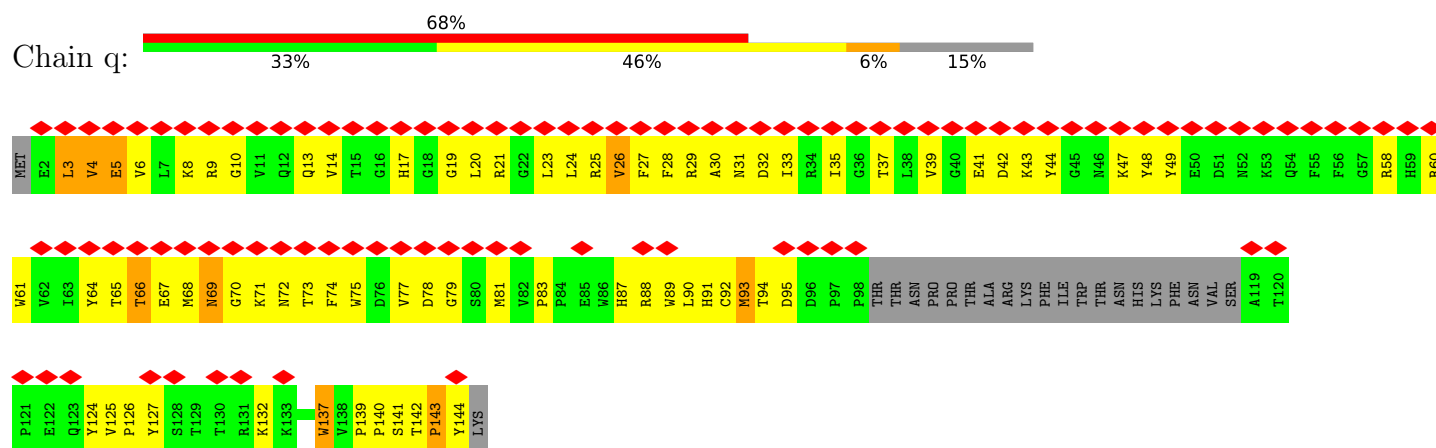
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



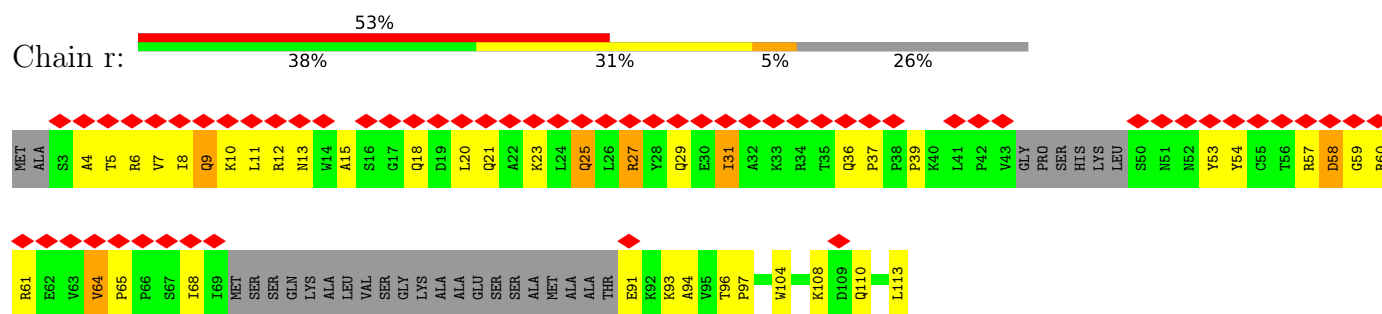
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



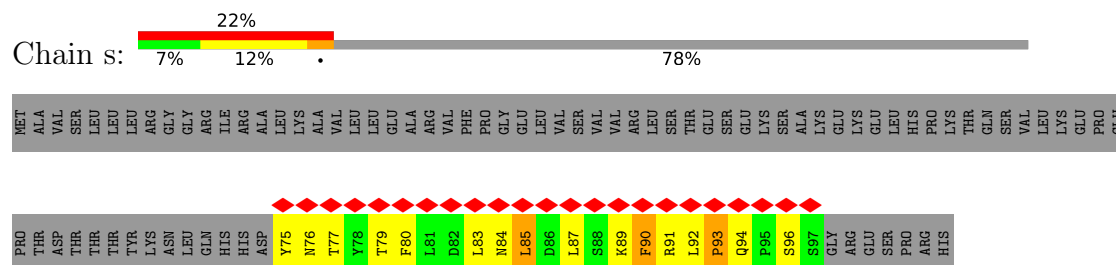
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- 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	177076	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 ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.925	Depositor
Minimum map value	-2.073	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.086	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: SF4, FES, CDL, 3PE, UQ1, UQ9, NDP, PC1, FMN, EHZ, ZN

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	0.94	1/820 (0.1%)	1.18	8/1118 (0.7%)
2	B	1.16	6/1272 (0.5%)	1.73	26/1722 (1.5%)
3	C	1.04	1/1689 (0.1%)	1.42	24/2300 (1.0%)
4	D	0.99	3/3162 (0.1%)	1.50	49/4276 (1.1%)
5	E	0.82	2/1675 (0.1%)	1.30	26/2282 (1.1%)
6	F	0.96	6/3363 (0.2%)	1.54	66/4543 (1.5%)
7	G	0.97	13/5374 (0.2%)	1.59	112/7281 (1.5%)
8	H	0.87	2/2608 (0.1%)	1.23	30/3563 (0.8%)
9	I	0.80	3/1409 (0.2%)	1.27	21/1904 (1.1%)
10	P	0.77	2/2793 (0.1%)	1.19	23/3787 (0.6%)
11	Q	0.97	3/963 (0.3%)	1.40	11/1302 (0.8%)
12	R	0.63	0/671	1.06	4/903 (0.4%)
13	S	0.86	2/678 (0.3%)	1.37	13/915 (1.4%)
14	T	0.75	0/613	1.11	7/826 (0.8%)
15	V	0.82	0/937	1.24	4/1270 (0.3%)
16	W	0.89	2/993 (0.2%)	0.99	7/1335 (0.5%)
17	X	0.62	0/1191	1.01	8/1605 (0.5%)
18	Z	0.75	2/1176 (0.2%)	1.17	10/1587 (0.6%)
19	a	0.89	0/561	1.60	14/755 (1.9%)
20	b	0.69	0/651	1.11	7/895 (0.8%)
21	q	0.83	5/1059 (0.5%)	1.25	15/1439 (1.0%)
22	r	0.94	2/701 (0.3%)	1.56	12/948 (1.3%)
23	s	1.11	0/198	1.68	5/269 (1.9%)
All	All	0.90	55/34557 (0.2%)	1.38	502/46825 (1.1%)

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	532	PRO	N-CD	-12.62	1.30	1.47
16	W	131	PRO	N-CD	-12.39	1.30	1.47
1	A	36	PRO	N-CD	-11.09	1.32	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	q	143	PRO	N-CD	-10.52	1.33	1.47
6	F	234	GLY	CA-C	-10.22	1.41	1.52
10	P	333	PRO	N-CD	-10.15	1.33	1.47
6	F	227	PRO	N-CD	10.13	1.61	1.47
2	B	121	PHE	C-O	-10.09	1.11	1.23
6	F	235	VAL	N-CA	-9.71	1.34	1.46
4	D	365	PRO	N-CD	-9.60	1.34	1.47
2	B	92	PRO	N-CD	9.41	1.60	1.47
7	G	275	PRO	N-CD	-9.40	1.34	1.47
6	F	319	PRO	N-CD	9.03	1.60	1.47
11	Q	106	ARG	C-O	8.93	1.34	1.24
9	I	154	TYR	C-O	8.83	1.35	1.23
18	Z	102	PRO	N-CD	-8.76	1.35	1.47
9	I	107	PRO	N-CD	8.61	1.59	1.47
18	Z	143	TYR	CA-C	-8.47	1.42	1.52
9	I	118	LEU	CA-C	8.16	1.64	1.52
21	q	139	PRO	N-CD	-7.95	1.36	1.47
5	E	218	ARG	CA-C	7.86	1.62	1.53
2	B	121	PHE	CA-C	-7.75	1.42	1.52
7	G	31	LEU	CA-C	-7.25	1.43	1.52
22	r	65	PRO	N-CD	7.17	1.57	1.47
2	B	122	ARG	CA-CB	-7.08	1.41	1.53
8	H	196	ALA	C-N	6.90	1.41	1.34
3	C	203	LEU	CA-C	-6.90	1.43	1.52
7	G	449	PRO	N-CD	6.85	1.57	1.47
7	G	541	PRO	N-CD	-6.82	1.38	1.47
7	G	203	ASP	CA-C	6.71	1.62	1.52
6	F	233	VAL	CA-C	-6.68	1.44	1.52
21	q	69	ASN	CA-C	6.60	1.61	1.52
7	G	600	GLU	CA-C	6.47	1.61	1.52
11	Q	155	PRO	N-CD	-6.32	1.38	1.47
21	q	69	ASN	C-O	6.19	1.31	1.24
7	G	127	ASP	CA-C	6.17	1.62	1.52
6	F	384	PRO	N-CD	-6.14	1.39	1.47
7	G	76	ARG	CA-C	6.14	1.61	1.53
10	P	292	PRO	N-CD	-6.13	1.39	1.47
4	D	359	ASP	CA-C	6.11	1.60	1.52
2	B	170	TYR	CA-CB	-6.04	1.43	1.53
7	G	192	VAL	CA-C	-6.04	1.47	1.53
5	E	93	PRO	N-CD	-5.96	1.39	1.47
4	D	392	PRO	C-O	-5.88	1.20	1.25
7	G	361	VAL	CA-C	5.80	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S	50	ASN	CA-C	5.70	1.60	1.53
13	S	63	PRO	N-CD	-5.64	1.39	1.47
11	Q	82	PRO	N-CD	-5.58	1.40	1.47
22	r	37	PRO	N-CD	5.41	1.55	1.47
7	G	683	PRO	N-CD	-5.38	1.40	1.47
16	W	111	HIS	C-O	5.30	1.30	1.23
8	H	51	ASP	CA-C	5.25	1.59	1.52
2	B	195	PRO	CA-C	-5.09	1.47	1.52
7	G	83	GLU	CA-C	5.08	1.59	1.52
21	q	4	VAL	CA-C	5.07	1.58	1.52

All (502) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	231	ILE	N-CA-C	-19.19	90.97	113.42
2	B	99	CYS	N-CA-C	-18.00	91.45	113.41
2	B	170	TYR	N-CA-C	-17.69	89.93	111.33
7	G	174	THR	N-CA-C	-16.82	89.07	114.64
2	B	122	ARG	N-CA-CB	-16.68	85.52	110.04
2	B	121	PHE	N-CA-C	-16.25	86.23	110.28
6	F	125	CYS	N-CA-C	-15.66	93.43	113.17
6	F	332	CYS	N-CA-C	15.64	130.11	111.02
7	G	380	ASP	N-CA-C	15.31	129.32	111.71
8	H	196	ALA	CA-C-N	-14.42	105.69	119.82
8	H	196	ALA	C-N-CA	-14.42	105.69	119.82
18	Z	102	PRO	N-CA-C	13.52	130.15	111.22
7	G	251	ILE	N-CA-C	13.30	126.79	108.17
7	G	77	MET	N-CA-C	-13.08	97.29	113.38
4	D	360	ASP	N-CA-C	-12.88	87.74	108.73
9	I	64	THR	N-CA-C	-12.74	98.38	114.56
18	Z	143	TYR	N-CA-C	12.73	129.48	108.73
10	P	115	SER	N-CA-C	-12.59	97.38	113.12
23	s	85	LEU	N-CA-C	-12.55	97.65	111.07
7	G	500	ILE	N-CA-C	-12.47	98.81	110.53
19	a	3	PHE	CB-CA-C	-12.34	89.71	110.68
6	F	171	VAL	N-CA-C	-11.85	99.39	110.53
7	G	204	MET	N-CA-C	-11.66	91.41	109.25
6	F	449	ARG	N-CA-C	-11.59	98.73	111.36
6	F	334	THR	N-CA-CB	11.51	127.31	109.82
9	I	118	LEU	N-CA-C	11.47	126.77	113.01
7	G	599	THR	N-CA-C	11.28	126.14	112.38
7	G	83	GLU	N-CA-C	11.12	127.43	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	197	PRO	N-CA-C	-10.97	99.82	113.98
4	D	358	VAL	N-CA-C	-10.93	95.26	109.80
2	B	121	PHE	CA-C-O	-10.82	109.04	121.16
4	D	257	GLU	N-CA-C	-10.81	99.47	111.14
2	B	122	ARG	N-CA-C	10.74	124.96	110.35
8	H	197	PRO	N-CA-CB	10.74	113.73	103.52
8	H	231	ILE	N-CA-CB	10.56	126.93	112.35
8	H	196	ALA	N-CA-C	10.48	132.97	109.81
22	r	64	VAL	N-CA-CB	-10.41	96.63	111.21
4	D	365	PRO	N-CA-CB	-10.31	97.42	103.19
7	G	280	ASP	N-CA-C	10.28	122.48	111.28
21	q	5	GLU	N-CA-C	10.13	123.59	111.33
9	I	119	CYS	N-CA-C	10.11	126.86	113.72
7	G	414	PHE	N-CA-C	-10.08	101.49	113.88
2	B	80	ASP	N-CA-C	-10.06	100.31	111.28
19	a	4	GLU	N-CA-C	10.04	124.79	112.54
13	S	57	GLU	N-CA-C	9.97	126.02	109.46
7	G	325	ARG	N-CA-C	-9.88	100.20	110.97
6	F	178	GLU	N-CA-C	-9.81	99.34	111.11
6	F	144	VAL	N-CA-C	-9.76	101.36	110.53
6	F	103	ASN	N-CA-C	-9.75	101.08	113.16
6	F	141	GLY	N-CA-C	-9.73	101.21	112.50
7	G	35	PHE	N-CA-C	9.69	124.37	108.96
7	G	694	PHE	N-CA-C	9.68	121.42	111.07
18	Z	144	THR	N-CA-CB	-9.68	95.05	111.50
5	E	64	ALA	N-CA-C	-9.65	99.53	111.11
6	F	418	GLN	N-CA-C	-9.60	100.77	111.14
7	G	337	ALA	N-CA-C	-9.59	100.79	114.12
8	H	207	LEU	N-CA-C	-9.56	94.75	109.95
4	D	427	PRO	N-CA-C	-9.54	95.52	110.50
19	a	2	TRP	N-CA-C	-9.53	101.66	113.28
22	r	31	ILE	N-CA-C	9.51	121.76	109.30
20	b	78	LEU	CB-CA-C	-9.48	98.04	112.07
2	B	155	PRO	N-CA-C	-9.43	95.68	110.95
21	q	3	LEU	N-CA-C	-9.43	100.55	112.90
7	G	692	LYS	N-CA-C	-9.32	100.48	112.23
7	G	640	ASP	N-CA-C	-9.27	101.26	111.36
9	I	95	PRO	N-CA-C	-9.23	102.32	113.86
5	E	85	ALA	N-CA-C	-9.18	101.36	111.36
4	D	223	HIS	N-CA-C	-9.16	98.69	111.52
20	b	26	TRP	N-CA-C	-8.96	101.48	111.07
22	r	65	PRO	N-CA-CB	8.93	107.86	103.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	61	VAL	N-CA-C	-8.92	96.04	108.27
3	C	149	LEU	N-CA-C	8.90	124.20	113.16
3	C	180	HIS	N-CA-C	-8.90	95.76	109.64
2	B	122	ARG	CB-CA-C	8.89	125.53	109.62
6	F	411	SER	N-CA-C	-8.87	101.58	111.07
7	G	212	LYS	N-CA-C	-8.80	94.56	108.90
7	G	365	ASN	N-CA-C	-8.79	102.11	112.92
19	a	66	LEU	N-CA-C	-8.78	102.35	113.23
7	G	133	GLN	N-CA-CB	8.76	121.48	110.45
21	q	66	THR	N-CA-C	-8.70	101.88	111.36
9	I	62	MET	N-CA-C	-8.67	92.12	107.73
13	S	51	LEU	N-CA-C	-8.67	91.07	109.01
7	G	310	GLU	CB-CA-C	-8.63	106.62	116.54
19	a	3	PHE	CA-CB-CG	8.57	122.37	113.80
11	Q	59	LEU	N-CA-CB	-8.49	99.13	111.70
22	r	25	GLN	N-CA-C	-8.40	103.04	113.28
4	D	258	VAL	N-CA-C	-8.35	102.28	110.72
7	G	532	PRO	CA-N-CD	8.35	123.69	112.00
22	r	58	ASP	N-CA-C	8.35	123.62	108.17
21	q	64	TYR	N-CA-C	8.35	121.10	110.33
7	G	452	LEU	N-CA-C	-8.33	102.20	111.28
22	r	29	GLN	N-CA-C	-8.33	102.31	114.39
16	W	131	PRO	CA-N-CD	8.32	123.65	112.00
18	Z	90	ASN	N-CA-C	-8.32	103.26	113.41
7	G	691	ILE	N-CA-C	8.22	123.72	111.89
7	G	387	LEU	N-CA-C	-8.20	98.00	110.30
6	F	298	GLU	N-CA-C	8.17	120.19	111.28
3	C	196	PRO	N-CA-C	8.17	124.89	113.53
5	E	218	ARG	CB-CA-C	-8.16	99.87	112.12
15	V	87	GLU	N-CA-C	-8.16	102.38	111.28
7	G	484	ASP	N-CA-C	8.15	121.08	111.71
6	F	411	SER	N-CA-CB	8.12	121.79	110.01
7	G	500	ILE	N-CA-CB	8.11	120.95	110.57
6	F	191	TYR	N-CA-C	8.10	121.67	110.24
10	P	143	ASP	N-CA-C	8.10	119.74	111.07
8	H	99	ASN	N-CA-C	-8.09	99.35	110.35
11	Q	155	PRO	N-CA-CB	-8.08	96.83	103.30
8	H	52	ALA	N-CA-C	-8.08	100.82	111.24
5	E	219	SER	N-CA-CB	8.05	124.04	111.56
8	H	193	THR	N-CA-C	-8.02	102.53	112.88
4	D	457	VAL	N-CA-C	-8.01	96.90	108.11
7	G	534	VAL	N-CA-C	-7.99	104.80	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	THR	N-CA-C	-7.99	102.52	111.07
22	r	10	LYS	N-CA-C	-7.98	103.00	112.89
7	G	664	TYR	N-CA-C	-7.97	97.67	109.62
6	F	364	VAL	N-CA-C	7.94	118.72	110.62
1	A	36	PRO	N-CA-CB	-7.93	94.28	103.00
4	D	359	ASP	CB-CA-C	-7.90	94.71	110.42
7	G	270	VAL	N-CA-CB	-7.89	100.61	110.31
2	B	165	ALA	N-CA-C	-7.85	104.19	114.31
9	I	118	LEU	CA-C-O	7.79	129.18	119.05
11	Q	72	ILE	N-CA-C	-7.79	105.90	113.53
5	E	193	GLU	N-CA-C	7.78	120.55	108.96
7	G	377	ALA	N-CA-C	-7.75	102.92	112.38
10	P	95	ARG	N-CA-C	7.75	120.62	111.71
8	H	230	ASN	N-CA-C	-7.74	101.89	112.03
18	Z	102	PRO	N-CA-CB	-7.74	93.20	103.42
2	B	195	PRO	N-CA-C	-7.73	101.27	110.70
11	Q	139	GLU	N-CA-C	-7.70	102.83	111.07
6	F	334	THR	N-CA-C	-7.67	101.66	111.02
6	F	58	ARG	N-CA-C	-7.66	103.01	111.36
7	G	56	VAL	N-CA-C	-7.63	103.01	110.72
10	P	50	SER	N-CA-C	-7.63	98.25	109.63
4	D	184	ILE	N-CA-C	-7.62	102.84	110.62
5	E	235	GLU	N-CA-C	-7.59	98.34	109.50
7	G	569	GLN	N-CA-C	7.58	121.97	108.24
6	F	171	VAL	N-CA-CB	7.57	120.26	110.57
5	E	166	LYS	N-CA-C	-7.57	102.22	113.72
18	Z	142	TRP	N-CA-C	-7.54	99.12	110.28
15	V	41	HIS	N-CA-CB	-7.54	101.91	110.35
9	I	190	LEU	N-CA-C	-7.53	104.70	114.04
12	R	74	HIS	N-CA-C	7.53	121.11	110.50
1	A	36	PRO	CA-N-CD	7.51	122.52	112.00
7	G	467	LYS	N-CA-C	-7.51	102.24	111.33
7	G	277	MET	N-CA-C	7.50	120.62	109.59
6	F	430	GLY	N-CA-C	7.46	121.69	112.73
2	B	169	GLY	N-CA-C	7.46	120.80	111.85
7	G	510	TRP	N-CA-CB	7.42	120.90	109.85
7	G	303	THR	N-CA-C	7.39	123.01	113.18
6	F	259	GLY	N-CA-C	-7.31	103.91	112.83
17	X	69	ASN	N-CA-C	-7.26	102.97	111.03
4	D	365	PRO	N-CA-C	7.26	117.44	110.47
14	T	99	SER	N-CA-C	-7.23	99.18	109.96
13	S	33	VAL	N-CA-C	-7.22	103.25	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	497	VAL	N-CA-C	-7.18	103.29	110.62
4	D	257	GLU	N-CA-CB	7.18	120.48	110.07
6	F	73	PRO	N-CA-C	-7.17	103.79	113.40
4	D	303	ARG	N-CA-C	-7.17	104.16	114.12
8	H	198	PHE	CB-CA-C	-7.16	101.19	111.14
3	C	195	HIS	CB-CA-C	7.15	117.25	110.17
6	F	81	LYS	N-CA-C	-7.13	103.58	111.36
8	H	198	PHE	N-CA-C	7.11	121.92	112.25
10	P	97	MET	N-CA-CB	7.10	121.32	110.60
7	G	465	VAL	N-CA-CB	7.09	118.38	110.51
7	G	461	SER	N-CA-C	7.09	119.91	111.33
6	F	78	GLY	N-CA-C	-7.08	104.24	112.73
7	G	217	GLU	N-CA-C	-7.07	101.71	110.41
1	A	67	LEU	N-CA-C	-7.05	103.64	111.82
2	B	194	CYS	N-CA-C	-7.05	102.58	112.17
7	G	148	SER	N-CA-C	7.05	120.89	109.40
8	H	52	ALA	N-CA-CB	7.03	120.40	110.07
6	F	246	GLU	N-CA-C	-7.00	103.65	111.28
6	F	169	LEU	N-CA-C	6.99	118.90	111.28
3	C	80	LEU	N-CA-C	-6.97	104.65	113.02
6	F	455	GLN	N-CA-C	6.97	118.53	111.07
6	F	428	GLY	N-CA-C	-6.97	103.85	112.77
15	V	74	GLY	N-CA-C	-6.96	104.43	112.79
4	D	193	ASP	N-CA-C	-6.95	103.63	111.07
6	F	418	GLN	N-CA-CB	6.94	120.14	110.07
21	q	137	TRP	N-CA-C	-6.94	99.55	109.96
19	a	57	VAL	N-CA-C	-6.93	105.97	112.83
8	H	156	MET	N-CA-C	6.93	118.91	111.36
4	D	255	ILE	N-CA-C	6.93	117.07	110.42
7	G	294	TYR	N-CA-C	-6.92	104.64	113.23
6	F	103	ASN	N-CA-CB	6.92	121.03	110.44
8	H	194	ASN	N-CA-C	-6.92	101.84	111.39
7	G	582	VAL	N-CA-C	6.92	118.44	108.48
16	W	131	PRO	N-CA-CB	-6.91	95.40	103.00
6	F	148	ALA	N-CA-C	-6.90	103.84	111.36
3	C	233	ASP	CB-CA-C	-6.89	102.16	111.88
5	E	152	GLN	N-CA-C	-6.89	103.70	111.07
8	H	77	LEU	N-CA-C	-6.88	103.47	110.97
7	G	133	GLN	N-CA-C	-6.88	101.11	110.68
7	G	300	GLN	N-CA-CB	6.88	122.46	112.08
11	Q	61	ILE	N-CA-C	-6.87	105.79	111.91
5	E	235	GLU	N-CA-CB	6.86	122.23	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	362	ASP	N-CA-C	6.86	125.41	110.80
7	G	385	TYR	N-CA-C	6.85	120.94	111.55
6	F	233	VAL	O-C-N	6.85	131.11	123.10
22	r	65	PRO	N-CA-C	-6.84	103.26	110.58
6	F	329	LYS	N-CA-C	6.83	119.59	111.33
7	G	268	GLY	N-CA-C	6.81	124.76	115.30
12	R	46	VAL	N-CA-C	-6.80	103.68	110.62
6	F	244	ASN	N-CA-C	-6.79	100.93	110.50
13	S	49	PRO	N-CA-C	6.78	120.71	111.22
10	P	333	PRO	CA-N-CD	6.78	121.49	112.00
17	X	104	GLN	N-CA-C	6.77	118.45	111.14
9	I	119	CYS	N-CA-CB	-6.77	100.70	110.65
3	C	204	THR	N-CA-C	6.77	120.51	112.93
7	G	434	SER	N-CA-C	-6.74	100.99	110.29
8	H	203	GLY	N-CA-C	-6.73	97.22	113.18
6	F	233	VAL	CA-C-O	-6.73	113.33	120.53
11	Q	58	LYS	CA-C-O	6.72	128.81	119.80
4	D	329	ARG	CB-CA-C	6.72	121.95	110.79
9	I	86	TYR	CB-CA-C	-6.70	101.29	113.49
17	X	57	LEU	N-CA-C	-6.70	104.20	112.38
9	I	49	ASP	N-CA-C	-6.69	99.77	110.14
7	G	640	ASP	N-CA-CB	6.67	120.03	110.16
3	C	49	ARG	N-CA-C	6.67	120.38	109.85
2	B	121	PHE	CA-C-N	6.66	130.81	120.75
2	B	121	PHE	C-N-CA	6.66	130.81	120.75
6	F	344	GLN	N-CA-C	-6.66	104.03	111.28
19	a	65	GLY	N-CA-C	-6.65	105.57	114.95
7	G	287	SER	N-CA-C	6.64	119.30	110.53
2	B	88	SER	N-CA-C	-6.64	103.97	111.14
8	H	311	THR	N-CA-C	-6.64	104.81	113.17
9	I	51	LYS	N-CA-C	-6.63	103.97	111.07
7	G	601	GLY	N-CA-C	6.62	124.84	115.30
2	B	124	SER	N-CA-C	6.62	119.54	109.41
6	F	228	PRO	N-CA-C	-6.61	98.85	112.47
6	F	206	CYS	N-CA-C	-6.60	105.08	113.01
5	E	166	LYS	CB-CA-C	6.60	123.52	110.65
16	W	98	LYS	N-CA-C	-6.59	102.01	110.19
6	F	336	LEU	N-CA-CB	-6.58	100.97	111.43
11	Q	58	LYS	CB-CA-C	-6.57	101.12	111.17
7	G	435	PRO	N-CA-C	-6.56	100.20	110.50
13	S	50	ASN	CA-C-O	6.56	129.28	121.08
9	I	98	ARG	N-CA-C	6.55	118.96	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ALA	N-CA-C	6.55	118.42	111.28
6	F	234	GLY	CA-C-N	-6.54	111.73	120.50
6	F	234	GLY	C-N-CA	-6.54	111.73	120.50
7	G	275	PRO	CB-CA-C	-6.54	102.41	110.98
2	B	163	SER	N-CA-C	-6.53	105.28	112.72
19	a	16	LEU	CA-C-N	-6.53	112.96	122.69
19	a	16	LEU	C-N-CA	-6.53	112.96	122.69
7	G	605	GLN	N-CA-C	6.52	119.14	108.52
4	D	365	PRO	CA-N-CD	6.50	121.09	112.00
19	a	58	ASN	N-CA-C	6.49	119.31	108.73
13	S	61	VAL	N-CA-CB	6.49	123.05	111.63
7	G	189	ILE	N-CA-C	-6.49	105.38	111.48
7	G	653	LEU	N-CA-CB	6.48	121.45	110.49
14	T	95	PRO	N-CA-C	-6.46	106.41	114.68
7	G	190	ALA	N-CA-C	-6.45	99.13	109.96
7	G	275	PRO	CA-N-CD	6.45	121.02	112.00
13	S	41	TYR	N-CA-C	-6.44	103.95	110.97
6	F	178	GLU	N-CA-CB	6.44	119.53	109.94
7	G	250	SER	N-CA-C	6.43	116.77	108.34
7	G	273	ILE	N-CA-C	-6.43	98.36	107.75
10	P	224	LEU	CB-CA-C	-6.43	109.15	116.54
7	G	662	THR	N-CA-C	-6.41	96.45	107.61
10	P	119	ALA	N-CA-C	-6.40	104.22	111.14
21	q	143	PRO	CA-N-CD	6.37	120.91	112.00
22	r	27	ARG	N-CA-C	6.36	118.66	108.41
6	F	416	SER	N-CA-C	6.36	117.87	111.07
8	H	288	LEU	N-CA-C	-6.35	103.65	111.40
6	F	144	VAL	N-CA-CB	6.34	118.68	110.57
6	F	370	LEU	N-CA-C	-6.34	104.45	111.36
4	D	337	MET	N-CA-C	-6.33	104.38	111.28
11	Q	105	GLU	N-CA-C	6.30	119.35	109.96
23	s	93	PRO	N-CA-C	6.30	120.97	111.14
7	G	176	CYS	N-CA-C	6.30	119.61	110.42
5	E	64	ALA	N-CA-CB	6.28	119.30	109.94
19	a	26	ILE	N-CA-C	-6.28	104.53	113.07
3	C	47	ARG	N-CA-C	6.27	116.81	109.60
3	C	149	LEU	N-CA-CB	-6.26	100.86	110.44
8	H	217	ALA	CB-CA-C	-6.24	109.36	116.54
9	I	66	LEU	N-CA-C	-6.24	105.67	113.28
5	E	50	THR	N-CA-CB	6.23	121.47	110.37
6	F	409	ILE	N-CA-C	6.23	116.40	110.42
6	F	415	ILE	N-CA-C	-6.22	104.43	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	192	ASP	N-CA-C	6.22	119.08	109.07
7	G	356	ASP	N-CA-CB	6.22	119.26	110.12
3	C	223	VAL	N-CA-C	6.21	117.03	108.84
6	F	101	PHE	N-CA-C	6.21	118.84	111.33
2	B	135	GLY	CA-C-O	-6.20	117.99	122.45
4	D	262	LEU	N-CA-CB	-6.18	102.37	110.59
7	G	389	THR	N-CA-C	-6.18	101.27	110.23
7	G	451	ILE	N-CA-C	-6.17	104.97	113.00
7	G	418	ILE	N-CA-C	-6.17	103.40	112.04
9	I	86	TYR	N-CA-C	6.17	120.88	112.55
7	G	325	ARG	N-CA-CB	6.16	118.90	109.91
2	B	80	ASP	N-CA-CB	6.15	119.16	110.12
4	D	145	MET	N-CA-C	6.14	123.88	110.80
23	s	83	LEU	N-CA-C	6.13	117.63	111.07
7	G	420	LYS	N-CA-C	6.12	118.74	111.33
11	Q	71	HIS	N-CA-C	-6.12	105.10	113.30
2	B	194	CYS	N-CA-CB	6.11	116.19	110.39
4	D	147	ASN	N-CA-C	-6.10	104.55	111.07
10	P	361	TRP	N-CA-C	-6.06	106.86	114.56
10	P	268	PRO	N-CA-C	6.06	121.95	113.53
20	b	80	TRP	N-CA-CB	6.06	119.72	110.39
21	q	141	SER	N-CA-C	6.04	117.86	111.28
7	G	508	ALA	N-CA-C	6.03	117.85	111.28
10	P	85	ARG	N-CA-C	-6.01	105.53	112.92
7	G	353	ALA	N-CA-C	-6.00	104.67	112.23
7	G	532	PRO	N-CA-CB	-5.98	97.10	103.38
21	q	132	LYS	N-CA-CB	-5.98	107.35	114.17
7	G	638	THR	N-CA-C	-5.97	100.23	109.24
6	F	291	GLU	N-CA-C	5.96	118.23	110.43
10	P	76	MET	N-CA-C	-5.95	106.07	113.15
17	X	60	GLY	N-CA-C	-5.95	105.60	112.50
16	W	33	ARG	N-CA-C	-5.93	104.81	111.28
18	Z	101	VAL	CA-C-N	-5.93	114.52	120.21
18	Z	101	VAL	C-N-CA	-5.93	114.52	120.21
4	D	350	LYS	CB-CA-C	-5.92	103.14	111.85
17	X	16	GLU	N-CA-C	-5.92	102.30	110.35
7	G	651	PRO	N-CA-C	5.92	121.31	114.03
6	F	127	ASP	N-CA-C	5.91	118.51	111.71
5	E	233	LEU	CB-CA-C	-5.90	101.61	111.23
17	X	76	SER	N-CA-C	-5.90	101.89	111.04
10	P	331	ASP	CB-CA-C	-5.89	103.41	111.95
4	D	455	ASP	CB-CA-C	-5.86	103.56	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	333	PRO	N-CA-CB	-5.86	97.10	103.25
9	I	85	ASN	N-CA-C	-5.85	100.72	109.15
8	H	2	PHE	N-CA-C	-5.84	104.87	112.23
13	S	51	LEU	N-CA-CB	5.84	119.52	110.12
7	G	639	LEU	N-CA-C	5.83	118.58	111.82
23	s	90	PHE	N-CA-CB	5.82	118.50	110.07
16	W	97	ILE	N-CA-C	-5.80	104.85	110.42
7	G	672	ALA	N-CA-C	-5.79	104.97	111.28
4	D	232	VAL	N-CA-C	-5.79	101.47	109.46
18	Z	26	PRO	N-CA-C	5.79	120.34	110.74
4	D	414	ASP	N-CA-C	-5.78	101.40	110.36
11	Q	57	GLU	N-CA-C	-5.78	100.63	109.41
7	G	275	PRO	N-CA-CB	-5.77	97.97	103.33
7	G	289	LYS	N-CA-C	5.76	117.56	111.28
4	D	114	GLY	N-CA-C	-5.76	99.53	113.18
7	G	181	ARG	N-CA-C	-5.76	104.61	111.69
6	F	102	MET	CB-CA-C	-5.75	101.45	110.94
6	F	299	LEU	N-CA-C	5.75	118.49	111.82
6	F	393	ASN	N-CA-C	-5.74	104.92	111.07
14	T	77	ASP	N-CA-C	-5.74	107.27	114.56
10	P	375	VAL	N-CA-C	5.74	117.94	108.99
9	I	64	THR	N-CA-CB	-5.74	103.37	111.00
20	b	61	GLY	N-CA-C	-5.73	107.76	115.21
10	P	44	GLY	N-CA-C	5.72	119.49	110.96
1	A	61	THR	N-CA-CB	5.71	118.29	110.01
19	a	3	PHE	N-CA-CB	5.71	118.62	110.06
5	E	183	PRO	N-CA-C	-5.70	102.19	110.80
5	E	119	THR	N-CA-C	-5.70	105.82	112.89
1	A	65	PHE	N-CA-C	-5.68	106.27	113.43
11	Q	64	LEU	N-CA-C	-5.67	106.50	113.41
7	G	59	GLN	N-CA-C	5.66	118.02	107.99
9	I	65	GLU	N-CA-C	5.66	120.19	113.28
3	C	117	ASP	CA-C-N	-5.65	116.41	122.85
3	C	117	ASP	C-N-CA	-5.65	116.41	122.85
9	I	106	TYR	N-CA-C	-5.65	101.99	109.84
6	F	176	ALA	N-CA-C	5.63	118.14	111.33
6	F	457	HIS	N-CA-CB	-5.62	100.95	110.50
7	G	475	VAL	N-CA-C	5.61	115.94	107.75
6	F	304	ALA	CB-CA-C	-5.61	110.09	116.54
7	G	599	THR	CA-C-N	-5.61	114.20	122.83
7	G	599	THR	C-N-CA	-5.61	114.20	122.83
4	D	136	PHE	N-CA-C	5.60	119.29	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	24	SER	N-CA-C	-5.60	107.08	114.31
4	D	186	ALA	N-CA-C	5.60	117.06	111.07
5	E	222	PHE	CB-CA-C	-5.60	100.62	109.80
9	I	189	LYS	N-CA-C	-5.59	106.12	113.17
4	D	143	SER	CB-CA-C	5.59	120.80	111.30
7	G	615	LEU	N-CA-C	-5.59	106.23	113.16
4	D	221	ARG	N-CA-C	-5.59	106.23	113.16
7	G	530	TYR	N-CA-C	-5.59	102.01	110.28
10	P	177	SER	CB-CA-C	-5.58	103.66	111.80
4	D	309	ASP	CB-CA-C	-5.57	109.65	117.23
8	H	50	ALA	N-CA-C	5.57	117.81	111.02
4	D	267	ILE	N-CA-C	5.57	120.92	109.34
1	A	80	GLN	CB-CA-C	-5.56	102.66	111.17
2	B	88	SER	N-CA-CB	5.56	118.14	110.07
22	r	108	LYS	N-CA-C	5.55	117.33	111.28
3	C	153	ASP	N-CA-C	5.55	117.23	110.41
14	T	78	GLY	N-CA-C	-5.54	106.08	112.73
5	E	233	LEU	N-CA-C	5.54	119.86	113.38
10	P	110	ALA	N-CA-CB	-5.53	101.70	110.28
10	P	141	PHE	N-CA-C	-5.53	104.67	111.75
4	D	137	ASP	N-CA-C	-5.53	106.49	113.18
7	G	127	ASP	CA-C-O	5.53	129.02	121.89
8	H	192	GLU	N-CA-C	-5.52	105.76	112.88
20	b	25	VAL	N-CA-C	-5.52	106.96	113.42
4	D	91	ALA	CB-CA-C	-5.51	110.23	116.63
4	D	182	ASN	N-CA-CB	5.51	118.06	110.07
6	F	118	ASP	N-CA-C	-5.51	102.13	110.28
6	F	294	VAL	CA-C-N	-5.50	114.09	119.76
6	F	294	VAL	C-N-CA	-5.50	114.09	119.76
19	a	25	TYR	N-CA-C	-5.50	107.83	114.75
4	D	292	MET	N-CA-C	-5.47	105.39	111.36
7	G	363	SER	N-CA-C	-5.46	100.28	109.07
20	b	79	ASP	CA-C-O	5.46	127.64	119.23
21	q	33	ILE	N-CA-C	-5.46	107.96	113.20
13	S	50	ASN	CB-CA-C	-5.44	103.12	111.66
4	D	200	PHE	CA-CB-CG	5.43	119.23	113.80
7	G	82	ILE	N-CA-C	-5.43	104.08	110.21
3	C	228	GLU	N-CA-C	-5.40	103.35	110.43
22	r	9	GLN	N-CA-C	5.39	118.08	111.82
16	W	21	LYS	CA-C-N	-5.39	114.17	119.99
16	W	21	LYS	C-N-CA	-5.39	114.17	119.99
7	G	420	LYS	N-CA-CB	-5.38	101.99	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	227	GLU	N-CA-C	-5.38	107.09	113.97
4	D	223	HIS	N-CA-CB	-5.37	103.75	111.91
10	P	53	GLY	N-CA-C	5.37	121.32	113.48
7	G	682	ASP	CA-C-N	-5.37	114.23	119.76
7	G	682	ASP	C-N-CA	-5.37	114.23	119.76
4	D	142	VAL	N-CA-C	-5.36	105.62	110.82
7	G	510	TRP	N-CA-C	-5.36	101.92	109.96
12	R	48	PHE	N-CA-C	5.36	119.57	113.19
7	G	652	ASN	CB-CA-C	-5.36	102.12	111.23
4	D	86	PRO	N-CA-C	-5.35	106.56	113.57
21	q	143	PRO	N-CA-CB	-5.34	96.26	103.15
6	F	199	ARG	N-CA-C	5.33	117.43	109.59
7	G	654	VAL	N-CA-C	-5.33	105.82	113.07
18	Z	102	PRO	CA-N-CD	5.33	119.46	112.00
5	E	219	SER	N-CA-C	-5.32	100.65	108.79
2	B	141	MET	N-CA-C	-5.32	106.79	113.28
4	D	344	ILE	N-CA-C	-5.32	105.20	110.62
5	E	48	PRO	N-CA-C	5.31	120.75	113.84
10	P	229	VAL	N-CA-C	-5.30	104.22	110.21
7	G	356	ASP	N-CA-C	-5.30	105.51	111.28
8	H	87	VAL	CA-C-N	-5.29	114.90	120.94
8	H	87	VAL	C-N-CA	-5.29	114.90	120.94
13	S	51	LEU	CA-C-N	-5.29	113.23	119.84
13	S	51	LEU	C-N-CA	-5.29	113.23	119.84
7	G	362	ASP	CA-CB-CG	5.28	117.88	112.60
5	E	66	VAL	N-CA-C	5.27	116.63	110.62
9	I	96	ARG	N-CA-C	5.26	119.55	113.18
4	D	248	SER	N-CA-C	-5.25	105.63	111.36
7	G	449	PRO	N-CA-CB	5.25	109.06	103.39
21	q	93	MET	N-CA-C	-5.25	105.73	111.82
5	E	48	PRO	CB-CA-C	-5.25	104.40	111.85
6	F	412	LEU	N-CA-C	-5.25	105.73	111.82
7	G	277	MET	N-CA-CB	-5.24	101.64	109.71
6	F	300	ILE	N-CA-CB	5.23	119.30	110.56
7	G	435	PRO	CB-CA-C	-5.22	105.87	111.56
10	P	96	LEU	CB-CA-C	-5.22	99.70	109.72
3	C	235	ASN	N-CA-C	-5.21	99.70	110.80
2	B	76	THR	N-CA-C	-5.21	105.04	111.40
5	E	221	ARG	N-CA-C	5.21	117.78	110.23
17	X	20	VAL	N-CA-C	-5.21	100.70	108.46
3	C	237	PRO	CB-CA-C	-5.20	104.19	109.92
19	a	17	VAL	CB-CA-C	-5.20	104.75	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	137	LYS	N-CA-C	5.20	117.85	111.82
3	C	235	ASN	N-CA-CB	5.20	119.27	110.49
4	D	133	LEU	CA-C-N	-5.19	113.45	119.47
4	D	133	LEU	C-N-CA	-5.19	113.45	119.47
7	G	63	PHE	CA-C-O	-5.19	115.04	121.06
13	S	45	LYS	N-CA-C	-5.19	105.52	111.07
3	C	109	SER	N-CA-C	5.18	118.26	109.76
7	G	83	GLU	N-CA-CB	-5.18	101.93	109.95
4	D	132	ALA	N-CA-C	-5.17	107.99	114.56
7	G	600	GLU	CB-CA-C	-5.17	103.04	111.06
21	q	26	VAL	N-CA-CB	5.17	119.76	111.23
21	q	87	HIS	N-CA-C	-5.17	105.73	111.36
21	q	139	PRO	CA-N-CD	5.16	119.23	112.00
17	X	25	LEU	N-CA-C	-5.16	105.66	111.28
4	D	439	SER	CB-CA-C	-5.15	104.39	112.12
6	F	337	MET	CB-CA-C	-5.15	103.03	111.68
7	G	172	ILE	N-CA-C	-5.15	98.63	109.34
7	G	713	ALA	N-CA-C	-5.15	105.56	111.07
6	F	131	MET	N-CA-C	-5.14	105.84	112.68
7	G	192	VAL	CB-CA-C	-5.14	105.25	111.88
7	G	569	GLN	CB-CA-C	-5.14	104.23	112.05
3	C	240	ALA	N-CA-CB	-5.14	102.30	110.06
8	H	189	THR	N-CA-C	-5.14	107.04	113.72
7	G	458	GLY	N-CA-C	-5.14	108.23	115.32
7	G	150	ARG	N-CA-CB	-5.13	101.81	110.49
6	F	60	GLY	N-CA-C	-5.11	106.00	114.48
7	G	203	ASP	CA-C-O	5.11	127.25	121.32
23	s	85	LEU	N-CA-CB	5.11	117.41	110.01
8	H	202	GLU	N-CA-C	-5.10	105.17	111.90
15	V	87	GLU	N-CA-CB	5.09	117.61	110.12
4	D	352	PRO	N-CA-C	5.09	116.91	110.70
7	G	660	GLU	N-CA-C	5.08	118.10	109.76
22	r	59	GLY	N-CA-C	-5.08	106.61	112.50
14	T	89	LEU	N-CA-C	-5.08	105.75	111.28
4	D	106	VAL	N-CA-CB	-5.08	105.27	111.21
21	q	8	LYS	N-CA-C	-5.07	105.66	111.14
5	E	222	PHE	N-CA-C	5.07	117.88	109.46
7	G	280	ASP	N-CA-CB	-5.07	102.67	110.12
3	C	241	PHE	CB-CA-C	5.06	117.99	109.69
14	T	149	ALA	N-CA-C	5.06	116.48	110.97
3	C	237	PRO	N-CD-CG	-5.05	95.62	103.20
5	E	225	GLU	CA-C-N	-5.05	114.37	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	225	GLU	C-N-CA	-5.05	114.37	119.83
3	C	108	LYS	N-CA-C	5.05	116.78	111.28
5	E	213	PRO	CB-CA-C	-5.05	106.28	112.89
6	F	366	ALA	N-CA-C	-5.05	105.47	110.97
3	C	139	ARG	N-CA-CB	-5.04	102.19	111.37
9	I	117	LYS	N-CA-C	-5.04	103.03	113.31
2	B	194	CYS	CA-C-N	-5.03	115.19	120.38
2	B	194	CYS	C-N-CA	-5.03	115.19	120.38
7	G	388	ASN	N-CA-C	-5.03	103.86	111.56
4	D	419	PRO	N-CA-C	5.02	118.51	111.33
12	R	53	LYS	N-CA-C	5.00	116.56	108.41
10	P	52	SER	N-CA-C	-5.00	106.43	112.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	799	0	851	126	0
2	B	1241	0	1252	179	0
3	C	1643	0	1598	133	0
4	D	3088	0	3059	351	0
5	E	1635	0	1625	183	0
6	F	3288	0	3243	373	0
7	G	5287	0	5322	583	0
8	H	2532	0	2621	314	0
9	I	1380	0	1339	169	0
10	P	2720	0	2740	256	0
11	Q	940	0	930	96	0
12	R	660	0	639	69	0
13	S	667	0	685	75	0
14	T	604	0	596	70	0
15	V	915	0	954	78	0
16	W	970	0	991	92	0
17	X	1164	0	1150	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Z	1145	0	1139	110	0
19	a	548	0	562	75	0
20	b	628	0	628	72	0
21	q	1025	0	980	80	0
22	r	686	0	710	70	0
23	s	193	0	187	36	0
24	A	42	0	58	8	0
24	H	48	0	73	12	0
24	I	51	0	82	8	0
25	B	8	0	0	6	0
25	F	8	0	0	10	0
25	G	16	0	0	8	0
25	I	16	0	0	9	0
26	B	18	0	18	11	0
27	B	78	0	107	23	0
28	E	4	0	0	3	0
28	G	4	0	0	4	0
29	F	31	0	19	3	0
30	H	35	0	43	4	0
31	P	48	0	26	7	0
32	R	1	0	0	0	0
33	W	32	0	0	3	0
34	a	57	0	58	12	0
All	All	34255	0	34285	3090	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 45.

All (3090) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:SER:HB2	1:A:55:PHE:CD2	1.31	1.61
1:A:52:SER:CB	1:A:55:PHE:CD2	2.10	1.33
1:A:52:SER:CB	1:A:55:PHE:HD2	1.41	1.32
4:D:181:LEU:CD1	4:D:210:MET:SD	2.27	1.23
4:D:181:LEU:HD11	4:D:210:MET:SD	1.79	1.23
3:C:234:LEU:HD12	3:C:234:LEU:O	1.36	1.22
7:G:130:ILE:HA	9:I:140:ARG:NH1	1.56	1.21
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
7:G:571:HIS:HD2	7:G:572:HIS:CD2	1.60	1.19
4:D:360:ASP:OD1	4:D:360:ASP:O	1.60	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:ILE:HG13	3:C:144:THR:HG22	1.25	1.18
7:G:544:MET:HE3	7:G:546:PHE:CZ	1.78	1.17
3:C:223:VAL:CG2	3:C:225:LEU:CD1	2.22	1.16
8:H:260:MET:HE3	19:a:13:GLY:O	1.43	1.16
3:C:229:PHE:CE1	9:I:126:GLN:HG3	1.80	1.15
13:S:95:LEU:HD12	13:S:95:LEU:O	1.46	1.14
1:A:35:ASN:OD1	1:A:36:PRO:HD2	1.49	1.12
1:A:18:ILE:CD1	8:H:76:THR:CG2	2.27	1.11
9:I:152:CYS:SG	25:I:302:SF4:FE1	1.41	1.11
9:I:210:LEU:HD13	22:r:39:PRO:O	1.47	1.11
4:D:144:MET:SD	4:D:222:MET:HA	1.91	1.11
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.14	1.11
6:F:266:GLY:CA	6:F:271:SER:HA	1.79	1.10
3:C:229:PHE:HE1	9:I:126:GLN:HG3	0.99	1.10
1:A:18:ILE:HD12	8:H:76:THR:CG2	1.82	1.10
18:Z:120:LEU:HD23	18:Z:122:GLY:H	1.15	1.10
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.09
7:G:130:ILE:C	9:I:140:ARG:HH12	1.61	1.09
1:A:79:ILE:HD11	8:H:155:LEU:HD22	1.27	1.09
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.08
10:P:171:ASN:HB3	10:P:327:VAL:HB	1.26	1.08
2:B:92:PRO:HB2	2:B:122:ARG:NH1	1.68	1.07
6:F:266:GLY:HA3	6:F:271:SER:CA	1.84	1.07
22:r:27:ARG:HB3	22:r:31:ILE:HG23	1.32	1.07
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.08	1.07
1:A:49:LEU:HB3	1:A:50:PRO:HD2	1.30	1.06
7:G:571:HIS:CD2	7:G:572:HIS:CD2	2.44	1.06
4:D:267:ILE:HG22	8:H:278:PRO:HG2	1.32	1.05
3:C:120:THR:HG21	15:V:116:ILE:HG21	1.37	1.05
4:D:348:LEU:O	18:Z:11:PRO:HG3	1.57	1.05
5:E:131:ILE:HD11	5:E:185:VAL:HB	1.37	1.05
6:F:379:CYS:SG	25:F:502:SF4:FE4	1.46	1.05
10:P:350:ILE:HD11	10:P:366:ILE:HB	1.35	1.05
7:G:130:ILE:O	9:I:140:ARG:NH1	1.89	1.04
4:D:299:GLN:NE2	9:I:36:TYR:CE2	2.26	1.04
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.36	1.03
8:H:90:PRO:HD3	8:H:162:LEU:HD13	1.37	1.03
3:C:186:ILE:HG23	3:C:187:LEU:HG	1.35	1.03
4:D:238:LEU:HB3	22:r:36:GLN:HG3	1.37	1.03
4:D:256:ASP:HA	4:D:259:GLU:CB	1.89	1.02
7:G:130:ILE:CA	9:I:140:ARG:NH1	2.22	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:184:MET:HG2	8:H:293:PHE:CD2	1.95	1.02
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.35	1.02
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.41	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
21:q:71:LYS:HB3	21:q:73:THR:HG23	1.40	1.02
4:D:217:VAL:CG1	4:D:240:LEU:HD22	1.89	1.01
6:F:382:CYS:SG	25:F:502:SF4:FE3	1.50	1.01
1:A:18:ILE:CD1	8:H:76:THR:HG22	1.90	1.01
4:D:261:MET:HE1	9:I:73:THR:HG23	1.42	1.01
23:s:92:LEU:HB2	23:s:93:PRO:HD2	1.39	1.00
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	1.00
2:B:97:LEU:HD13	4:D:94:VAL:HG13	1.42	0.99
3:C:223:VAL:HG22	3:C:225:LEU:CD1	1.90	0.99
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	0.99
8:H:184:MET:HG2	8:H:293:PHE:CE2	1.98	0.99
16:W:74:ALA:HA	33:W:201:EHZ:O4	1.61	0.99
21:q:142:THR:OG1	21:q:143:PRO:HD2	1.62	0.99
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.98
3:C:149:LEU:HD21	11:Q:64:LEU:CD2	1.93	0.98
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.28	0.98
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.98
4:D:376:GLU:HG3	7:G:121:LEU:HD12	1.46	0.98
21:q:78:ASP:HB2	21:q:81:MET:HG3	1.42	0.98
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.98
3:C:223:VAL:CG2	3:C:225:LEU:HD11	1.92	0.98
4:D:181:LEU:HD12	4:D:210:MET:SD	2.00	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.97
6:F:118:ASP:HA	6:F:159:ARG:HG3	1.45	0.97
3:C:152:ILE:HD11	3:C:177:PHE:CE2	1.99	0.97
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.05	0.97
1:A:80:GLN:C	20:b:46:ASN:HD21	1.73	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
1:A:68:GLU:CG	1:A:98:LEU:HD13	1.93	0.96
7:G:75:CYS:SG	28:G:803:FES:FE1	1.57	0.96
9:I:171:PRO:CB	21:q:93:MET:HE1	1.96	0.96
19:a:58:ASN:HD22	19:a:60:TYR:HE1	1.10	0.96
7:G:611:THR:HG21	11:Q:105:GLU:CA	1.95	0.96
4:D:256:ASP:HA	4:D:259:GLU:HB3	1.45	0.96
6:F:196:PHE:CE1	23:s:91:ARG:HD3	2.00	0.96
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.95
14:T:138:LEU:HD12	14:T:138:LEU:O	1.66	0.95
2:B:166:ASN:O	9:I:150:THR:HB	1.66	0.95
1:A:18:ILE:HD12	8:H:76:THR:HG22	1.43	0.95
2:B:122:ARG:HB2	26:B:302:UQ1:H72	1.47	0.95
7:G:130:ILE:C	9:I:140:ARG:NH1	2.25	0.95
6:F:382:CYS:HG	25:F:502:SF4:FE3	0.77	0.95
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.95
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.95
7:G:114:GLU:OE2	22:r:53:TYR:HA	1.66	0.95
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.94
5:E:134:CYS:HG	28:E:301:FES:FE1	0.65	0.94
14:T:99:SER:HB2	14:T:102:SER:HB3	1.48	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
8:H:117:LEU:CD2	8:H:136:VAL:HG11	1.97	0.94
8:H:260:MET:HE2	19:a:17:VAL:HG13	1.47	0.94
1:A:68:GLU:HG2	1:A:98:LEU:HD13	1.49	0.94
4:D:259:GLU:HG3	18:Z:25:LEU:HD21	1.50	0.94
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.94
1:A:79:ILE:HA	1:A:87:MET:SD	2.06	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.93
6:F:196:PHE:HE1	23:s:91:ARG:HD3	1.31	0.93
7:G:382:ARG:NE	7:G:652:ASN:HD21	1.67	0.93
20:b:78:LEU:HD22	20:b:80:TRP:HE1	1.33	0.93
2:B:170:TYR:HE2	4:D:135:TYR:CG	1.87	0.93
4:D:238:LEU:HD23	22:r:36:GLN:HB2	1.47	0.93
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.82	0.93
7:G:544:MET:HE3	7:G:546:PHE:CE1	2.03	0.93
9:I:152:CYS:HG	25:I:302:SF4:FE1	0.62	0.93
10:P:220:TYR:HD2	10:P:226:VAL:HG13	1.32	0.93
18:Z:97:ILE:HG23	18:Z:98:MET:HG3	1.51	0.93
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.51	0.93
7:G:674:LEU:HD11	13:S:46:LYS:HE2	1.49	0.93
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.92
17:X:18:VAL:HG21	18:Z:74:LEU:HD11	1.51	0.92
7:G:338:VAL:CG1	7:G:546:PHE:HE1	1.81	0.92
4:D:267:ILE:HG21	8:H:278:PRO:O	1.67	0.92
7:G:182:CYS:SG	25:G:802:SF4:FE2	1.61	0.92
7:G:661:GLU:O	7:G:661:GLU:HG2	1.68	0.92
10:P:306:GLY:HA2	10:P:312:PRO:HB3	1.48	0.92
8:H:17:MET:HE1	30:H:400:UQ9:H17	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.52	0.91
8:H:260:MET:HE3	19:a:13:GLY:C	1.95	0.91
2:B:98:ALA:HB2	2:B:134:ALA:O	1.69	0.91
3:C:87:ILE:HG13	3:C:144:THR:CG2	2.00	0.91
4:D:256:ASP:HB2	18:Z:25:LEU:HD12	1.52	0.91
7:G:611:THR:CG2	11:Q:105:GLU:HA	1.99	0.91
9:I:113:CYS:HG	25:I:303:SF4:FE3	0.61	0.91
6:F:379:CYS:HG	25:F:502:SF4:FE4	0.61	0.91
4:D:361:ALA:O	4:D:384:LEU:HD11	1.71	0.91
4:D:376:GLU:HG3	7:G:121:LEU:CD1	2.00	0.91
19:a:64:LYS:HE2	19:a:66:LEU:HB2	1.51	0.90
2:B:141:MET:HE2	4:D:115:LEU:HB3	1.54	0.90
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.53	0.90
7:G:662:THR:HG23	7:G:662:THR:O	1.71	0.90
10:P:168:SER:O	10:P:202:ARG:HA	1.71	0.90
3:C:234:LEU:O	3:C:234:LEU:CD1	2.20	0.90
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.85	0.89
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.89
10:P:268:PRO:HG3	10:P:342:PRO:HB2	1.54	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.89
22:r:12:ARG:NH2	22:r:21:GLN:HE22	1.69	0.89
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.53	0.89
7:G:404:GLY:HA2	7:G:684:LEU:HD13	1.52	0.89
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.37	0.89
10:P:292:PRO:O	10:P:293:LEU:HG	1.72	0.89
4:D:269:ARG:O	4:D:273:VAL:HG12	1.72	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
8:H:19:PHE:CE2	19:a:11:ILE:HG21	2.08	0.88
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.88
7:G:176:CYS:HG	25:G:802:SF4:FE4	0.62	0.88
17:X:20:VAL:HG23	17:X:25:LEU:CD1	2.03	0.88
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.39	0.88
1:A:79:ILE:HD11	8:H:155:LEU:CD2	2.01	0.88
19:a:58:ASN:HB3	19:a:60:TYR:CD1	2.08	0.88
2:B:194:CYS:SG	25:B:301:SF4:FE4	1.65	0.88
4:D:120:THR:HG23	4:D:135:TYR:CD1	2.09	0.88
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.37	0.88
3:C:223:VAL:HG21	3:C:225:LEU:HD11	1.56	0.87
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.56	0.87
2:B:82:ILE:HD11	27:B:304:PC1:H362	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:327:ILE:HD11	6:F:331:VAL:HG11	1.56	0.87
3:C:229:PHE:HE1	9:I:126:GLN:CG	1.86	0.87
7:G:608:VAL:HG23	11:Q:103:THR:HB	1.57	0.87
6:F:266:GLY:HA3	6:F:271:SER:HA	0.89	0.87
6:F:110:PRO:HB3	6:F:152:ARG:HE	1.40	0.87
7:G:615:LEU:HG	10:P:41:ILE:HG23	1.56	0.86
22:r:12:ARG:HH21	22:r:21:GLN:HE22	1.18	0.86
4:D:256:ASP:HB2	18:Z:25:LEU:CD1	2.05	0.86
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.86
11:Q:52:LEU:HD22	16:W:19:SER:HB3	1.58	0.86
18:Z:58:ARG:HG2	20:b:45:ILE:HG12	1.57	0.86
3:C:87:ILE:CG1	3:C:144:THR:HG22	2.05	0.86
1:A:18:ILE:CD1	8:H:76:THR:HG23	2.04	0.86
4:D:451:ILE:HG23	4:D:456:ILE:HD11	1.57	0.86
4:D:137:ASP:OD2	4:D:223:HIS:HA	1.76	0.86
18:Z:120:LEU:HD23	18:Z:122:GLY:N	1.90	0.86
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.85
8:H:19:PHE:HE2	19:a:11:ILE:HG21	1.39	0.85
22:r:27:ARG:HB3	22:r:31:ILE:CG2	2.05	0.85
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.85
1:A:80:GLN:CA	20:b:46:ASN:HD21	1.90	0.85
8:H:45:ILE:HD11	19:a:11:ILE:HD11	1.57	0.85
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.58	0.85
10:P:55:VAL:HG21	12:R:43:TYR:HB2	1.58	0.85
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.85
7:G:662:THR:O	7:G:662:THR:CG2	2.25	0.85
4:D:261:MET:O	4:D:265:ASN:ND2	2.10	0.85
14:T:117:GLU:HA	14:T:120:MET:HE2	1.58	0.85
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.85
6:F:300:ILE:HD13	6:F:307:VAL:H	1.40	0.85
9:I:123:CYS:HG	25:I:302:SF4:FE2	0.60	0.85
4:D:137:ASP:OD2	4:D:223:HIS:CA	2.24	0.85
4:D:266:ARG:HH21	9:I:60:ILE:HA	1.42	0.85
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.58	0.85
7:G:388:ASN:H	7:G:514:ASN:CB	1.90	0.85
19:a:52:ARG:HG3	19:a:57:VAL:O	1.76	0.84
1:A:7:ILE:HD13	24:H:401:3PE:H371	1.56	0.84
4:D:192:LEU:HD11	4:D:200:PHE:HB2	1.59	0.84
7:G:544:MET:CE	7:G:546:PHE:CZ	2.60	0.84
2:B:98:ALA:HB2	2:B:134:ALA:C	2.02	0.84
4:D:96:ARG:HG3	4:D:115:LEU:HD11	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:HD11	8:H:76:THR:CG2	2.07	0.84
7:G:377:ALA:HB3	7:G:384:ASN:HD21	1.43	0.84
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.84
10:P:220:TYR:CD2	10:P:226:VAL:HG13	2.13	0.84
10:P:96:LEU:C	10:P:96:LEU:HD12	2.03	0.83
2:B:94:THR:H	26:B:302:UQ1:H113	1.43	0.83
13:S:95:LEU:O	13:S:95:LEU:CD1	2.26	0.83
10:P:293:LEU:HB2	10:P:298:TYR:CZ	2.14	0.83
3:C:223:VAL:CG2	3:C:225:LEU:HD12	2.08	0.83
4:D:144:MET:SD	4:D:222:MET:HG3	2.19	0.83
1:A:25:PRO:HG2	8:H:60:PRO:HD3	1.61	0.83
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.83
6:F:425:CYS:SG	25:F:502:SF4:FE1	1.70	0.83
7:G:75:CYS:HG	28:G:803:FES:FE1	0.90	0.83
12:R:47:ARG:HB2	21:q:125:VAL:HG11	1.61	0.83
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.14	0.83
7:G:617:ARG:HH12	16:W:128:GLY:C	1.86	0.82
10:P:293:LEU:HB2	10:P:298:TYR:CE2	2.14	0.82
1:A:68:GLU:CD	1:A:98:LEU:HD13	2.04	0.82
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.10	0.82
8:H:203:GLY:O	8:H:207:LEU:O	1.96	0.82
4:D:236:LEU:HD22	4:D:240:LEU:HD23	1.59	0.82
4:D:256:ASP:CA	4:D:259:GLU:HB3	2.09	0.82
7:G:403:VAL:HG23	7:G:432:ILE:HB	1.61	0.82
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.59	0.82
2:B:194:CYS:HG	25:B:301:SF4:FE4	0.54	0.82
8:H:80:THR:HG21	24:H:401:3PE:H3D2	1.62	0.82
11:Q:154:LYS:HB2	11:Q:155:PRO:HD2	1.61	0.82
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.82
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.44	0.82
10:P:104:THR:HG21	12:R:46:VAL:HG12	1.60	0.82
4:D:129:TYR:HE1	4:D:411:LEU:HD21	1.43	0.82
8:H:199:ASP:HB2	8:H:279:ARG:HD3	1.59	0.82
2:B:92:PRO:HB2	2:B:122:ARG:HH12	1.45	0.82
4:D:390:GLN:OE1	7:G:145:MET:HE1	1.80	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
2:B:170:TYR:HE2	4:D:135:TYR:CD1	1.97	0.81
11:Q:131:LYS:HG2	11:Q:135:ILE:CD1	2.09	0.81
18:Z:58:ARG:HG2	20:b:45:ILE:CG1	2.10	0.81
3:C:149:LEU:HD21	11:Q:64:LEU:HD22	1.62	0.81
2:B:122:ARG:CB	26:B:302:UQ1:H72	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
9:I:89:GLU:HG2	21:q:61:TRP:HB3	1.62	0.81
2:B:92:PRO:HD2	2:B:119:VAL:HG13	1.61	0.81
4:D:192:LEU:HD11	4:D:200:PHE:CB	2.10	0.81
1:A:25:PRO:O	1:A:26:GLN:HB2	1.78	0.81
6:F:228:PRO:HG2	11:Q:160:TYR:HD2	1.45	0.81
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.63	0.81
8:H:54:LYS:HE2	8:H:58:LYS:HD2	1.62	0.81
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.61	0.81
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.81
15:V:72:LEU:HD13	15:V:80:VAL:HG11	1.62	0.81
18:Z:120:LEU:CD2	18:Z:122:GLY:H	1.94	0.81
8:H:229:THR:O	8:H:229:THR:HG22	1.81	0.81
6:F:425:CYS:HG	25:F:502:SF4:FE1	0.53	0.81
7:G:388:ASN:H	7:G:514:ASN:HB3	1.45	0.80
10:P:171:ASN:HB3	10:P:327:VAL:CB	2.10	0.80
2:B:92:PRO:HG3	2:B:130:VAL:CG1	2.10	0.80
2:B:170:TYR:CE1	4:D:134:PRO:HB2	2.17	0.80
6:F:109:ARG:NH1	6:F:237:GLY:O	2.13	0.80
7:G:89:VAL:HB	7:G:94:MET:HG3	1.62	0.80
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.45	0.80
8:H:117:LEU:HD21	8:H:136:VAL:HG11	1.60	0.80
6:F:234:GLY:HA3	6:F:238:CYS:O	1.81	0.80
7:G:617:ARG:HH12	16:W:129:HIS:N	1.79	0.80
4:D:241:LEU:HB3	18:Z:16:TYR:OH	1.82	0.80
8:H:90:PRO:HG2	8:H:240:ILE:HD13	1.61	0.80
1:A:33:LYS:HA	2:B:150:ASP:O	1.81	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
17:X:18:VAL:HG12	17:X:20:VAL:HG22	1.63	0.80
1:A:72:LEU:HD21	1:A:94:LEU:HD23	1.64	0.80
3:C:147:ASP:OD1	3:C:148:GLU:OE1	2.00	0.80
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.63	0.80
13:S:62:GLN:HB2	13:S:80:ASN:HB2	1.64	0.80
14:T:82:ARG:HD2	14:T:125:GLU:HG3	1.61	0.80
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.22	0.80
10:P:363:SER:HA	16:W:54:GLN:HE22	1.46	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
21:q:43:LYS:HZ3	21:q:44:TYR:HE2	1.28	0.79
4:D:177:ILE:O	4:D:181:LEU:HD13	1.81	0.79
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
7:G:73:GLY:HA2	28:G:803:FES:S1	2.22	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.79
10:P:51:VAL:HG22	10:P:53:GLY:H	1.48	0.79
7:G:338:VAL:HG13	7:G:546:PHE:HE1	1.47	0.79
8:H:28:LEU:HD21	8:H:274:ARG:HD3	1.65	0.79
14:T:106:LYS:H	14:T:106:LYS:HD2	1.48	0.79
3:C:170:TRP:CG	3:C:183:LEU:HD21	2.18	0.79
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.98	0.79
10:P:88:VAL:HG13	10:P:91:ILE:HD11	1.63	0.79
10:P:225:ALA:CB	10:P:289:ILE:HB	2.13	0.79
7:G:544:MET:HE3	7:G:546:PHE:HZ	1.39	0.78
9:I:211:TYR:CZ	22:r:39:PRO:HG3	2.17	0.78
7:G:130:ILE:HA	9:I:140:ARG:HH11	1.45	0.78
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.15	0.78
10:P:188:GLU:HG2	10:P:200:ILE:HD13	1.64	0.78
4:D:137:ASP:OD1	4:D:138:ARG:HG3	1.83	0.78
6:F:224:ARG:HD3	11:Q:164:PHE:CE1	2.18	0.78
8:H:196:ALA:HB1	8:H:197:PRO:CD	2.13	0.78
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.13	0.78
10:P:226:VAL:HG12	10:P:228:LEU:HG	1.64	0.78
1:A:72:LEU:CD2	1:A:94:LEU:HD23	2.13	0.78
1:A:52:SER:HB2	1:A:55:PHE:CE2	2.14	0.78
3:C:160:ILE:HD12	4:D:285:ASN:HD22	1.49	0.78
2:B:136:THR:HG21	4:D:118:ARG:HD3	1.66	0.78
3:C:103:THR:HG21	15:V:55:LYS:HE3	1.66	0.78
6:F:424:ILE:HD11	7:G:73:GLY:O	1.84	0.78
6:F:36:LYS:HB3	6:F:38:GLU:HG2	1.66	0.77
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.77
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.77
9:I:210:LEU:HD12	22:r:39:PRO:HD2	1.66	0.77
1:A:68:GLU:HG2	1:A:98:LEU:CD1	2.13	0.77
4:D:256:ASP:HA	4:D:259:GLU:HB2	1.63	0.77
1:A:73:LEU:O	1:A:76:PRO:HD2	1.84	0.77
5:E:196:THR:H	5:E:199:ASP:HB2	1.47	0.77
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.66	0.77
8:H:184:MET:CG	8:H:293:PHE:CD2	2.66	0.77
8:H:227:GLU:O	8:H:231:ILE:HG13	1.83	0.77
14:T:123:GLU:HG2	14:T:130:ILE:HG12	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:ILE:HG21	8:H:150:LEU:HD21	1.65	0.77
1:A:3:LEU:HD23	24:H:401:3PE:H31	1.66	0.77
4:D:137:ASP:CG	4:D:223:HIS:HA	2.09	0.77
10:P:266:THR:HG21	10:P:329:PRO:HG3	1.67	0.77
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.77
18:Z:101:VAL:HB	18:Z:102:PRO:HD2	1.67	0.77
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77
22:r:27:ARG:HD2	22:r:31:ILE:HG22	1.67	0.77
3:C:89:PRO:O	3:C:92:VAL:HG23	1.85	0.77
13:S:25:GLN:HG3	13:S:57:GLU:OE1	1.84	0.77
8:H:117:LEU:HD23	8:H:136:VAL:HG11	1.67	0.77
3:C:70:LYS:HD3	15:V:101:GLU:HB2	1.67	0.76
4:D:299:GLN:NE2	9:I:36:TYR:CD2	2.53	0.76
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.76
17:X:20:VAL:HG23	17:X:25:LEU:HD11	1.66	0.76
4:D:259:GLU:HB3	18:Z:25:LEU:HD11	1.66	0.76
8:H:86:TRP:HE1	8:H:229:THR:HG22	1.48	0.76
10:P:225:ALA:HB1	10:P:289:ILE:HB	1.68	0.76
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.21	0.76
2:B:202:LEU:HD23	9:I:86:TYR:CG	2.20	0.76
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.66	0.76
6:F:109:ARG:CZ	6:F:237:GLY:O	2.34	0.76
7:G:652:ASN:HB3	7:G:655:ARG:NH2	2.01	0.76
10:P:221:ARG:HD2	10:P:286:ARG:HD2	1.68	0.76
22:r:12:ARG:HH21	22:r:21:GLN:NE2	1.82	0.76
2:B:170:TYR:HE2	4:D:135:TYR:CD2	2.03	0.76
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.21	0.76
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.76
8:H:92:PRO:HG3	8:H:255:TYR:HB3	1.68	0.76
17:X:36:CYS:O	17:X:40:ASN:ND2	2.19	0.76
3:C:160:ILE:HD12	4:D:285:ASN:ND2	1.99	0.76
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.75
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.75
10:P:226:VAL:HG11	10:P:277:VAL:HG11	1.68	0.75
13:S:22:HIS:C	13:S:58:CYS:SG	2.69	0.75
11:Q:64:LEU:HG	16:W:84:LEU:HD12	1.68	0.75
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.04	0.75
8:H:260:MET:SD	19:a:13:GLY:HA2	2.25	0.75
2:B:94:THR:O	26:B:302:UQ1:H111	1.86	0.75
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:184:LYS:HB3	23:s:92:LEU:HD22	1.67	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
4:D:97:LEU:O	4:D:97:LEU:HG	1.85	0.75
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.75
21:q:25:ARG:HB3	21:q:29:ARG:HH12	1.52	0.75
1:A:80:GLN:HA	20:b:46:ASN:ND2	2.00	0.75
7:G:127:ASP:HA	12:R:106:TYR:OH	1.86	0.75
8:H:304:HIS:O	8:H:308:PRO:HD3	1.87	0.75
10:P:217:PHE:HB2	10:P:280:ILE:HD13	1.66	0.75
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.75
26:B:302:UQ1:HM22	26:B:302:UQ1:HM33	1.67	0.75
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.74
10:P:228:LEU:HD21	10:P:277:VAL:HG21	1.68	0.74
15:V:35:LEU:HD13	15:V:48:THR:HG23	1.68	0.74
17:X:128:VAL:O	17:X:128:VAL:HG23	1.87	0.74
9:I:90:LYS:HB2	21:q:90:LEU:CD2	2.17	0.74
9:I:180:HIS:CD2	10:P:100:LEU:HD21	2.21	0.74
12:R:31:ILE:HG12	12:R:37:VAL:HB	1.70	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
10:P:359:TYR:O	10:P:360:ARG:HB3	1.86	0.74
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.69	0.74
10:P:272:LEU:HG	10:P:375:VAL:HG21	1.68	0.74
11:Q:69:GLU:O	11:Q:72:ILE:HG22	1.86	0.74
17:X:49:GLU:HG3	17:X:50:GLU:HG3	1.70	0.74
2:B:170:TYR:CE2	4:D:135:TYR:CG	2.75	0.74
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.01	0.74
4:D:261:MET:HE1	9:I:73:THR:CG2	2.16	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
8:H:200:LEU:HD21	8:H:282:TYR:HA	1.69	0.74
5:E:176:LEU:HD12	5:E:184:MET:HE3	1.69	0.74
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.74
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.74
4:D:259:GLU:HG3	18:Z:25:LEU:CD2	2.17	0.74
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.22	0.74
8:H:90:PRO:HG2	8:H:240:ILE:HG21	1.69	0.74
10:P:55:VAL:HG21	12:R:43:TYR:CB	2.18	0.74
3:C:118:VAL:HG12	3:C:120:THR:HG22	1.69	0.73
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.22	0.73
6:F:392:MET:CE	6:F:419:ILE:HD12	2.18	0.73
6:F:293:SER:HA	6:F:336:LEU:HD13	1.68	0.73
13:S:42:VAL:HG13	13:S:43:GLU:CD	2.13	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:368:ARG:NH2	9:I:165:ASP:OD1	2.21	0.73
3:C:223:VAL:HG22	3:C:225:LEU:HD12	1.69	0.73
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.73
8:H:92:PRO:CG	8:H:255:TYR:HB3	2.17	0.73
2:B:161:MET:HG2	2:B:196:PRO:HG2	1.70	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.52	0.73
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.70	0.73
1:A:99:SER:HB3	24:A:201:3PE:H392	1.71	0.73
3:C:149:LEU:CD2	11:Q:64:LEU:CD2	2.67	0.73
6:F:67:GLU:HG3	6:F:71:LYS:HE3	1.70	0.73
9:I:61:LEU:O	24:I:301:3PE:H362	1.89	0.73
17:X:7:LEU:HD12	18:Z:91:LEU:HD22	1.69	0.73
7:G:226:CYS:HG	25:G:802:SF4:FE1	1.05	0.73
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.73
4:D:203:MET:HE1	4:D:254:ARG:HB3	1.70	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
10:P:96:LEU:HD12	10:P:97:MET:N	2.01	0.73
2:B:115:ASP:HA	2:B:119:VAL:O	1.88	0.72
2:B:90:LEU:O	2:B:92:PRO:HD3	1.89	0.72
10:P:134:TRP:HB3	10:P:312:PRO:HG3	1.71	0.72
4:D:215:GLU:OE2	9:I:94:SER:HB3	1.89	0.72
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
10:P:274:PHE:HE1	10:P:290:PRO:HG3	1.54	0.72
18:Z:129:THR:HB	18:Z:132:GLU:HG3	1.71	0.72
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.72
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.23	0.72
10:P:263:PHE:CD1	10:P:333:PRO:HB2	2.24	0.72
10:P:270:ARG:HH21	10:P:327:VAL:C	1.98	0.72
27:B:303:PC1:H341	27:B:303:PC1:H222	1.70	0.72
3:C:45:THR:HG22	4:D:358:VAL:CG2	2.20	0.72
8:H:260:MET:HE1	19:a:16:LEU:HB2	1.70	0.72
14:T:104:PHE:HB3	14:T:110:LEU:HD22	1.71	0.72
1:A:65:PHE:O	1:A:68:GLU:HB2	1.90	0.72
5:E:185:VAL:HG22	5:E:195:LEU:HD13	1.72	0.72
7:G:544:MET:CE	7:G:546:PHE:HZ	2.01	0.72
9:I:154:TYR:HA	9:I:169:GLU:OE2	1.89	0.72
10:P:73:LEU:HA	10:P:76:MET:HE2	1.71	0.72
15:V:28:TYR:OH	15:V:55:LYS:HD3	1.89	0.72
4:D:217:VAL:HG11	4:D:240:LEU:HD22	1.72	0.72
4:D:320:ILE:HD11	9:I:38:TYR:CE1	2.25	0.72
10:P:64:PHE:HE1	10:P:209:ARG:O	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:124:ASN:OD1	10:P:125:VAL:HG23	1.89	0.72
4:D:144:MET:SD	4:D:222:MET:CA	2.73	0.72
4:D:267:ILE:CG2	8:H:278:PRO:HG2	2.15	0.72
4:D:320:ILE:HD11	9:I:38:TYR:CD1	2.24	0.72
8:H:90:PRO:CG	8:H:162:LEU:HB3	2.20	0.72
19:a:58:ASN:ND2	19:a:60:TYR:HE1	1.84	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.20	0.72
7:G:541:PRO:HB2	7:G:561:PRO:HD3	1.72	0.72
19:a:64:LYS:HE2	19:a:66:LEU:CB	2.19	0.72
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.90	0.72
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.72
6:F:327:ILE:HG23	6:F:332:CYS:SG	2.29	0.72
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.72
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.72
2:B:97:LEU:HD22	2:B:141:MET:HG2	1.72	0.71
2:B:170:TYR:CE2	4:D:135:TYR:CD1	2.77	0.71
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.71
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.71	0.71
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.71	0.71
4:D:97:LEU:HD11	4:D:109:CYS:HB3	1.70	0.71
4:D:146:CYS:SG	4:D:178:THR:OG1	2.48	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
10:P:276:LEU:HD23	10:P:280:ILE:HD12	1.72	0.71
13:S:79:LEU:HA	13:S:82:LEU:HG	1.73	0.71
17:X:7:LEU:HD22	18:Z:87:LEU:CD1	2.19	0.71
1:A:22:PHE:HA	8:H:60:PRO:HG3	1.71	0.71
1:A:52:SER:OG	1:A:55:PHE:HB2	1.90	0.71
4:D:238:LEU:HB3	22:r:36:GLN:CG	2.16	0.71
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
8:H:45:ILE:CD1	19:a:11:ILE:HD11	2.19	0.71
8:H:51:ASP:HA	8:H:54:LYS:HB3	1.73	0.71
4:D:202:TRP:HH2	4:D:261:MET:CE	2.03	0.71
7:G:266:ARG:HH12	9:I:131:GLU:HG2	1.54	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
8:H:157:ASN:ND2	8:H:165:LEU:HD11	2.06	0.71
1:A:84:THR:HG22	20:b:43:SER:HB2	1.72	0.71
3:C:120:THR:HG23	3:C:121:ARG:N	2.05	0.71
3:C:152:ILE:HD11	3:C:177:PHE:HE2	1.50	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:386:THR:CG2	9:I:118:LEU:HD13	2.21	0.71
7:G:651:PRO:HB2	13:S:57:GLU:O	1.89	0.71
34:a:101:CDL:HA32	21:q:10:GLY:HA3	1.72	0.71
8:H:288:LEU:HD11	24:I:301:3PE:H2	1.71	0.71
8:H:18:ALA:O	8:H:21:THR:OG1	2.07	0.71
5:E:240:PRO:HB3	6:F:60:GLY:HA3	1.73	0.71
8:H:196:ALA:HB1	8:H:197:PRO:HD3	1.73	0.71
21:q:25:ARG:O	21:q:29:ARG:HB3	1.91	0.71
21:q:26:VAL:HG12	21:q:32:ASP:O	1.91	0.71
5:E:71:GLU:HG3	23:s:94:GLN:HE21	1.54	0.70
5:E:131:ILE:HD13	5:E:187:ILE:HG12	1.72	0.70
7:G:382:ARG:CZ	7:G:652:ASN:HD21	2.03	0.70
8:H:265:LEU:O	8:H:269:THR:N	2.24	0.70
17:X:47:ARG:NH2	18:Z:80:ASP:OD1	2.24	0.70
4:D:129:TYR:CE1	4:D:411:LEU:HD21	2.25	0.70
4:D:436:ASP:OD1	4:D:437:LYS:N	2.24	0.70
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.71	0.70
10:P:64:PHE:CZ	10:P:242:VAL:HG21	2.26	0.70
1:A:18:ILE:HD11	8:H:76:THR:HG22	1.69	0.70
7:G:359:ASN:OD1	13:S:68:ARG:NH1	2.24	0.70
10:P:157:LYS:HB2	10:P:195:PHE:HD1	1.55	0.70
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.21	0.70
10:P:174:MET:O	10:P:175:LYS:HG2	1.91	0.70
4:D:94:VAL:HG11	4:D:116:LEU:HB2	1.73	0.70
4:D:202:TRP:HH2	4:D:261:MET:HE2	1.57	0.70
7:G:617:ARG:NH1	16:W:128:GLY:C	2.50	0.70
1:A:80:GLN:HA	20:b:46:ASN:HD21	1.53	0.70
4:D:359:ASP:C	4:D:359:ASP:OD1	2.34	0.70
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.70
1:A:49:LEU:HB3	1:A:50:PRO:CD	2.15	0.70
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.70
5:E:221:ARG:NH2	5:E:227:ALA:HB2	2.07	0.70
8:H:260:MET:CE	19:a:17:VAL:HG13	2.20	0.70
13:S:42:VAL:HG22	13:S:46:LYS:HE3	1.72	0.70
17:X:130:LYS:HD3	20:b:63:MET:HG3	1.74	0.70
4:D:277:VAL:HA	4:D:324:GLY:O	1.91	0.70
4:D:304:LYS:HG3	4:D:316:PHE:CZ	2.26	0.70
9:I:54:THR:HA	20:b:13:TRP:HE1	1.57	0.70
21:q:26:VAL:CG1	21:q:32:ASP:O	2.40	0.70
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.70
1:A:35:ASN:CG	1:A:36:PRO:HD2	2.16	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:228:PRO:CG	11:Q:160:TYR:HD2	2.05	0.69
7:G:83:GLU:O	7:G:84:LYS:HG2	1.90	0.69
16:W:87:ILE:HG22	16:W:91:MET:HE3	1.73	0.69
7:G:628:GLU:OE1	16:W:122:LEU:HB2	1.92	0.69
8:H:197:PRO:HD3	8:H:273:ILE:HG21	1.74	0.69
17:X:142:TYR:HA	18:Z:115:ARG:HE	1.57	0.69
1:A:33:LYS:HE2	8:H:61:MET:HE2	1.74	0.69
10:P:165:ILE:HD13	10:P:253:THR:HG22	1.73	0.69
2:B:97:LEU:HD13	4:D:94:VAL:CG1	2.20	0.69
8:H:287:HIS:CD2	8:H:291:LYS:HD2	2.28	0.69
10:P:91:ILE:HG13	10:P:95:ARG:HH12	1.57	0.69
10:P:236:VAL:CG2	10:P:270:ARG:HG2	2.22	0.69
15:V:113:LYS:O	15:V:116:ILE:HG13	1.93	0.69
23:s:89:LYS:NZ	23:s:90:PHE:CZ	2.60	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
1:A:35:ASN:OD1	1:A:36:PRO:CD	2.36	0.69
4:D:259:GLU:HG2	18:Z:23:ARG:HD2	1.74	0.69
5:E:185:VAL:HG22	5:E:195:LEU:CD1	2.23	0.69
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
10:P:226:VAL:CG1	10:P:228:LEU:HG	2.22	0.69
15:V:19:THR:HB	15:V:22:GLU:HG3	1.74	0.69
17:X:59:GLU:HA	17:X:62:LEU:HG	1.73	0.69
1:A:35:ASN:HA	8:H:64:LEU:HD12	1.75	0.69
3:C:87:ILE:CG1	3:C:144:THR:CG2	2.69	0.69
4:D:220:ALA:HB2	9:I:98:ARG:HH21	1.58	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
14:T:82:ARG:HD2	14:T:125:GLU:CG	2.23	0.69
17:X:7:LEU:HD22	18:Z:87:LEU:HD11	1.74	0.69
5:E:221:ARG:HH21	5:E:227:ALA:HB2	1.58	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
3:C:120:THR:CG2	15:V:116:ILE:HG21	2.18	0.69
11:Q:99:MET:HE2	11:Q:126:LEU:HD12	1.73	0.69
23:s:92:LEU:HB2	23:s:93:PRO:CD	2.22	0.69
4:D:255:ILE:HG12	4:D:337:MET:HE2	1.74	0.68
6:F:194:ASP:OD2	23:s:91:ARG:HB3	1.93	0.68
7:G:617:ARG:NH1	16:W:129:HIS:N	2.39	0.68
8:H:203:GLY:O	8:H:207:LEU:HB2	1.93	0.68
5:E:178:ALA:HB3	5:E:184:MET:SD	2.34	0.68
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.68
8:H:196:ALA:C	8:H:198:PHE:N	2.47	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:155:LEU:O	8:H:315:PRO:HG2	1.94	0.68
14:T:111:ASP:H	14:T:114:ASP:HB2	1.58	0.68
15:V:106:GLU:HG3	15:V:107:PRO:HD2	1.74	0.68
1:A:84:THR:O	1:A:87:MET:HG2	1.93	0.68
7:G:652:ASN:HB3	7:G:655:ARG:HH22	1.57	0.68
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.68
18:Z:92:GLU:O	18:Z:96:ILE:N	2.26	0.68
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.68
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.75	0.68
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.76	0.68
10:P:252:ALA:HB2	10:P:338:LEU:HD21	1.76	0.68
17:X:48:TRP:CE2	20:b:55:VAL:HG22	2.29	0.68
19:a:58:ASN:HB3	19:a:60:TYR:HD1	1.58	0.68
20:b:31:ILE:HA	20:b:34:MET:HE2	1.76	0.68
21:q:137:TRP:CH2	21:q:140:PRO:HD3	2.29	0.68
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.68
7:G:382:ARG:HH21	7:G:386:LEU:HD11	1.59	0.68
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.76	0.68
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.74	0.68
19:a:18:ILE:N	19:a:19:PRO:CD	2.55	0.68
3:C:63:TYR:CZ	3:C:67:ILE:HD11	2.28	0.68
3:C:223:VAL:HG22	3:C:225:LEU:HD13	1.74	0.68
2:B:202:LEU:HD23	9:I:86:TYR:CD1	2.30	0.67
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
2:B:171:TYR:CD1	4:D:135:TYR:HE1	2.12	0.67
9:I:89:GLU:OE1	21:q:58:ARG:HG2	1.94	0.67
9:I:123:CYS:SG	25:I:302:SF4:FE2	1.79	0.67
1:A:31:SER:HB2	1:A:33:LYS:HG3	1.76	0.67
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.67
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.28	0.67
10:P:266:THR:HG21	10:P:329:PRO:HB3	1.76	0.67
19:a:32:GLY:HA3	19:a:60:TYR:CD2	2.30	0.67
21:q:39:VAL:HG21	21:q:89:TRP:CH2	2.30	0.67
6:F:199:ARG:HD3	23:s:80:PHE:CE2	2.30	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
8:H:314:VAL:HG23	18:Z:58:ARG:HH21	1.59	0.67
10:P:266:THR:HG21	10:P:329:PRO:CG	2.25	0.67
4:D:86:PRO:HG3	4:D:96:ARG:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:129:TYR:HA	5:E:188:ASN:HD21	1.60	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.48	0.67
8:H:198:PHE:CD1	8:H:285:LEU:HD13	2.29	0.67
13:S:40:ARG:HA	13:S:43:GLU:OE1	1.95	0.67
18:Z:105:LYS:HD3	18:Z:108:GLU:OE1	1.94	0.67
6:F:300:ILE:HD13	6:F:307:VAL:HG23	1.77	0.67
9:I:171:PRO:HB3	21:q:93:MET:CE	2.04	0.67
10:P:166:HIS:CD2	10:P:191:VAL:HG21	2.29	0.67
1:A:68:GLU:OE2	1:A:98:LEU:HD22	1.95	0.67
2:B:169:GLY:O	2:B:170:TYR:C	2.36	0.67
2:B:195:PRO:O	2:B:196:PRO:C	2.35	0.67
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.67
6:F:117:ALA:HB1	6:F:131:MET:SD	2.35	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
3:C:223:VAL:HG21	3:C:225:LEU:CD1	2.17	0.67
5:E:131:ILE:HG23	5:E:170:LEU:HA	1.77	0.67
5:E:197:PRO:HA	5:E:200:ILE:HD12	1.77	0.67
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.67
9:I:210:LEU:CD1	22:r:39:PRO:O	2.35	0.67
22:r:8:ILE:O	22:r:11:LEU:HB2	1.95	0.67
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.66
2:B:107:MET:HE3	2:B:114:MET:HE2	1.77	0.66
5:E:192:TYR:HB3	5:E:195:LEU:HD21	1.78	0.66
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.77	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.95	0.66
1:A:26:GLN:HG3	27:B:304:PC1:H232	1.77	0.66
2:B:113:ASP:OD1	8:H:34:ARG:HD3	1.94	0.66
8:H:230:ASN:CB	8:H:233:LEU:HD12	2.25	0.66
10:P:176:SER:H	10:P:182:ARG:HG2	1.60	0.66
1:A:25:PRO:CG	8:H:60:PRO:HD3	2.26	0.66
2:B:92:PRO:HB3	2:B:130:VAL:HG13	1.78	0.66
2:B:124:SER:HB3	2:B:125:PRO:HD2	1.76	0.66
2:B:170:TYR:CE2	4:D:135:TYR:CD2	2.84	0.66
13:S:44:LEU:HD11	13:S:95:LEU:HD21	1.78	0.66
8:H:87:VAL:HG22	8:H:88:PRO:HD3	1.78	0.66
8:H:203:GLY:O	8:H:207:LEU:C	2.38	0.66
1:A:2:ASN:HB2	18:Z:143:TYR:HE1	1.60	0.66
2:B:164:CYS:HA	2:B:168:GLY:O	1.95	0.66
2:B:202:LEU:CD2	9:I:86:TYR:CG	2.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.26	0.66
10:P:227:PRO:HB2	10:P:298:TYR:CE1	2.30	0.66
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.78	0.66
22:r:6:ARG:O	22:r:9:GLN:HG2	1.96	0.66
2:B:168:GLY:HA3	2:B:172:HIS:CD2	2.30	0.66
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.66
8:H:92:PRO:HG3	8:H:255:TYR:CB	2.25	0.66
10:P:187:GLY:HA2	10:P:190:GLU:HG2	1.78	0.66
14:T:93:ILE:HG13	14:T:110:LEU:HG	1.78	0.66
17:X:133:THR:HG22	17:X:134:ASP:H	1.60	0.66
4:D:266:ARG:HH21	9:I:60:ILE:CA	2.08	0.66
6:F:109:ARG:HE	6:F:239:PRO:HD3	1.61	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
10:P:171:ASN:CB	10:P:327:VAL:HB	2.16	0.66
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.66
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.66
10:P:209:ARG:HA	10:P:352:VAL:HG12	1.78	0.66
14:T:123:GLU:CD	14:T:130:ILE:H	2.03	0.66
19:a:7:PRO:O	19:a:11:ILE:HD12	1.95	0.66
6:F:110:PRO:O	6:F:238:CYS:HB3	1.96	0.66
8:H:10:LEU:HD22	8:H:83:LEU:HG	1.78	0.66
10:P:301:ILE:HG22	10:P:305:PHE:HE2	1.61	0.66
27:B:303:PC1:H112	21:q:75:TRP:CE3	2.31	0.65
8:H:184:MET:HA	8:H:293:PHE:HE2	1.62	0.65
9:I:90:LYS:HD3	21:q:91:HIS:CE1	2.31	0.65
5:E:151:LEU:CD1	5:E:200:ILE:HG21	2.26	0.65
6:F:227:PRO:HG3	7:G:94:MET:SD	2.35	0.65
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65
8:H:99:ASN:O	8:H:100:LEU:HB2	1.96	0.65
9:I:89:GLU:HG2	21:q:61:TRP:CB	2.26	0.65
17:X:18:VAL:HA	17:X:68:LEU:HD21	1.76	0.65
17:X:24:VAL:HG12	17:X:86:TRP:CD1	2.31	0.65
21:q:67:GLU:HG2	21:q:72:ASN:HA	1.78	0.65
2:B:100:CYS:HB2	2:B:134:ALA:HB1	1.77	0.65
2:B:170:TYR:HD1	9:I:153:ILE:HD13	1.60	0.65
10:P:64:PHE:CZ	10:P:242:VAL:CG2	2.79	0.65
14:T:87:LEU:HD13	14:T:98:LEU:HD11	1.79	0.65
14:T:105:MET:HE2	14:T:139:MET:HG2	1.79	0.65
2:B:98:ALA:HB3	2:B:101:ALA:H	1.61	0.65
4:D:192:LEU:CD1	4:D:200:PHE:HB2	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.78	0.65
7:G:338:VAL:CG1	7:G:546:PHE:CE1	2.72	0.65
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.65
17:X:132:LYS:HB3	20:b:59:ASP:HB3	1.78	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
7:G:652:ASN:CB	7:G:655:ARG:NH2	2.60	0.65
2:B:109:ALA:HB1	2:B:110:PRO:HD2	1.79	0.65
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.78	0.65
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.77	0.65
7:G:614:GLY:O	16:W:129:HIS:HE1	1.80	0.65
8:H:92:PRO:HG3	8:H:255:TYR:CG	2.32	0.65
8:H:303:TRP:HE3	20:b:29:ALA:HB2	1.61	0.65
11:Q:75:ARG:HH22	11:Q:104:ARG:HG3	1.61	0.65
1:A:17:LEU:HD13	8:H:225:MET:HE1	1.78	0.65
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.27	0.65
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.65
8:H:198:PHE:HD1	8:H:285:LEU:HD13	1.61	0.65
8:H:311:THR:HG22	18:Z:51:MET:HG3	1.79	0.65
2:B:126:ARG:NH2	8:H:63:PRO:HB3	2.12	0.64
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.64
8:H:90:PRO:CG	8:H:240:ILE:HD13	2.27	0.64
3:C:152:ILE:HD12	3:C:153:ASP:O	1.97	0.64
4:D:259:GLU:CG	18:Z:25:LEU:HD11	2.27	0.64
4:D:136:PHE:HA	4:D:139:LEU:HD12	1.80	0.64
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.62	0.64
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.80	0.64
2:B:169:GLY:C	2:B:171:TYR:N	2.51	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
7:G:572:HIS:HB2	7:G:699:SER:OG	1.97	0.64
22:r:68:ILE:HG13	22:r:68:ILE:O	1.97	0.64
4:D:113:ILE:HG21	4:D:432:LEU:CD2	2.27	0.64
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.79	0.64
8:H:98:LEU:HD21	24:H:401:3PE:H2	1.78	0.64
10:P:114:ASP:HA	10:P:117:ARG:HB2	1.80	0.64
17:X:133:THR:HG21	17:X:135:ARG:CZ	2.26	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
7:G:401:LEU:HD21	7:G:432:ILE:CD1	2.28	0.64
18:Z:59:ARG:HG2	20:b:81:LEU:HG	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.33	0.64
8:H:145:THR:O	8:H:149:ILE:HG12	1.97	0.64
2:B:92:PRO:CB	2:B:122:ARG:HH12	2.11	0.64
2:B:138:THR:HG21	4:D:116:LEU:HA	1.80	0.64
3:C:124:ARG:HD2	3:C:148:GLU:OE2	1.98	0.64
4:D:266:ARG:HH22	9:I:63:TRP:HA	1.62	0.64
5:E:176:LEU:HB2	5:E:184:MET:HE1	1.80	0.64
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.80	0.64
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.64
1:A:24:LEU:CD1	27:B:304:PC1:H3B2	2.28	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
7:G:571:HIS:CD2	7:G:572:HIS:HD2	2.11	0.64
12:R:36:GLN:NE2	21:q:127:TYR:HB3	2.13	0.64
3:C:63:TYR:CE2	3:C:67:ILE:HD11	2.33	0.64
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.77	0.64
6:F:224:ARG:NH1	11:Q:164:PHE:CD1	2.66	0.64
6:F:388:GLY:HA3	6:F:419:ILE:HD11	1.80	0.64
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.13	0.64
8:H:307:LEU:HD23	8:H:310:PHE:CZ	2.33	0.64
13:S:44:LEU:HD11	13:S:95:LEU:CD2	2.28	0.64
14:T:106:LYS:HD2	14:T:106:LYS:N	2.13	0.64
15:V:8:THR:HG23	15:V:8:THR:O	1.97	0.64
1:A:23:TRP:CZ3	1:A:24:LEU:HD23	2.33	0.63
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.80	0.63
13:S:63:PRO:HB2	13:S:79:LEU:HD12	1.80	0.63
34:a:101:CDL:H521	21:q:3:LEU:HD13	1.80	0.63
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.80	0.63
5:E:230:LEU:HD21	6:F:48:ARG:NE	2.13	0.63
6:F:174:ARG:HB2	23:s:87:LEU:HD11	1.80	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
4:D:116:LEU:HG	4:D:116:LEU:O	1.97	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
10:P:227:PRO:HB2	10:P:298:TYR:CZ	2.33	0.63
17:X:83:THR:O	17:X:87:THR:OG1	2.10	0.63
1:A:32:GLU:OE2	1:A:35:ASN:HB2	1.98	0.63
4:D:137:ASP:OD2	4:D:223:HIS:HB3	1.98	0.63
5:E:230:LEU:HD21	6:F:48:ARG:HE	1.63	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
7:G:449:PRO:HG3	7:G:483:ARG:HH22	1.62	0.63
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.80	0.63
17:X:7:LEU:CD2	18:Z:87:LEU:CD1	2.77	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:6:ARG:HA	22:r:9:GLN:HG2	1.81	0.63
2:B:108:ALA:HA	2:B:114:MET:HG2	1.80	0.63
6:F:35:LEU:HD23	6:F:40:ARG:HG2	1.81	0.63
7:G:126:LEU:HD23	7:G:126:LEU:H	1.64	0.63
7:G:130:ILE:CA	9:I:140:ARG:HH12	2.01	0.63
8:H:95:LEU:HG	8:H:96:ILE:HG23	1.80	0.63
20:b:65:ASP:O	20:b:66:VAL:C	2.41	0.63
4:D:217:VAL:HG11	4:D:240:LEU:CD2	2.29	0.63
4:D:315:GLU:HB3	4:D:346:GLN:HE22	1.62	0.63
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.63
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.33	0.63
10:P:335:LEU:HB3	10:P:340:VAL:HB	1.81	0.63
23:s:87:LEU:HA	23:s:90:PHE:HD2	1.64	0.63
1:A:18:ILE:HD11	8:H:76:THR:HG23	1.73	0.63
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.63	0.63
10:P:207:PHE:CE2	10:P:241:TYR:HD1	2.17	0.63
17:X:142:TYR:HB3	18:Z:115:ARG:HH21	1.62	0.63
1:A:52:SER:OG	1:A:55:PHE:CD2	2.52	0.63
2:B:137:LEU:HD22	2:B:145:LEU:CD2	2.29	0.63
3:C:189:ASP:OD1	3:C:190:TYR:N	2.32	0.63
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.81	0.63
4:D:386:THR:HG23	9:I:118:LEU:HD13	1.81	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.63
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.29	0.63
8:H:70:LEU:HA	8:H:73:ILE:HG22	1.79	0.63
14:T:102:SER:O	14:T:141:PRO:HD3	1.98	0.63
19:a:4:GLU:O	19:a:7:PRO:HD2	1.99	0.63
5:E:183:PRO:HB2	5:E:195:LEU:N	2.14	0.62
22:r:5:THR:HG22	22:r:7:VAL:HG12	1.81	0.62
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.98	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
8:H:189:THR:HB	8:H:234:MET:HB3	1.80	0.62
10:P:169:HIS:H	10:P:184:LYS:HE3	1.64	0.62
11:Q:59:LEU:N	11:Q:59:LEU:HD12	2.15	0.62
17:X:31:HIS:HB2	17:X:70:PHE:HZ	1.64	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.28	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
13:S:20:ARG:HG2	13:S:66:TRP:HB2	1.81	0.62
2:B:106:HIS:CE1	4:D:211:PHE:HE2	2.17	0.62
4:D:376:GLU:OE1	7:G:151:SER:HB2	1.99	0.62
6:F:254:ILE:HA	6:F:262:PHE:CE1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.29	0.62
11:Q:82:PRO:HD3	11:Q:98:LYS:HG3	1.81	0.62
19:a:52:ARG:HG3	19:a:57:VAL:C	2.23	0.62
3:C:126:GLU:OE2	3:C:143:LYS:HD3	1.99	0.62
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
7:G:136:GLU:HG2	11:Q:85:ASN:HD21	1.64	0.62
7:G:176:CYS:SG	25:G:802:SF4:FE4	1.78	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.62
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.62
10:P:244:ASP:HB3	10:P:335:LEU:HD13	1.82	0.62
10:P:266:THR:HG21	10:P:329:PRO:CB	2.29	0.62
10:P:276:LEU:HD23	10:P:280:ILE:CD1	2.30	0.62
17:X:86:TRP:CZ2	19:a:64:LYS:HA	2.34	0.62
20:b:78:LEU:HD22	20:b:80:TRP:NE1	2.10	0.62
2:B:81:LEU:HG	8:H:53:MET:SD	2.39	0.62
6:F:228:PRO:HG2	11:Q:160:TYR:CD2	2.31	0.62
7:G:388:ASN:H	7:G:514:ASN:HB2	1.65	0.62
7:G:652:ASN:C	7:G:652:ASN:OD1	2.42	0.62
15:V:27:LEU:O	15:V:31:THR:HG23	2.00	0.62
17:X:7:LEU:HD13	18:Z:87:LEU:HD12	1.81	0.62
4:D:250:ASN:HA	22:r:23:LYS:HD3	1.82	0.62
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.82	0.62
17:X:8:PRO:HD2	18:Z:84:LEU:HD11	1.81	0.62
2:B:97:LEU:HA	4:D:94:VAL:HG22	1.80	0.62
3:C:103:THR:HG21	15:V:55:LYS:CE	2.28	0.62
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.62
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.62
9:I:51:LYS:HA	18:Z:33:TYR:CE2	2.35	0.62
10:P:297:VAL:O	10:P:301:ILE:HG12	2.00	0.62
10:P:363:SER:HB3	16:W:51:HIS:CE1	2.35	0.62
2:B:184:ILE:HG22	2:B:185:VAL:HG13	1.82	0.62
2:B:207:GLN:HG3	2:B:210:ARG:HH21	1.65	0.62
3:C:186:ILE:HG23	3:C:187:LEU:N	2.14	0.62
8:H:260:MET:CE	19:a:13:GLY:C	2.70	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
4:D:202:TRP:CD2	9:I:76:TYR:HE2	2.18	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
10:P:263:PHE:HD1	10:P:333:PRO:HB2	1.65	0.62
16:W:104:THR:O	16:W:108:ARG:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:MET:HB3	4:D:101:LEU:HB2	1.82	0.61
4:D:259:GLU:CB	18:Z:25:LEU:HD11	2.30	0.61
7:G:306:MET:HG2	7:G:316:TYR:HA	1.82	0.61
13:S:22:HIS:O	13:S:58:CYS:SG	2.58	0.61
22:r:9:GLN:HA	22:r:12:ARG:HG2	1.80	0.61
2:B:171:TYR:CE1	4:D:135:TYR:CE1	2.88	0.61
4:D:217:VAL:CG1	4:D:240:LEU:CD2	2.74	0.61
5:E:71:GLU:OE1	23:s:96:SER:HB3	2.00	0.61
5:E:222:PHE:H	5:E:225:GLU:CD	2.08	0.61
12:R:98:GLU:CD	12:R:98:GLU:H	2.07	0.61
15:V:9:THR:HG21	15:V:78:GLU:HB2	1.81	0.61
3:C:120:THR:HG21	15:V:116:ILE:CG2	2.22	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.30	0.61
11:Q:69:GLU:HA	11:Q:72:ILE:HG22	1.82	0.61
2:B:175:TYR:OH	4:D:117:HIS:HE1	1.83	0.61
3:C:63:TYR:CE2	3:C:67:ILE:CD1	2.83	0.61
4:D:84:PHE:HZ	4:D:90:ALA:HB3	1.65	0.61
7:G:473:MET:CE	7:G:514:ASN:HD21	2.12	0.61
8:H:288:LEU:HG	8:H:293:PHE:CE1	2.35	0.61
17:X:46:CYS:HB2	17:X:135:ARG:CZ	2.29	0.61
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.82	0.61
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.61
10:P:320:GLU:O	10:P:324:ILE:HG22	2.00	0.61
18:Z:82:ARG:HD2	19:a:53:ARG:NH1	2.16	0.61
1:A:80:GLN:C	20:b:46:ASN:ND2	2.53	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
8:H:90:PRO:CG	8:H:240:ILE:HG21	2.30	0.61
10:P:321:ARG:O	10:P:325:SER:HB3	2.01	0.61
13:S:42:VAL:CG1	13:S:43:GLU:OE2	2.48	0.61
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.30	0.61
4:D:220:ALA:CB	9:I:98:ARG:HH21	2.14	0.61
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	0.61
16:W:58:THR:HG23	16:W:61:GLN:H	1.65	0.61
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.35	0.61
1:A:13:LEU:HD21	8:H:14:LEU:HD11	1.82	0.61
3:C:73:GLN:HG2	15:V:103:LEU:HD21	1.83	0.61
3:C:195:HIS:HE1	16:W:88:LYS:NZ	1.99	0.61
4:D:86:PRO:HA	4:D:95:LEU:O	2.00	0.61
4:D:360:ASP:OD1	4:D:360:ASP:C	2.37	0.61
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	0.61
7:G:614:GLY:O	16:W:129:HIS:CE1	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:90:PRO:HD2	8:H:240:ILE:HD13	1.81	0.61
23:s:92:LEU:CB	23:s:93:PRO:HD2	2.23	0.61
2:B:97:LEU:CD1	4:D:94:VAL:HG13	2.25	0.61
3:C:223:VAL:HG23	3:C:225:LEU:CD1	2.26	0.61
5:E:243:GLY:O	6:F:257:ARG:HG3	2.00	0.61
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.61
8:H:138:GLN:NE2	8:H:191:ALA:O	2.31	0.61
8:H:190:LEU:HD13	8:H:270:PHE:CD1	2.36	0.61
21:q:68:MET:HG3	21:q:71:LYS:HB2	1.83	0.61
3:C:84:GLU:HG2	3:C:141:ARG:HD2	1.83	0.61
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.61
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.61
10:P:235:THR:HG21	10:P:323:HIS:O	2.00	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
10:P:209:ARG:O	10:P:210:GLU:HG2	2.00	0.60
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.83	0.60
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.60
5:E:136:THR:HB	28:E:301:FES:S2	2.41	0.60
5:E:142:ARG:HG2	5:E:183:PRO:HD3	1.83	0.60
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.60
8:H:45:ILE:HD11	19:a:11:ILE:CD1	2.27	0.60
10:P:97:MET:O	10:P:103:LEU:HD11	2.00	0.60
14:T:92:LYS:HE3	16:W:67:ARG:NH1	2.16	0.60
20:b:63:MET:HB2	20:b:66:VAL:HG12	1.83	0.60
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.60
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.82	0.60
10:P:228:LEU:HD13	10:P:232:GLY:HA3	1.82	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
9:I:189:LYS:HG3	9:I:189:LYS:O	2.02	0.60
18:Z:125:TYR:HA	18:Z:128:ARG:HD2	1.83	0.60
4:D:124:ILE:HG13	4:D:135:TYR:CD2	2.36	0.60
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.82	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.60
9:I:135:ARG:O	9:I:135:ARG:HG2	2.00	0.60
19:a:58:ASN:CB	19:a:60:TYR:CE1	2.84	0.60
1:A:52:SER:HB2	1:A:55:PHE:HD2	0.53	0.60
9:I:87:PRO:HG2	9:I:88:PHE:CD2	2.37	0.60
9:I:106:TYR:OH	12:R:88:HIS:HB3	2.01	0.60
10:P:236:VAL:HG21	10:P:270:ARG:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:O	1:A:4:TYR:N	2.35	0.60
7:G:382:ARG:O	7:G:383:SER:C	2.44	0.60
15:V:75:GLY:HA3	15:V:79:GLU:OE1	2.01	0.60
7:G:145:MET:O	22:r:61:ARG:NH2	2.35	0.60
7:G:375:GLU:O	7:G:675:VAL:HG21	2.02	0.60
13:S:18:GLU:CB	13:S:52:PRO:HB2	2.32	0.60
16:W:26:ARG:HB2	16:W:26:ARG:NH1	2.16	0.60
27:B:304:PC1:H3B1	8:H:57:MET:CE	2.32	0.60
3:C:208:GLU:CG	3:C:221:GLU:HG3	2.31	0.60
4:D:149:GLN:HE21	4:D:171:ARG:HB3	1.65	0.60
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.82	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
8:H:200:LEU:CD2	8:H:282:TYR:HA	2.31	0.60
12:R:47:ARG:HB2	21:q:125:VAL:CG1	2.31	0.60
12:R:84:GLY:O	12:R:85:ALA:HB3	2.02	0.60
23:s:89:LYS:NZ	23:s:90:PHE:CE2	2.62	0.60
4:D:137:ASP:OD2	4:D:223:HIS:CB	2.50	0.60
4:D:353:PRO:HA	18:Z:10:MET:HE1	1.84	0.60
5:E:223:CYS:SG	6:F:133:HIS:CE1	2.95	0.60
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.37	0.60
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.60
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.60
2:B:171:TYR:CE1	4:D:135:TYR:HE1	2.20	0.59
6:F:297:LYS:HB2	6:F:333:GLU:CB	2.31	0.59
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.67	0.59
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.59
9:I:93:LEU:HD11	9:I:173:PHE:CE2	2.37	0.59
20:b:69:HIS:CD2	20:b:70:PRO:HD2	2.36	0.59
4:D:238:LEU:CB	22:r:36:GLN:HG3	2.23	0.59
4:D:241:LEU:CB	18:Z:16:TYR:OH	2.48	0.59
5:E:147:ILE:HD11	5:E:195:LEU:HB2	1.84	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
6:F:225:LEU:HD22	7:G:93:ALA:HB3	1.84	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
10:P:292:PRO:O	10:P:293:LEU:CG	2.47	0.59
1:A:79:ILE:CG1	1:A:87:MET:HE1	2.31	0.59
2:B:153:PRO:HG3	8:H:58:LYS:HE3	1.83	0.59
2:B:167:GLY:H	2:B:180:GLY:HA2	1.67	0.59
6:F:224:ARG:HD3	11:Q:164:PHE:CZ	2.37	0.59
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.59
10:P:238:GLN:HG2	10:P:270:ARG:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:61:ILE:O	11:Q:65:THR:HG23	2.02	0.59
15:V:14:LEU:CD2	15:V:79:GLU:HG2	2.32	0.59
1:A:106:TRP:CH2	20:b:19:LEU:HD21	2.38	0.59
5:E:162:THR:CG2	5:E:166:LYS:HA	2.33	0.59
6:F:119:GLU:HB3	6:F:124:THR:CG2	2.32	0.59
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.65	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.37	0.59
4:D:81:THR:HG23	4:D:98:VAL:HG13	1.85	0.59
10:P:217:PHE:CB	10:P:280:ILE:HD13	2.33	0.59
4:D:222:MET:O	4:D:223:HIS:HB2	2.03	0.59
5:E:143:ASP:O	5:E:146:SER:HB3	2.02	0.59
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.84	0.59
7:G:310:GLU:OE1	7:G:313:LEU:HD21	2.01	0.59
8:H:307:LEU:HA	8:H:310:PHE:CE2	2.37	0.59
9:I:105:ARG:NH2	9:I:191:LEU:HD22	2.17	0.59
10:P:192:ARG:HH12	10:P:260:GLY:HA2	1.67	0.59
12:R:33:HIS:CD2	12:R:34:THR:HG23	2.37	0.59
19:a:55:SER:HB3	19:a:61:TYR:CD2	2.38	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.67	0.59
7:G:401:LEU:HD21	7:G:432:ILE:HD12	1.83	0.59
8:H:187:ILE:HG23	8:H:198:PHE:CZ	2.38	0.59
17:X:130:LYS:HB2	20:b:66:VAL:HG21	1.84	0.59
1:A:88:MET:HE1	8:H:309:ILE:HB	1.85	0.59
6:F:261:TRP:HE3	6:F:262:PHE:CD1	2.21	0.59
7:G:32:ILE:HG12	7:G:45:PRO:HG3	1.85	0.59
2:B:93:MET:O	2:B:93:MET:HG3	2.02	0.59
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.85	0.59
8:H:196:ALA:C	8:H:198:PHE:H	2.10	0.59
13:S:14:LEU:HB3	13:S:70:ALA:HB2	1.85	0.59
15:V:38:PHE:CE1	15:V:95:LEU:HB2	2.37	0.59
2:B:170:TYR:CE2	4:D:135:TYR:CE1	2.90	0.59
5:E:188:ASN:O	5:E:189:ASP:HB3	2.03	0.59
6:F:410:ASP:OD1	6:F:411:SER:N	2.36	0.59
7:G:126:LEU:CD2	7:G:157:LYS:HE3	2.33	0.59
7:G:182:CYS:HG	25:G:802:SF4:FE2	0.43	0.59
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.59
8:H:81:LEU:HD23	24:H:401:3PE:H391	1.85	0.59
9:I:38:TYR:CD2	9:I:41:LYS:HD3	2.38	0.59
10:P:302:GLY:HA2	10:P:305:PHE:HD2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.27	0.58
5:E:184:MET:HG3	5:E:192:TYR:O	2.03	0.58
7:G:136:GLU:HG2	11:Q:85:ASN:ND2	2.17	0.58
10:P:227:PRO:HB2	10:P:298:TYR:OH	2.01	0.58
1:A:23:TRP:CZ3	1:A:24:LEU:CD2	2.87	0.58
2:B:92:PRO:HG3	2:B:130:VAL:HG11	1.85	0.58
7:G:136:GLU:OE2	7:G:272:ARG:NH1	2.36	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.85	0.58
8:H:200:LEU:HD23	8:H:282:TYR:HD1	1.68	0.58
13:S:42:VAL:HG13	13:S:43:GLU:OE2	2.03	0.58
14:T:80:LYS:HG3	14:T:145:VAL:HG21	1.84	0.58
2:B:92:PRO:HG3	2:B:130:VAL:HG12	1.85	0.58
2:B:194:CYS:O	25:B:301:SF4:S3	2.61	0.58
4:D:144:MET:SD	4:D:223:HIS:N	2.74	0.58
4:D:232:VAL:HG22	4:D:356:ILE:HB	1.85	0.58
9:I:51:LYS:HA	18:Z:33:TYR:HE2	1.68	0.58
9:I:90:LYS:H	21:q:90:LEU:HD21	1.67	0.58
17:X:15:VAL:HG21	17:X:61:LYS:HG2	1.84	0.58
2:B:90:LEU:C	2:B:92:PRO:HD3	2.27	0.58
27:B:303:PC1:H112	21:q:75:TRP:HE3	1.68	0.58
4:D:253:LEU:HD22	22:r:23:LYS:HB2	1.85	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
6:F:379:CYS:SG	25:F:502:SF4:S1	3.02	0.58
11:Q:161:GLY:HA2	11:Q:164:PHE:CD2	2.38	0.58
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.63	0.58
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.10	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
8:H:157:ASN:C	8:H:157:ASN:OD1	2.47	0.58
8:H:196:ALA:CB	8:H:197:PRO:CD	2.81	0.58
8:H:287:HIS:HD2	8:H:291:LYS:HD2	1.67	0.58
10:P:170:LEU:O	10:P:171:ASN:OD1	2.21	0.58
13:S:42:VAL:CG1	13:S:43:GLU:CD	2.76	0.58
15:V:114:TRP:CD2	15:V:114:TRP:O	2.56	0.58
2:B:157:TYR:HB3	2:B:188:ASP:OD2	2.03	0.58
6:F:133:HIS:O	6:F:134:ASP:C	2.46	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
9:I:68:ARG:HH12	18:Z:28:ARG:HG2	1.69	0.58
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:230:LEU:HD21	6:F:48:ARG:NH2	2.19	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.16	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
10:P:236:VAL:HG22	10:P:270:ARG:HG2	1.85	0.58
1:A:64:LEU:O	1:A:68:GLU:HG3	2.03	0.58
2:B:106:HIS:CE1	4:D:211:PHE:CE2	2.91	0.58
5:E:134:CYS:SG	5:E:175:CYS:HA	2.43	0.58
5:E:189:ASP:OD1	6:F:163:TYR:HB3	2.04	0.58
8:H:90:PRO:HB3	8:H:162:LEU:HB3	1.85	0.58
10:P:209:ARG:CA	10:P:352:VAL:HG12	2.34	0.58
10:P:282:GLY:O	10:P:285:HIS:CE1	2.56	0.58
15:V:6:LYS:CG	15:V:16:VAL:HG23	2.34	0.58
19:a:18:ILE:N	19:a:19:PRO:HD3	2.19	0.58
4:D:202:TRP:CH2	4:D:261:MET:CE	2.86	0.58
6:F:184:LYS:HB3	23:s:92:LEU:CD2	2.33	0.58
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.58
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.58
17:X:9:THR:HB	17:X:12:GLU:HG3	1.86	0.58
2:B:81:LEU:HD21	8:H:53:MET:HE1	1.85	0.58
27:B:304:PC1:H3C1	8:H:53:MET:HG3	1.85	0.58
5:E:165:ASP:C	5:E:167:LEU:H	2.09	0.58
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.04	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
12:R:47:ARG:HG3	12:R:48:PHE:CD2	2.38	0.58
16:W:42:TRP:CZ2	33:W:201:EHZ:O1	2.57	0.58
2:B:126:ARG:HH21	8:H:63:PRO:HB3	1.69	0.57
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.67	0.57
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.86	0.57
8:H:305:ILE:O	8:H:308:PRO:HD2	2.04	0.57
9:I:113:CYS:SG	25:I:303:SF4:FE3	1.80	0.57
15:V:50:GLN:HE22	22:r:93:LYS:HA	1.69	0.57
8:H:158:GLY:HA3	8:H:315:PRO:HB2	1.86	0.57
11:Q:64:LEU:HD12	16:W:85:LEU:HD21	1.86	0.57
15:V:111:GLN:HG3	15:V:111:GLN:O	2.04	0.57
17:X:24:VAL:HG12	17:X:86:TRP:CG	2.39	0.57
21:q:88:ARG:HG2	21:q:94:THR:OG1	2.03	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.57
8:H:62:ARG:HD3	8:H:68:MET:SD	2.45	0.57
8:H:150:LEU:C	8:H:150:LEU:HD13	2.29	0.57
9:I:163:PRO:O	12:R:89:PRO:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:15:VAL:CG2	17:X:61:LYS:HG2	2.35	0.57
22:r:13:ASN:OD1	22:r:20:LEU:HB2	2.05	0.57
7:G:386:LEU:O	7:G:387:LEU:C	2.46	0.57
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.68	0.57
8:H:260:MET:CE	19:a:16:LEU:HB2	2.35	0.57
10:P:91:ILE:HD12	10:P:105:PHE:CD2	2.39	0.57
4:D:267:ILE:CG2	8:H:278:PRO:O	2.48	0.57
5:E:183:PRO:HB2	5:E:195:LEU:H	1.68	0.57
10:P:128:ASN:ND2	10:P:149:PRO:HB3	2.20	0.57
14:T:90:TYR:CE2	14:T:93:ILE:HG12	2.38	0.57
34:a:101:CDL:HB61	21:q:6:VAL:HG21	1.86	0.57
21:q:60:ARG:HH12	21:q:95:ASP:CA	2.15	0.57
2:B:81:LEU:HD11	8:H:53:MET:SD	2.45	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.68	0.57
7:G:372:PHE:H	7:G:532:PRO:HB2	1.69	0.57
14:T:104:PHE:HE2	14:T:144:ILE:HD11	1.69	0.57
2:B:199:GLU:HB2	9:I:173:PHE:CE1	2.40	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.40	0.57
10:P:293:LEU:HB2	10:P:298:TYR:OH	2.05	0.57
13:S:42:VAL:O	13:S:46:LYS:HG3	2.04	0.57
18:Z:101:VAL:HB	18:Z:102:PRO:CD	2.33	0.57
4:D:192:LEU:HD11	4:D:200:PHE:HB3	1.85	0.57
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.57
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.87	0.57
9:I:180:HIS:CD2	10:P:100:LEU:CD2	2.87	0.57
11:Q:163:ASN:OD1	11:Q:164:PHE:CD1	2.58	0.57
3:C:45:THR:HG22	4:D:358:VAL:HG23	1.87	0.57
4:D:267:ILE:HG22	8:H:278:PRO:CG	2.22	0.57
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.70	0.57
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.57
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.87	0.57
9:I:36:TYR:HD2	22:r:104:TRP:HB2	1.70	0.57
10:P:169:HIS:ND1	31:P:401:NDP:H5N	2.20	0.57
21:q:68:MET:O	21:q:71:LYS:HB2	2.05	0.57
1:A:1:MET:O	1:A:2:ASN:C	2.48	0.56
2:B:81:LEU:HD21	8:H:53:MET:CE	2.35	0.56
4:D:356:ILE:HD11	4:D:357:LYS:HE3	1.87	0.56
7:G:330:LEU:HD13	7:G:546:PHE:CZ	2.39	0.56
9:I:64:THR:HG21	18:Z:35:MET:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:249:ILE:O	10:P:253:THR:HG23	2.05	0.56
15:V:45:ARG:O	15:V:49:GLU:HB2	2.04	0.56
3:C:45:THR:OG1	22:r:57:ARG:HD2	2.04	0.56
3:C:184:ARG:NH2	4:D:110:ASP:OD2	2.38	0.56
4:D:137:ASP:OD1	4:D:137:ASP:C	2.48	0.56
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.56
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.84	0.56
9:I:79:ARG:HH21	22:r:20:LEU:HD13	1.69	0.56
13:S:44:LEU:HD12	13:S:48:HIS:CD2	2.40	0.56
15:V:81:ILE:O	15:V:82:LEU:C	2.48	0.56
17:X:20:VAL:HG23	17:X:25:LEU:HD12	1.83	0.56
17:X:130:LYS:HD2	20:b:59:ASP:OD1	2.05	0.56
23:s:76:ASN:O	23:s:79:THR:HG22	2.05	0.56
1:A:75:LEU:HD13	8:H:305:ILE:HD11	1.86	0.56
4:D:90:ALA:HB2	8:H:205:SER:O	2.05	0.56
4:D:235:ASP:HA	4:D:356:ILE:HG21	1.86	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
7:G:330:LEU:HA	7:G:544:MET:HE1	1.86	0.56
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.17	0.56
12:R:38:TYR:HE1	12:R:44:ARG:HE	1.53	0.56
17:X:8:PRO:HG2	18:Z:84:LEU:HD21	1.88	0.56
19:a:37:ARG:HH11	19:a:59:ARG:HD2	1.70	0.56
3:C:210:ARG:NH2	10:P:75:ARG:HD3	2.21	0.56
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
10:P:258:ALA:O	10:P:261:LYS:HB2	2.05	0.56
10:P:271:TYR:HA	10:P:375:VAL:HG22	1.86	0.56
4:D:158:LEU:HD12	4:D:411:LEU:HD23	1.87	0.56
4:D:375:MET:HE1	7:G:126:LEU:HA	1.86	0.56
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.56
10:P:88:VAL:HA	10:P:91:ILE:HG12	1.86	0.56
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.56
9:I:90:LYS:HE2	21:q:79:GLY:O	2.06	0.56
11:Q:62:THR:HB	11:Q:72:ILE:HD11	1.88	0.56
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.40	0.56
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.56
23:s:84:ASN:OD1	23:s:85:LEU:N	2.38	0.56
2:B:77:LYS:HE3	27:B:303:PC1:H271	1.88	0.56
2:B:168:GLY:HA3	2:B:172:HIS:HD2	1.71	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
10:P:54:VAL:O	10:P:54:VAL:HG23	2.05	0.56
10:P:96:LEU:C	10:P:96:LEU:CD1	2.72	0.56
20:b:69:HIS:HB3	20:b:72:ASP:OD1	2.06	0.56
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.56
7:G:652:ASN:OD1	7:G:652:ASN:O	2.23	0.56
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.41	0.56
10:P:192:ARG:HE	10:P:200:ILE:HD12	1.70	0.56
12:R:33:HIS:HD2	12:R:34:THR:HG23	1.70	0.56
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.56
20:b:11:ASN:OD1	20:b:12:ALA:N	2.39	0.56
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.35	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
8:H:87:VAL:HG23	8:H:96:ILE:HD11	1.88	0.56
12:R:69:VAL:CG1	12:R:112:LYS:HB2	2.35	0.56
18:Z:129:THR:HG22	18:Z:131:GLU:H	1.70	0.56
2:B:224:ARG:HD3	10:P:85:ARG:HH12	1.70	0.56
3:C:67:ILE:HA	15:V:43:ALA:HB3	1.87	0.56
3:C:184:ARG:HH22	4:D:112:HIS:CD2	2.24	0.56
5:E:131:ILE:HD11	5:E:185:VAL:CB	2.24	0.56
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56
12:R:69:VAL:HG12	12:R:112:LYS:N	2.21	0.56
21:q:142:THR:HG1	21:q:143:PRO:HD2	1.68	0.56
2:B:81:LEU:HA	27:B:303:PC1:H242	1.88	0.55
5:E:91:TRP:CE3	5:E:125:PRO:HB3	2.41	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55
9:I:68:ARG:NH2	18:Z:26:PRO:O	2.39	0.55
12:R:35:GLY:O	12:R:36:GLN:HB3	2.05	0.55
6:F:42:PHE:HD2	6:F:275:LEU:HD11	1.70	0.55
8:H:102:ILE:CG2	8:H:150:LEU:HD11	2.35	0.55
11:Q:126:LEU:HD13	11:Q:137:PHE:CE2	2.40	0.55
17:X:20:VAL:CG2	17:X:25:LEU:HD11	2.33	0.55
1:A:49:LEU:HD23	4:D:80:MET:SD	2.46	0.55
2:B:94:THR:N	26:B:302:UQ1:H113	2.16	0.55
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.87	0.55
7:G:545:LEU:HD21	7:G:547:LEU:HD21	1.88	0.55
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.55
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.48	0.55
13:S:55:ILE:O	13:S:55:ILE:HG13	2.05	0.55
19:a:40:ARG:HG2	19:a:41:VAL:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:TYR:HE2	4:D:135:TYR:CE1	2.24	0.55
3:C:104:ASN:O	22:r:97:PRO:HD3	2.06	0.55
4:D:181:LEU:CD1	4:D:210:MET:CE	2.84	0.55
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.40	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
7:G:289:LYS:NZ	7:G:697:THR:OG1	2.36	0.55
7:G:400:VAL:HG22	7:G:473:MET:HG2	1.87	0.55
8:H:150:LEU:O	8:H:154:LEU:HG	2.07	0.55
8:H:161:SER:HB2	8:H:164:THR:HG23	1.87	0.55
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.87	0.55
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.21	0.55
18:Z:89:GLU:O	18:Z:93:GLU:HG2	2.06	0.55
18:Z:97:ILE:HG13	18:Z:98:MET:H	1.71	0.55
24:A:201:3PE:H272	20:b:23:PHE:CD2	2.41	0.55
3:C:120:THR:CG2	3:C:121:ARG:N	2.68	0.55
4:D:380:HIS:O	4:D:384:LEU:HG	2.07	0.55
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.18	0.55
20:b:69:HIS:CG	20:b:70:PRO:HD2	2.41	0.55
1:A:6:VAL:HG11	8:H:87:VAL:CG1	2.36	0.55
4:D:123:LEU:HB3	4:D:135:TYR:OH	2.07	0.55
4:D:163:PRO:HG2	4:D:168:GLN:HE21	1.71	0.55
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.42	0.55
6:F:77:LEU:O	6:F:81:LYS:HG2	2.06	0.55
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.55
8:H:68:MET:O	8:H:72:ILE:HG12	2.06	0.55
15:V:22:GLU:O	15:V:23:ARG:C	2.50	0.55
15:V:33:ASP:O	15:V:36:LYS:N	2.34	0.55
16:W:42:TRP:CE2	16:W:93:LEU:HG	2.41	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
8:H:181:MET:HE3	8:H:300:LEU:HD13	1.89	0.55
9:I:180:HIS:NE2	10:P:100:LEU:HD21	2.21	0.55
10:P:91:ILE:HD12	10:P:105:PHE:HD2	1.70	0.55
10:P:206:ILE:HG13	31:P:401:NDP:H42N	1.89	0.55
19:a:58:ASN:HB3	19:a:60:TYR:CE1	2.39	0.55
1:A:5:THR:O	1:A:9:ILE:HG12	2.07	0.55
4:D:171:ARG:HG2	4:D:227:ILE:HD12	1.88	0.55
5:E:130:HIS:NE2	5:E:132:GLN:HG2	2.21	0.55
6:F:300:ILE:HD11	6:F:311:TRP:HD1	1.72	0.55
7:G:304:GLU:HG3	7:G:305:PRO:HD2	1.89	0.55
8:H:157:ASN:OD1	8:H:158:GLY:N	2.40	0.55
10:P:232:GLY:HA2	10:P:273:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:LEU:CD2	2:B:141:MET:HG2	2.36	0.55
2:B:117:PHE:HZ	9:I:86:TYR:HB3	1.72	0.55
4:D:140:ASP:H	4:D:147:ASN:ND2	2.05	0.55
4:D:386:THR:CG2	9:I:118:LEU:CD1	2.85	0.55
6:F:48:ARG:HG2	6:F:48:ARG:O	2.06	0.55
7:G:377:ALA:HB3	7:G:384:ASN:ND2	2.19	0.55
10:P:272:LEU:HG	10:P:375:VAL:HG11	1.88	0.55
13:S:51:LEU:O	13:S:53:ILE:HG13	2.07	0.55
4:D:451:ILE:CG2	4:D:456:ILE:HD11	2.33	0.55
6:F:299:LEU:CD1	6:F:300:ILE:HG23	2.37	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
7:G:388:ASN:N	7:G:514:ASN:HB2	2.22	0.55
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.88	0.55
9:I:68:ARG:NH1	18:Z:28:ARG:HG2	2.22	0.55
9:I:211:TYR:CE1	22:r:39:PRO:HG3	2.41	0.55
17:X:64:ASN:OD1	17:X:64:ASN:O	2.25	0.55
4:D:80:MET:SD	4:D:101:LEU:HD12	2.46	0.54
4:D:174:PHE:CZ	4:D:240:LEU:HD21	2.43	0.54
4:D:202:TRP:CH2	4:D:261:MET:HE3	2.42	0.54
4:D:301:ASP:O	4:D:302:LEU:HB2	2.05	0.54
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.89	0.54
5:E:226:PRO:HD3	6:F:46:TYR:CE2	2.42	0.54
6:F:119:GLU:HG3	6:F:127:ASP:OD2	2.07	0.54
8:H:264:LEU:O	8:H:268:SER:N	2.37	0.54
12:R:44:ARG:HB3	12:R:47:ARG:NH1	2.22	0.54
2:B:175:TYR:OH	3:C:197:PHE:CE1	2.60	0.54
4:D:97:LEU:CD1	4:D:109:CYS:HB3	2.35	0.54
4:D:232:VAL:CG2	4:D:356:ILE:HB	2.37	0.54
10:P:304:LEU:H	10:P:304:LEU:HD12	1.71	0.54
13:S:51:LEU:O	13:S:52:PRO:C	2.48	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.07	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
8:H:90:PRO:CD	8:H:240:ILE:HD13	2.38	0.54
8:H:92:PRO:HG2	8:H:255:TYR:HB3	1.88	0.54
8:H:196:ALA:O	8:H:197:PRO:C	2.41	0.54
1:A:3:LEU:CD2	24:H:401:3PE:H31	2.35	0.54
2:B:84:TRP:CZ3	27:B:303:PC1:H371	2.42	0.54
2:B:107:MET:CE	2:B:114:MET:HE2	2.37	0.54
3:C:160:ILE:CD1	4:D:285:ASN:HD22	2.19	0.54
3:C:219:VAL:HG11	16:W:113:THR:CG2	2.37	0.54
4:D:411:LEU:HD11	4:D:419:PRO:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:167:SER:CB	23:s:75:TYR:CE2	2.91	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.40	0.54
7:G:330:LEU:HD13	7:G:546:PHE:HZ	1.71	0.54
7:G:629:ILE:CD1	16:W:122:LEU:HD21	2.37	0.54
8:H:197:PRO:HD2	8:H:198:PHE:CD2	2.42	0.54
2:B:81:LEU:CG	8:H:53:MET:SD	2.95	0.54
6:F:35:LEU:HB2	6:F:291:GLU:HB2	1.89	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
8:H:197:PRO:HD3	8:H:273:ILE:CG2	2.36	0.54
13:S:16:LEU:HD21	13:S:19:ILE:HD11	1.89	0.54
13:S:26:ARG:HA	13:S:34:ARG:NH1	2.23	0.54
13:S:44:LEU:HD22	13:S:91:MET:HG2	1.89	0.54
17:X:41:LYS:CB	17:X:131:VAL:HG11	2.38	0.54
18:Z:58:ARG:HG2	20:b:45:ILE:CD1	2.38	0.54
5:E:151:LEU:CD1	5:E:200:ILE:HD13	2.37	0.54
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.89	0.54
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.54
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
9:I:143:THR:HA	12:R:34:THR:HG21	1.89	0.54
16:W:27:ASP:HB2	16:W:30:GLU:HG3	1.89	0.54
17:X:9:THR:HG22	17:X:11:GLU:H	1.72	0.54
2:B:175:TYR:OH	4:D:117:HIS:CE1	2.61	0.54
4:D:159:LEU:HD21	4:D:391:VAL:HG12	1.90	0.54
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
7:G:557:ARG:HD3	21:q:144:TYR:CD2	2.43	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
8:H:157:ASN:ND2	8:H:165:LEU:CD1	2.71	0.54
11:Q:53:ILE:HG12	16:W:26:ARG:O	2.08	0.54
12:R:40:GLU:HA	12:R:45:ARG:HH11	1.72	0.54
2:B:171:TYR:HE1	4:D:120:THR:HG1	1.54	0.54
2:B:194:CYS:HB3	2:B:195:PRO:CD	2.33	0.54
4:D:133:LEU:HB3	4:D:134:PRO:HD3	1.88	0.54
4:D:255:ILE:HG22	4:D:338:ARG:NH2	2.22	0.54
5:E:87:ARG:HD2	23:s:77:THR:HB	1.89	0.54
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
8:H:68:MET:O	8:H:69:SER:C	2.49	0.54
10:P:302:GLY:O	10:P:303:LYS:C	2.50	0.54
13:S:63:PRO:HB2	13:S:79:LEU:CD1	2.37	0.54
4:D:311:TYR:HA	4:D:314:VAL:HG22	1.89	0.54
5:E:162:THR:HG22	5:E:166:LYS:HA	1.89	0.54
6:F:194:ASP:OD2	23:s:91:ARG:CB	2.55	0.54
7:G:179:CYS:HG	25:G:802:SF4:FE3	1.23	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
8:H:86:TRP:NE1	8:H:229:THR:HG22	2.20	0.54
8:H:317:TYR:O	8:H:318:MET:HB2	2.08	0.54
9:I:90:LYS:HD3	21:q:91:HIS:HE1	1.72	0.54
11:Q:81:VAL:O	11:Q:81:VAL:HG13	2.07	0.54
11:Q:161:GLY:HA2	11:Q:164:PHE:HD2	1.72	0.54
16:W:69:MET:C	16:W:71:MET:N	2.62	0.54
16:W:120:ASP:HB3	16:W:123:SER:OG	2.08	0.54
17:X:108:ASP:O	17:X:112:LEU:N	2.41	0.54
20:b:80:TRP:CG	20:b:81:LEU:N	2.76	0.54
1:A:87:MET:HG3	1:A:88:MET:N	2.23	0.54
1:A:92:PHE:CE1	8:H:302:MET:HG3	2.42	0.54
24:A:201:3PE:H361	20:b:23:PHE:CE1	2.43	0.54
2:B:219:LYS:HD2	2:B:223:ARG:CZ	2.38	0.54
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.43	0.54
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.54
8:H:93:HIS:HB2	19:a:24:ALA:HB2	1.90	0.54
9:I:72:MET:O	9:I:75:SER:OG	2.23	0.54
1:A:18:ILE:HD12	8:H:76:THR:HG21	1.86	0.53
3:C:70:LYS:HE3	3:C:71:TYR:CZ	2.43	0.53
6:F:80:MET:HE2	6:F:95:THR:HG21	1.89	0.53
6:F:388:GLY:CA	6:F:419:ILE:HD11	2.38	0.53
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.53
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.39	0.53
2:B:126:ARG:NH2	8:H:61:MET:SD	2.81	0.53
5:E:230:LEU:HD11	6:F:48:ARG:HH21	1.72	0.53
7:G:36:VAL:O	7:G:39:GLN:HG2	2.07	0.53
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.53
8:H:206:GLU:HG3	8:H:207:LEU:N	2.24	0.53
14:T:79:ILE:HD13	14:T:148:ILE:HG22	1.91	0.53
16:W:93:LEU:HD22	16:W:97:ILE:HG13	1.89	0.53
2:B:170:TYR:CE2	4:D:135:TYR:CE2	2.95	0.53
4:D:323:ARG:O	4:D:325:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:230:LEU:HD21	6:F:48:ARG:HH21	1.72	0.53
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.53
6:F:233:VAL:HG11	11:Q:164:PHE:HB2	1.90	0.53
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.53
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.53
7:G:541:PRO:HB2	7:G:561:PRO:CD	2.39	0.53
8:H:90:PRO:CB	8:H:162:LEU:HB3	2.37	0.53
8:H:181:MET:HE3	8:H:300:LEU:CD1	2.39	0.53
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.53
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.89	0.53
6:F:362:ASP:O	6:F:363:ILE:C	2.51	0.53
7:G:35:PHE:HB2	7:G:101:ASN:HA	1.90	0.53
8:H:245:PRO:HG2	8:H:255:TYR:CE2	2.44	0.53
10:P:122:HIS:CD2	12:R:45:ARG:HB2	2.43	0.53
10:P:366:ILE:O	10:P:369:THR:HG22	2.08	0.53
15:V:44:TYR:CE2	15:V:94:MET:HG3	2.44	0.53
20:b:27:GLY:O	20:b:28:LEU:C	2.51	0.53
4:D:390:GLN:HG3	4:D:415:GLY:O	2.09	0.53
6:F:166:ALA:HB1	23:s:80:PHE:CE1	2.44	0.53
6:F:382:CYS:SG	25:F:502:SF4:S4	3.06	0.53
8:H:261:MET:O	8:H:265:LEU:HD23	2.08	0.53
14:T:86:VAL:HG11	14:T:122:MET:SD	2.48	0.53
14:T:90:TYR:HD2	14:T:93:ILE:HB	1.73	0.53
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.09	0.53
7:G:243:TRP:NE1	9:I:121:ALA:HB2	2.23	0.53
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.53
9:I:54:THR:HA	20:b:13:TRP:NE1	2.24	0.53
9:I:57:ALA:HB2	20:b:13:TRP:O	2.09	0.53
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.90	0.53
10:P:143:ASP:O	10:P:148:ILE:HG12	2.09	0.53
2:B:170:TYR:CE2	4:D:135:TYR:CZ	2.97	0.53
26:B:302:UQ1:HM31	4:D:192:LEU:HB3	1.91	0.53
10:P:130:ILE:HD13	10:P:148:ILE:HG21	1.90	0.53
10:P:301:ILE:HG22	10:P:305:PHE:CE2	2.43	0.53
12:R:44:ARG:O	12:R:47:ARG:HG2	2.09	0.53
4:D:136:PHE:HZ	4:D:422:CYS:SG	2.31	0.53
5:E:165:ASP:C	5:E:167:LEU:N	2.64	0.53
7:G:382:ARG:HB3	7:G:386:LEU:HD12	1.89	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.09	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
10:P:48:ARG:NH2	10:P:98:GLY:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:76:MET:HE3	10:P:78:SER:OG	2.08	0.53
12:R:33:HIS:HB3	12:R:59:PHE:CD1	2.44	0.53
14:T:133:ILE:HG13	14:T:137:LYS:HZ2	1.73	0.53
15:V:35:LEU:CD1	15:V:48:THR:HG23	2.37	0.53
17:X:41:LYS:HB2	17:X:131:VAL:HG11	1.91	0.53
18:Z:24:ASN:O	18:Z:25:LEU:C	2.52	0.53
19:a:6:LEU:O	19:a:7:PRO:C	2.51	0.53
20:b:74:LEU:H	20:b:74:LEU:HD12	1.73	0.53
23:s:87:LEU:HB3	23:s:91:ARG:NH1	2.23	0.53
3:C:132:LEU:HD11	4:D:300:TRP:CZ2	2.44	0.53
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.53
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.53
9:I:210:LEU:HD12	22:r:39:PRO:CD	2.39	0.53
11:Q:79:ILE:H	11:Q:79:ILE:HD12	1.73	0.53
12:R:98:GLU:HA	12:R:113:GLN:CD	2.34	0.53
13:S:44:LEU:HD12	13:S:48:HIS:HD2	1.72	0.53
17:X:17:GLU:HA	17:X:64:ASN:HD21	1.74	0.53
17:X:57:LEU:HD11	18:Z:84:LEU:HD21	1.90	0.53
22:r:6:ARG:C	22:r:9:GLN:HG2	2.34	0.53
2:B:194:CYS:O	2:B:196:PRO:HD3	2.09	0.53
4:D:216:ARG:O	4:D:237:PRO:HG3	2.09	0.53
5:E:244:VAL:HG11	6:F:64:LYS:NZ	2.23	0.53
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.91	0.53
8:H:197:PRO:HB3	8:H:277:TYR:HB2	1.91	0.53
9:I:65:GLU:HG3	9:I:65:GLU:O	2.08	0.53
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.53
13:S:22:HIS:HB3	13:S:58:CYS:SG	2.48	0.53
16:W:130:ASP:O	16:W:130:ASP:OD1	2.26	0.53
17:X:13:LEU:O	17:X:15:VAL:HG23	2.08	0.53
17:X:18:VAL:HA	17:X:68:LEU:CD2	2.39	0.53
20:b:19:LEU:HB3	20:b:23:PHE:CE2	2.44	0.53
22:r:12:ARG:NH2	22:r:21:GLN:NE2	2.46	0.53
1:A:24:LEU:HD11	27:B:304:PC1:H3B2	1.91	0.52
4:D:154:ALA:HB2	4:D:398:THR:HG21	1.90	0.52
4:D:386:THR:HG23	9:I:118:LEU:CD1	2.39	0.52
5:E:143:ASP:HB3	5:E:146:SER:HB2	1.91	0.52
5:E:223:CYS:SG	6:F:133:HIS:NE2	2.81	0.52
5:E:230:LEU:HD21	6:F:48:ARG:CZ	2.40	0.52
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
7:G:364:ASP:C	7:G:364:ASP:OD1	2.51	0.52
8:H:288:LEU:HD21	24:I:301:3PE:H222	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:18:GLU:HB2	13:S:52:PRO:HB2	1.90	0.52
2:B:137:LEU:CD2	2:B:145:LEU:CD2	2.86	0.52
3:C:125:PHE:HZ	3:C:198:ARG:HE	1.56	0.52
4:D:259:GLU:CG	18:Z:25:LEU:CD1	2.87	0.52
4:D:266:ARG:NH1	9:I:66:LEU:HG	2.24	0.52
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.92	0.52
14:T:80:LYS:O	14:T:84:LEU:HG	2.08	0.52
16:W:31:ALA:O	16:W:34:ARG:N	2.40	0.52
17:X:54:ARG:HD3	18:Z:116:TRP:CZ3	2.44	0.52
22:r:6:ARG:HA	22:r:9:GLN:CD	2.34	0.52
1:A:79:ILE:HG12	1:A:87:MET:HE1	1.92	0.52
5:E:179:CYS:HA	28:E:301:FES:S1	2.49	0.52
6:F:126:LYS:HG3	6:F:275:LEU:CB	2.39	0.52
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.74	0.52
6:F:167:SER:HB3	23:s:75:TYR:CE2	2.43	0.52
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.75	0.52
7:G:67:GLU:HB3	11:Q:156:LYS:HD2	1.91	0.52
10:P:203:PRO:HG2	31:P:401:NDP:C5N	2.39	0.52
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.52
15:V:97:TRP:O	15:V:98:LYS:C	2.52	0.52
4:D:113:ILE:CG2	4:D:432:LEU:CD2	2.87	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
10:P:59:PHE:CD1	10:P:83:PRO:HG2	2.44	0.52
10:P:236:VAL:HG23	10:P:271:TYR:C	2.35	0.52
11:Q:111:LEU:HD12	12:R:47:ARG:HH21	1.75	0.52
17:X:133:THR:HG22	17:X:134:ASP:N	2.24	0.52
18:Z:50:MET:SD	18:Z:54:ASN:ND2	2.82	0.52
21:q:21:ARG:O	21:q:25:ARG:HG3	2.09	0.52
2:B:79:ASP:HA	2:B:82:ILE:HB	1.92	0.52
3:C:149:LEU:O	16:W:23:ILE:HD11	2.10	0.52
4:D:376:GLU:HG3	7:G:121:LEU:HD13	1.85	0.52
5:E:226:PRO:HG2	5:E:229:GLY:O	2.10	0.52
6:F:225:LEU:CD2	7:G:93:ALA:HB3	2.39	0.52
6:F:296:LEU:HD22	6:F:337:MET:CE	2.39	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
22:r:6:ARG:HA	22:r:9:GLN:CG	2.40	0.52
3:C:186:ILE:HG13	4:D:113:ILE:HD11	1.92	0.52
3:C:186:ILE:CG2	3:C:187:LEU:HG	2.23	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:238:CYS:O	6:F:239:PRO:C	2.50	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
7:G:313:LEU:O	7:G:313:LEU:HD12	2.10	0.52
7:G:557:ARG:CG	7:G:579:MET:HE3	2.38	0.52
1:A:57:LEU:O	1:A:58:VAL:C	2.52	0.52
1:A:106:TRP:NE1	24:A:201:3PE:H32	2.24	0.52
3:C:136:PHE:CE1	22:r:96:THR:HB	2.44	0.52
4:D:222:MET:HG2	4:D:223:HIS:CD2	2.44	0.52
4:D:358:VAL:O	4:D:364:SER:OG	2.25	0.52
5:E:198:LYS:O	5:E:201:GLU:HB3	2.10	0.52
7:G:35:PHE:CE1	7:G:40:SER:HB2	2.45	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
8:H:200:LEU:HD22	8:H:285:LEU:HD23	1.90	0.52
8:H:253:GLU:O	8:H:254:LEU:C	2.52	0.52
13:S:90:ALA:O	13:S:94:VAL:HG23	2.09	0.52
14:T:110:LEU:HD21	14:T:118:ILE:HD12	1.91	0.52
17:X:7:LEU:CD2	18:Z:87:LEU:HD11	2.38	0.52
21:q:4:VAL:HG23	21:q:5:GLU:OE2	2.10	0.52
2:B:92:PRO:CG	2:B:130:VAL:CG1	2.87	0.52
3:C:209:LEU:HD21	16:W:108:ARG:NH1	2.25	0.52
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.24	0.52
9:I:79:ARG:NH2	22:r:20:LEU:HD13	2.24	0.52
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.75	0.52
17:X:45:LEU:HD23	20:b:56:PRO:O	2.09	0.52
17:X:142:TYR:O	17:X:143:HIS:C	2.52	0.52
22:r:27:ARG:HD2	22:r:31:ILE:CG2	2.40	0.52
2:B:122:ARG:NH1	2:B:132:ILE:HD12	2.25	0.52
3:C:170:TRP:CD1	3:C:183:LEU:HD21	2.44	0.52
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.92	0.52
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.45	0.52
5:E:143:ASP:HB3	5:E:146:SER:CB	2.40	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
7:G:402:LEU:O	7:G:431:LEU:HA	2.09	0.52
12:R:69:VAL:HG11	12:R:112:LYS:HB2	1.92	0.52
2:B:98:ALA:HB1	2:B:100:CYS:H	1.74	0.52
2:B:124:SER:HB3	2:B:125:PRO:CD	2.39	0.52
3:C:230:ARG:NH1	9:I:128:ILE:O	2.43	0.52
4:D:254:ARG:HE	22:r:25:GLN:HB3	1.74	0.52
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.52
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:524:ALA:HB2	7:G:597:VAL:HG22	1.91	0.52
10:P:279:TYR:CD1	10:P:372:ALA:HB2	2.45	0.52
11:Q:55:VAL:HB	11:Q:57:GLU:OE2	2.10	0.52
14:T:102:SER:HB2	14:T:107:ASP:HB2	1.90	0.52
15:V:42:ALA:O	15:V:43:ALA:C	2.53	0.52
16:W:110:PHE:O	16:W:111:HIS:C	2.53	0.52
19:a:52:ARG:HH21	19:a:57:VAL:HG23	1.75	0.52
4:D:451:ILE:HG23	4:D:456:ILE:CD1	2.35	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
3:C:63:TYR:OH	3:C:102:HIS:HE1	1.93	0.51
4:D:270:ASN:HB3	8:H:284:GLN:NE2	2.25	0.51
4:D:321:GLY:HA3	4:D:328:ASP:OD1	2.09	0.51
6:F:64:LYS:H	6:F:256:ARG:HE	1.58	0.51
6:F:119:GLU:CD	29:F:501:FMN:HN3	2.18	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.46	0.51
7:G:391:ILE:HG22	7:G:417:ARG:HE	1.75	0.51
7:G:473:MET:HE3	7:G:514:ASN:ND2	2.22	0.51
7:G:617:ARG:NH1	16:W:129:HIS:HA	2.24	0.51
14:T:104:PHE:CB	14:T:110:LEU:HD22	2.39	0.51
18:Z:87:LEU:O	18:Z:91:LEU:HB2	2.10	0.51
2:B:92:PRO:CB	2:B:122:ARG:NH1	2.57	0.51
2:B:200:ALA:O	2:B:201:LEU:C	2.53	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.51
4:D:385:TYR:HB2	9:I:118:LEU:HD11	1.93	0.51
5:E:178:ALA:HB2	5:E:191:TYR:CE2	2.45	0.51
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
7:G:338:VAL:HG13	7:G:546:PHE:CE1	2.37	0.51
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.53	0.51
7:G:670:GLU:HB2	13:S:42:VAL:CG2	2.40	0.51
10:P:137:ARG:HG3	10:P:138:ASN:OD1	2.10	0.51
10:P:206:ILE:H	31:P:401:NDP:H71N	1.58	0.51
10:P:316:LYS:O	10:P:320:GLU:HG3	2.10	0.51
18:Z:97:ILE:HG13	18:Z:98:MET:N	2.25	0.51
4:D:97:LEU:HA	4:D:111:PRO:HA	1.92	0.51
6:F:194:ASP:OD1	23:s:91:ARG:HG2	2.10	0.51
8:H:148:ILE:HB	8:H:297:THR:CG2	2.41	0.51
9:I:105:ARG:NH2	12:R:56:ASN:ND2	2.58	0.51
21:q:26:VAL:HG11	21:q:32:ASP:O	2.10	0.51
2:B:94:THR:N	26:B:302:UQ1:C11	2.73	0.51
2:B:182:ASP:HA	2:B:187:VAL:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:ILE:CG2	3:C:187:LEU:N	2.73	0.51
6:F:167:SER:OG	23:s:75:TYR:CE2	2.63	0.51
6:F:382:CYS:HA	7:G:74:ASN:O	2.11	0.51
7:G:238:PHE:CE1	9:I:140:ARG:HD2	2.46	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
8:H:136:VAL:O	8:H:137:ALA:C	2.54	0.51
17:X:52:ASP:OD1	17:X:53:PRO:HD2	2.11	0.51
21:q:19:GLY:O	21:q:23:LEU:N	2.41	0.51
24:A:201:3PE:H361	20:b:23:PHE:CZ	2.46	0.51
2:B:189:ILE:HD12	2:B:207:GLN:HB3	1.93	0.51
3:C:92:VAL:O	3:C:96:LEU:HD13	2.11	0.51
6:F:296:LEU:CD1	6:F:337:MET:HE3	2.34	0.51
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.08	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.51
7:G:611:THR:HG21	11:Q:105:GLU:N	2.25	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:39:ILE:HG12	21:q:31:ASN:OD1	2.11	0.51
8:H:98:LEU:CD2	24:H:401:3PE:H2	2.41	0.51
11:Q:135:ILE:HD11	11:Q:147:VAL:HG21	1.91	0.51
11:Q:154:LYS:CB	11:Q:155:PRO:HD2	2.39	0.51
15:V:31:THR:HG22	15:V:88:LEU:HB2	1.92	0.51
16:W:95:GLU:HB3	16:W:101:LYS:HG3	1.93	0.51
17:X:53:PRO:HD2	18:Z:116:TRP:CG	2.46	0.51
4:D:181:LEU:HD11	4:D:210:MET:CG	2.41	0.51
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.51
9:I:64:THR:CG2	18:Z:35:MET:HE1	2.41	0.51
10:P:215:ASN:O	10:P:216:HIS:C	2.54	0.51
11:Q:112:MET:SD	21:q:126:PRO:HB3	2.51	0.51
11:Q:131:LYS:HG2	11:Q:135:ILE:HD11	1.89	0.51
13:S:24:CYS:HB2	13:S:30:SER:HB3	1.92	0.51
3:C:70:LYS:O	15:V:103:LEU:HD12	2.10	0.51
4:D:179:ARG:NH2	4:D:401:GLU:O	2.43	0.51
4:D:256:ASP:O	4:D:260:GLU:N	2.33	0.51
4:D:259:GLU:HG2	18:Z:25:LEU:CD1	2.41	0.51
7:G:304:GLU:HG3	7:G:615:LEU:HD12	1.93	0.51
7:G:382:ARG:NH2	7:G:386:LEU:HD11	2.25	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
8:H:14:LEU:HB3	30:H:400:UQ9:H23	1.92	0.51
8:H:43:TYR:CE1	19:a:4:GLU:HG2	2.45	0.51
3:C:190:TYR:HB3	16:W:101:LYS:HG2	1.92	0.51
5:E:39:VAL:HG11	7:G:163:LYS:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
10:P:154:GLN:O	10:P:158:GLU:HG3	2.10	0.51
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.51
17:X:46:CYS:HB2	17:X:135:ARG:NE	2.26	0.51
18:Z:134:SER:O	18:Z:138:PHE:N	2.40	0.51
4:D:137:ASP:CB	4:D:223:HIS:HA	2.41	0.51
4:D:140:ASP:H	4:D:147:ASN:HD21	1.59	0.51
5:E:62:ILE:HG21	5:E:103:VAL:HG11	1.93	0.51
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.51
5:E:176:LEU:HB2	5:E:184:MET:CE	2.41	0.51
6:F:109:ARG:NE	6:F:239:PRO:HD3	2.25	0.51
7:G:130:ILE:CA	9:I:140:ARG:HH11	2.10	0.51
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
7:G:376:GLY:C	7:G:378:GLY:N	2.64	0.51
11:Q:58:LYS:O	11:Q:59:LEU:HB2	2.10	0.51
19:a:45:TRP:O	19:a:46:TYR:C	2.54	0.51
27:B:304:PC1:H3B1	8:H:57:MET:HE2	1.92	0.50
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.25	0.50
4:D:271:ARG:NH1	8:H:279:ARG:O	2.43	0.50
4:D:323:ARG:O	4:D:324:GLY:C	2.52	0.50
4:D:348:LEU:O	18:Z:11:PRO:CG	2.44	0.50
5:E:140:MET:HE1	6:F:366:ALA:HA	1.92	0.50
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.50
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.50
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.50
8:H:90:PRO:HB3	8:H:162:LEU:CB	2.41	0.50
9:I:63:TRP:CZ3	24:I:301:3PE:H322	2.45	0.50
9:I:105:ARG:NH2	12:R:56:ASN:HD21	2.09	0.50
10:P:153:ALA:HB2	10:P:164:PHE:CE2	2.46	0.50
10:P:157:LYS:HD3	10:P:195:PHE:CE1	2.46	0.50
11:Q:53:ILE:HG23	16:W:20:VAL:HG23	1.94	0.50
20:b:41:TYR:CD1	20:b:84:LEU:HD11	2.46	0.50
4:D:105:MET:HA	4:D:443:MET:HA	1.92	0.50
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.50
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.69	0.50
8:H:91:MET:O	8:H:92:PRO:C	2.50	0.50
9:I:111:GLU:OE2	9:I:187:LYS:HE3	2.11	0.50
10:P:270:ARG:HB3	10:P:375:VAL:O	2.11	0.50
13:S:23:LEU:HD12	13:S:23:LEU:O	2.12	0.50
16:W:67:ARG:O	16:W:71:MET:HB2	2.11	0.50
17:X:32:TYR:HE1	17:X:67:ALA:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:119:PRO:HA	18:Z:123:GLU:OE2	2.12	0.50
23:s:84:ASN:OD1	23:s:84:ASN:C	2.53	0.50
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
6:F:391:TRP:HH2	7:G:118:GLU:OE2	1.93	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
7:G:382:ARG:HB3	7:G:386:LEU:CD1	2.41	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
10:P:45:LYS:O	10:P:50:SER:HB3	2.11	0.50
15:V:67:LYS:O	15:V:68:LEU:C	2.52	0.50
1:A:49:LEU:N	1:A:49:LEU:HD12	2.26	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.50
7:G:382:ARG:NH1	7:G:527:ASP:CG	2.69	0.50
8:H:181:MET:CE	8:H:300:LEU:HD12	2.42	0.50
9:I:200:GLU:HG2	21:q:88:ARG:HB2	1.93	0.50
14:T:104:PHE:CG	14:T:110:LEU:HD22	2.46	0.50
14:T:144:ILE:O	14:T:148:ILE:HG12	2.12	0.50
1:A:2:ASN:HB2	18:Z:143:TYR:CE1	2.44	0.50
2:B:92:PRO:CD	2:B:119:VAL:HG13	2.38	0.50
2:B:170:TYR:HE2	4:D:135:TYR:CE2	2.30	0.50
5:E:178:ALA:HB2	5:E:191:TYR:HE2	1.76	0.50
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	0.50
11:Q:62:THR:HB	11:Q:72:ILE:CD1	2.42	0.50
22:r:6:ARG:O	22:r:9:GLN:CG	2.60	0.50
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.50
5:E:233:LEU:HD23	6:F:43:THR:O	2.10	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
7:G:403:VAL:HG13	7:G:403:VAL:O	2.12	0.50
7:G:406:ASN:O	7:G:407:PRO:C	2.53	0.50
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.50
8:H:86:TRP:CZ2	8:H:233:LEU:HG	2.47	0.50
8:H:181:MET:CE	8:H:300:LEU:CD1	2.90	0.50
8:H:224:PHE:CE2	30:H:400:UQ9:H11	2.46	0.50
10:P:301:ILE:CG2	10:P:305:PHE:HE2	2.22	0.50
14:T:79:ILE:HG23	14:T:126:PHE:CE1	2.47	0.50
15:V:8:THR:O	15:V:8:THR:CG2	2.59	0.50
15:V:9:THR:HG21	15:V:78:GLU:CB	2.41	0.50
20:b:67:PRO:HB3	20:b:74:LEU:HB2	1.93	0.50
22:r:7:VAL:O	22:r:11:LEU:HG	2.11	0.50
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.46	0.50
4:D:333:ARG:HH12	4:D:453:THR:HA	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:371:MET:CE	9:I:163:PRO:HB3	2.41	0.50
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.76	0.50
6:F:225:LEU:HB3	6:F:227:PRO:CD	2.37	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
8:H:231:ILE:O	8:H:235:ASN:ND2	2.45	0.50
9:I:78:PHE:CD1	22:r:8:ILE:HG23	2.47	0.50
10:P:68:TYR:CD2	10:P:242:VAL:HG11	2.46	0.50
10:P:165:ILE:HG21	10:P:249:ILE:HG23	1.93	0.50
11:Q:85:ASN:O	11:Q:86:ASN:C	2.52	0.50
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.50
14:T:92:LYS:NZ	14:T:92:LYS:HB3	2.27	0.50
18:Z:86:ILE:HG21	18:Z:124:MET:O	2.11	0.50
18:Z:92:GLU:O	18:Z:95:ALA:N	2.45	0.50
19:a:52:ARG:HD2	19:a:57:VAL:HG22	1.94	0.50
3:C:96:LEU:HD22	3:C:155:ILE:HG21	1.94	0.50
4:D:462:ASP:O	4:D:463:ARG:C	2.54	0.50
5:E:214:LYS:HG3	5:E:214:LYS:O	2.11	0.50
9:I:203:ALA:HB2	21:q:88:ARG:HH11	1.76	0.50
10:P:209:ARG:HG2	10:P:352:VAL:HG12	1.93	0.50
10:P:228:LEU:HD22	10:P:273:LEU:HD21	1.93	0.50
14:T:130:ILE:HG23	14:T:134:ASP:OD2	2.12	0.50
23:s:87:LEU:HB2	23:s:91:ARG:HH12	1.76	0.50
4:D:123:LEU:CB	4:D:135:TYR:OH	2.60	0.50
4:D:399:ALA:HB1	4:D:406:GLU:HG3	1.93	0.50
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.93	0.50
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.47	0.50
10:P:140:ASP:C	10:P:142:GLU:N	2.68	0.50
17:X:76:SER:OG	17:X:77:HIS:N	2.45	0.50
19:a:50:ARG:CZ	19:a:54:ILE:HD11	2.42	0.50
1:A:52:SER:HG	1:A:55:PHE:HB2	1.74	0.49
2:B:97:LEU:O	2:B:135:GLY:HA3	2.10	0.49
4:D:256:ASP:CG	22:r:18:GLN:HE22	2.20	0.49
5:E:229:GLY:O	5:E:231:THR:HG23	2.12	0.49
6:F:227:PRO:HB3	7:G:95:PRO:HD3	1.94	0.49
8:H:85:LEU:HD21	8:H:108:THR:HB	1.94	0.49
15:V:95:LEU:O	15:V:95:LEU:HD23	2.12	0.49
17:X:49:GLU:CG	17:X:50:GLU:HG3	2.40	0.49
2:B:194:CYS:CB	2:B:195:PRO:HD3	2.36	0.49
2:B:222:TYR:HA	10:P:137:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:112:HIS:HE1	16:W:100:TRP:CD1	2.30	0.49
5:E:193:GLU:OE1	5:E:217:PRO:HG3	2.13	0.49
5:E:240:PRO:HB3	6:F:60:GLY:CA	2.41	0.49
6:F:40:ARG:HB3	6:F:289:GLU:CD	2.37	0.49
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.11	0.49
8:H:102:ILE:HG21	8:H:150:LEU:HD11	1.93	0.49
10:P:150:ARG:HE	10:P:190:GLU:HB3	1.78	0.49
10:P:223:PHE:CG	10:P:223:PHE:O	2.64	0.49
17:X:45:LEU:HG	17:X:131:VAL:HG23	1.94	0.49
21:q:66:THR:HG23	21:q:74:PHE:CD1	2.47	0.49
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.49
5:E:200:ILE:HG22	5:E:204:ILE:HG13	1.92	0.49
6:F:185:ASN:HA	6:F:189:SER:O	2.12	0.49
7:G:70:SER:O	7:G:184:ARG:NH1	2.45	0.49
7:G:181:ARG:HA	7:G:184:ARG:HH21	1.77	0.49
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.49
7:G:372:PHE:CZ	7:G:385:TYR:HB3	2.47	0.49
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.92	0.49
10:P:91:ILE:HG13	10:P:95:ARG:NH1	2.23	0.49
10:P:209:ARG:CG	10:P:352:VAL:HG12	2.43	0.49
14:T:84:LEU:HD22	14:T:98:LEU:CD2	2.42	0.49
16:W:49:THR:O	16:W:50:VAL:C	2.56	0.49
17:X:5:VAL:HG11	18:Z:109:SER:HB3	1.95	0.49
1:A:2:ASN:HB3	8:H:2:PHE:CZ	2.48	0.49
2:B:137:LEU:CD2	2:B:145:LEU:HD22	2.42	0.49
2:B:170:TYR:OH	4:D:135:TYR:CD2	2.64	0.49
6:F:42:PHE:HE1	6:F:137:LYS:HG2	1.76	0.49
6:F:296:LEU:HD23	6:F:332:CYS:HB3	1.95	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
14:T:90:TYR:HE2	14:T:93:ILE:HG12	1.77	0.49
14:T:115:GLN:O	14:T:119:ILE:HG12	2.12	0.49
14:T:134:ASP:HA	14:T:137:LYS:HZ3	1.76	0.49
18:Z:10:MET:HG3	18:Z:11:PRO:HD2	1.93	0.49
19:a:49:GLU:O	19:a:53:ARG:HG3	2.13	0.49
2:B:109:ALA:HB1	2:B:110:PRO:CD	2.41	0.49
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.49
5:E:73:HIS:ND1	6:F:236:PHE:CD1	2.81	0.49
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.41	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
8:H:151:LEU:O	8:H:152:SER:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:120:MET:HE1	16:W:43:TYR:CG	2.47	0.49
2:B:99:CYS:SG	25:B:301:SF4:S4	3.03	0.49
3:C:148:GLU:OE2	11:Q:140:LYS:NZ	2.30	0.49
3:C:234:LEU:O	3:C:234:LEU:CG	2.60	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
6:F:45:LEU:O	6:F:46:TYR:HB2	2.12	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.95	0.49
10:P:163:ARG:HH22	10:P:256:PRO:HA	1.76	0.49
17:X:24:VAL:HG23	17:X:25:LEU:HD12	1.95	0.49
3:C:80:LEU:O	3:C:81:ASP:HB2	2.12	0.49
4:D:163:PRO:HG2	4:D:168:GLN:HG2	1.94	0.49
7:G:382:ARG:CZ	7:G:652:ASN:ND2	2.74	0.49
10:P:132:ARG:HD2	10:P:134:TRP:CZ2	2.47	0.49
10:P:157:LYS:CB	10:P:195:PHE:HD1	2.24	0.49
12:R:88:HIS:O	12:R:89:PRO:C	2.56	0.49
18:Z:128:ARG:HB3	18:Z:132:GLU:OE1	2.13	0.49
4:D:260:GLU:OE1	9:I:72:MET:SD	2.71	0.49
4:D:304:LYS:HD3	4:D:318:VAL:HG23	1.95	0.49
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.27	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
7:G:617:ARG:HH22	16:W:128:GLY:N	2.11	0.49
8:H:183:MET:SD	24:I:301:3PE:H331	2.53	0.49
12:R:48:PHE:HD1	12:R:52:GLN:O	1.95	0.49
13:S:30:SER:O	13:S:31:GLN:C	2.56	0.49
2:B:126:ARG:HH12	2:B:151:GLN:HG2	1.78	0.49
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.49
7:G:648:GLU:O	13:S:22:HIS:HE1	1.95	0.49
9:I:76:TYR:CE1	9:I:79:ARG:CZ	2.95	0.49
10:P:113:LYS:C	10:P:115:SER:H	2.21	0.49
10:P:157:LYS:HD3	10:P:195:PHE:CD1	2.48	0.49
11:Q:154:LYS:HB2	11:Q:155:PRO:CD	2.39	0.49
16:W:102:GLN:H	16:W:105:HIS:CD2	2.30	0.49
16:W:107:MET:HE3	16:W:112:GLU:OE2	2.11	0.49
20:b:60:ASP:HB2	20:b:62:ASN:OD1	2.12	0.49
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.96	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.49
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.76	0.49
9:I:144:ARG:NE	9:I:146:ASP:OD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:18:GLU:HB3	13:S:52:PRO:HB2	1.94	0.49
17:X:93:ASN:HB2	19:a:38:VAL:HG23	1.93	0.49
21:q:65:THR:HG22	21:q:81:MET:HE1	1.95	0.49
1:A:52:SER:HG	1:A:55:PHE:CB	2.26	0.48
2:B:98:ALA:HB1	2:B:100:CYS:N	2.28	0.48
6:F:67:GLU:O	6:F:71:LYS:HG2	2.13	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
8:H:229:THR:O	8:H:229:THR:CG2	2.52	0.48
8:H:277:TYR:CE2	24:I:301:3PE:H272	2.48	0.48
17:X:5:VAL:CG1	18:Z:109:SER:HB3	2.43	0.48
18:Z:144:THR:HG23	19:a:37:ARG:O	2.12	0.48
20:b:35:ILE:HG12	20:b:35:ILE:O	2.13	0.48
27:B:304:PC1:H382	8:H:57:MET:HE2	1.95	0.48
4:D:253:LEU:O	4:D:256:ASP:OD1	2.31	0.48
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.48
8:H:19:PHE:CD2	19:a:11:ILE:HG21	2.48	0.48
9:I:180:HIS:HD2	10:P:100:LEU:CD2	2.26	0.48
10:P:80:VAL:HB	10:P:103:LEU:HD22	1.94	0.48
10:P:236:VAL:HG23	10:P:271:TYR:O	2.13	0.48
13:S:16:LEU:HD13	13:S:94:VAL:HG12	1.95	0.48
15:V:31:THR:O	15:V:35:LEU:HG	2.12	0.48
15:V:77:VAL:C	15:V:79:GLU:N	2.67	0.48
16:W:93:LEU:O	16:W:94:GLN:C	2.55	0.48
17:X:49:GLU:CG	17:X:50:GLU:N	2.76	0.48
17:X:74:ILE:O	17:X:77:HIS:O	2.31	0.48
17:X:129:THR:HA	20:b:67:PRO:O	2.13	0.48
19:a:3:PHE:CE2	34:a:101:CDL:HA4	2.48	0.48
1:A:81:THR:N	20:b:46:ASN:HD21	2.10	0.48
2:B:96:GLY:O	2:B:134:ALA:O	2.31	0.48
2:B:99:CYS:HG	25:B:301:SF4:FE1	1.30	0.48
27:B:304:PC1:H241	10:P:310:PHE:HE1	1.79	0.48
3:C:223:VAL:HG23	3:C:225:LEU:HD12	1.88	0.48
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.48
8:H:147:ALA:O	8:H:151:LEU:N	2.42	0.48
8:H:152:SER:O	8:H:153:VAL:C	2.55	0.48
16:W:46:VAL:HB	16:W:47:PRO:HD3	1.95	0.48
22:r:27:ARG:CB	22:r:31:ILE:CG2	2.87	0.48
1:A:49:LEU:CB	1:A:50:PRO:HD2	2.17	0.48
1:A:108:GLN:O	1:A:109:LYS:HB2	2.14	0.48
2:B:90:LEU:O	2:B:119:VAL:HA	2.12	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.78	0.48
8:H:51:ASP:C	8:H:51:ASP:OD1	2.55	0.48
8:H:68:MET:HG2	8:H:72:ILE:HD13	1.95	0.48
8:H:197:PRO:HB3	8:H:277:TYR:CB	2.43	0.48
10:P:94:LEU:O	10:P:97:MET:HG2	2.14	0.48
14:T:110:LEU:CD2	14:T:118:ILE:HD12	2.44	0.48
1:A:7:ILE:CD1	24:H:401:3PE:H371	2.36	0.48
2:B:97:LEU:CD1	4:D:94:VAL:CG1	2.88	0.48
2:B:104:MET:SD	2:B:122:ARG:NE	2.86	0.48
3:C:149:LEU:CD2	11:Q:64:LEU:HD21	2.43	0.48
6:F:296:LEU:HD13	6:F:337:MET:CE	2.34	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
7:G:475:VAL:HG11	7:G:516:LEU:HD23	1.95	0.48
9:I:154:TYR:CA	9:I:169:GLU:OE2	2.61	0.48
12:R:51:ARG:O	12:R:52:GLN:HG3	2.13	0.48
14:T:80:LYS:HB2	14:T:145:VAL:HG11	1.96	0.48
14:T:95:PRO:HG2	14:T:97:LYS:HB3	1.95	0.48
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.78	0.48
4:D:181:LEU:HD11	4:D:210:MET:CB	2.43	0.48
4:D:181:LEU:HD12	4:D:210:MET:CE	2.43	0.48
5:E:223:CYS:HB3	6:F:132:ARG:NH1	2.28	0.48
6:F:226:LYS:O	6:F:227:PRO:C	2.56	0.48
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.48
12:R:67:GLN:HG3	12:R:68:PRO:HD2	1.96	0.48
2:B:94:THR:HG22	2:B:96:GLY:H	1.79	0.48
2:B:176:SER:O	2:B:177:VAL:HG23	2.14	0.48
5:E:131:ILE:CD1	5:E:185:VAL:HB	2.25	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.48
6:F:297:LYS:HB2	6:F:333:GLU:HB3	1.95	0.48
7:G:170:LYS:O	7:G:231:LEU:HA	2.13	0.48
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
9:I:62:MET:O	9:I:63:TRP:C	2.56	0.48
14:T:120:MET:HE1	16:W:43:TYR:CD2	2.49	0.48
18:Z:143:TYR:O	18:Z:144:THR:C	2.55	0.48
4:D:99:LEU:HD22	4:D:106:VAL:HG11	1.95	0.48
4:D:299:GLN:NE2	9:I:36:TYR:CZ	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:147:ILE:CD1	5:E:195:LEU:HB2	2.43	0.48
5:E:227:ALA:HB3	6:F:284:HIS:ND1	2.29	0.48
7:G:183:ILE:HD11	7:G:197:THR:HG23	1.95	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
8:H:140:ILE:HG13	8:H:141:SER:N	2.28	0.48
8:H:154:LEU:O	8:H:155:LEU:C	2.55	0.48
8:H:218:GLY:O	8:H:219:PRO:C	2.57	0.48
8:H:313:GLY:O	8:H:314:VAL:C	2.56	0.48
9:I:41:LYS:HG2	9:I:41:LYS:O	2.13	0.48
13:S:87:VAL:O	13:S:88:THR:C	2.55	0.48
17:X:10:LEU:H	17:X:10:LEU:HD12	1.77	0.48
17:X:49:GLU:O	17:X:51:LYS:HD2	2.13	0.48
2:B:97:LEU:HA	4:D:94:VAL:CG2	2.44	0.48
2:B:98:ALA:CB	2:B:101:ALA:H	2.27	0.48
5:E:45:GLU:H	5:E:45:GLU:CD	2.21	0.48
5:E:71:GLU:HG3	23:s:94:GLN:NE2	2.27	0.48
5:E:206:GLU:HB3	5:E:213:PRO:HB3	1.96	0.48
6:F:126:LYS:HG3	6:F:275:LEU:HB3	1.94	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.96	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
7:G:277:MET:HE1	11:Q:153:PRO:HD3	1.96	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
7:G:403:VAL:HG23	7:G:432:ILE:CB	2.38	0.48
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.95	0.48
8:H:51:ASP:OD1	8:H:52:ALA:N	2.47	0.48
10:P:146:VAL:HG13	10:P:190:GLU:HG3	1.95	0.48
10:P:376:ASN:O	10:P:377:TYR:C	2.57	0.48
11:Q:78:ARG:O	11:Q:80:PHE:HD1	1.96	0.48
22:r:6:ARG:CA	22:r:9:GLN:HG2	2.42	0.48
27:B:304:PC1:H3B1	8:H:57:MET:HE3	1.94	0.48
3:C:130:ASN:HD21	3:C:141:ARG:HE	1.62	0.48
3:C:221:GLU:O	3:C:222:PRO:C	2.56	0.48
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.95	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	0.48
8:H:17:MET:HG2	8:H:228:TYR:HB2	1.94	0.48
9:I:93:LEU:HD11	9:I:173:PHE:HE2	1.77	0.48
10:P:74:GLY:HA2	10:P:102:GLN:OE1	2.14	0.48
10:P:165:ILE:CD1	10:P:253:THR:HG22	2.42	0.48
10:P:169:HIS:HB2	10:P:184:LYS:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:285:HIS:HB3	10:P:361:TRP:CE3	2.47	0.48
14:T:119:ILE:HD12	14:T:138:LEU:CD1	2.40	0.48
22:r:110:GLN:HG2	22:r:113:LEU:HD22	1.95	0.48
4:D:84:PHE:HB3	4:D:96:ARG:O	2.13	0.47
4:D:240:LEU:HG	4:D:244:ILE:CD1	2.44	0.47
6:F:76:ILE:HG23	6:F:255:CYS:SG	2.54	0.47
6:F:134:ASP:CG	6:F:137:LYS:HB2	2.38	0.47
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.47
8:H:1:MET:HE2	19:a:26:ILE:HG23	1.96	0.47
16:W:65:LYS:O	16:W:69:MET:HG2	2.14	0.47
17:X:20:VAL:HB	17:X:24:VAL:HG21	1.95	0.47
19:a:12:MET:O	19:a:12:MET:HG2	2.14	0.47
1:A:6:VAL:HG11	8:H:87:VAL:HG11	1.96	0.47
4:D:384:LEU:HD21	7:G:144:MET:HE1	1.95	0.47
6:F:299:LEU:HD11	6:F:300:ILE:HG23	1.95	0.47
10:P:59:PHE:HA	10:P:83:PRO:HD2	1.96	0.47
10:P:365:GLU:N	10:P:365:GLU:OE1	2.46	0.47
18:Z:75:PHE:CE2	19:a:47:LEU:HD11	2.50	0.47
18:Z:120:LEU:HD23	18:Z:121:ILE:N	2.29	0.47
23:s:87:LEU:CB	23:s:91:ARG:NH1	2.76	0.47
3:C:219:VAL:HG11	16:W:113:THR:HG21	1.96	0.47
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.49	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
7:G:665:PHE:O	7:G:668:ALA:N	2.45	0.47
8:H:42:PRO:HB3	21:q:27:PHE:CZ	2.49	0.47
8:H:87:VAL:O	8:H:96:ILE:HG12	2.14	0.47
8:H:102:ILE:CG2	8:H:150:LEU:HD21	2.40	0.47
10:P:54:VAL:O	10:P:78:SER:HB3	2.14	0.47
10:P:76:MET:SD	10:P:254:LYS:HE3	2.54	0.47
10:P:307:LEU:O	10:P:308:SER:C	2.54	0.47
17:X:7:LEU:HD22	18:Z:87:LEU:HD12	1.93	0.47
3:C:123:ASN:HB2	15:V:111:GLN:OE1	2.14	0.47
4:D:203:MET:HE3	4:D:258:VAL:HG23	1.95	0.47
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.79	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:545:LEU:CD2	7:G:547:LEU:HD21	2.44	0.47
8:H:318:MET:HG2	19:a:40:ARG:HD2	1.96	0.47
9:I:152:CYS:SG	25:I:302:SF4:S4	3.12	0.47
16:W:84:LEU:HD11	16:W:88:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:48:TRP:O	17:X:51:LYS:HE3	2.15	0.47
24:A:201:3PE:H272	20:b:23:PHE:HD2	1.78	0.47
2:B:98:ALA:CB	2:B:134:ALA:C	2.82	0.47
2:B:182:ASP:HA	2:B:185:VAL:O	2.14	0.47
3:C:67:ILE:HD13	3:C:98:PHE:CZ	2.49	0.47
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.49	0.47
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.14	0.47
7:G:238:PHE:CD1	9:I:140:ARG:CZ	2.97	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
8:H:65:THR:HG21	8:H:71:PHE:HB2	1.96	0.47
19:a:3:PHE:HD2	34:a:101:CDL:H132	1.78	0.47
21:q:43:LYS:O	21:q:44:TYR:HB2	2.13	0.47
1:A:65:PHE:HA	1:A:68:GLU:CD	2.39	0.47
5:E:196:THR:O	5:E:197:PRO:C	2.56	0.47
6:F:313:ASN:OD1	6:F:359:ARG:NH1	2.48	0.47
8:H:230:ASN:HB3	8:H:233:LEU:HD12	1.97	0.47
9:I:77:LEU:O	19:a:2:TRP:HB3	2.14	0.47
13:S:35:ASP:O	13:S:38:VAL:HG22	2.15	0.47
21:q:69:ASN:CG	21:q:70:GLY:H	2.23	0.47
3:C:208:GLU:HG2	3:C:221:GLU:HG3	1.95	0.47
4:D:123:LEU:HD13	4:D:135:TYR:OH	2.14	0.47
4:D:256:ASP:HB2	18:Z:25:LEU:HD11	1.91	0.47
5:E:71:GLU:CG	23:s:94:GLN:HE21	2.26	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
6:F:128:ARG:HA	6:F:131:MET:HE2	1.96	0.47
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:258:GLY:O	6:F:259:GLY:C	2.58	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:385:TYR:CE2	7:G:526:LEU:HB2	2.49	0.47
8:H:213:VAL:HG13	8:H:214:GLU:HG2	1.96	0.47
9:I:76:TYR:HE1	9:I:79:ARG:NH2	2.12	0.47
13:S:95:LEU:HD12	13:S:95:LEU:C	2.33	0.47
14:T:116:VAL:O	14:T:120:MET:HG3	2.15	0.47
3:C:69:PRO:HD2	15:V:99:PRO:O	2.15	0.47
4:D:320:ILE:CD1	9:I:38:TYR:CD1	2.97	0.47
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.44	0.47
7:G:114:GLU:OE1	22:r:53:TYR:HB3	2.15	0.47
7:G:400:VAL:HG22	7:G:473:MET:CG	2.45	0.47
7:G:648:GLU:O	13:S:22:HIS:CE1	2.68	0.47
8:H:91:MET:HE1	8:H:259:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:57:LEU:HD11	18:Z:84:LEU:CD2	2.44	0.47
17:X:141:PRO:O	17:X:142:TYR:HB2	2.14	0.47
34:a:101:CDL:CA3	21:q:10:GLY:HA3	2.43	0.47
25:B:301:SF4:S2	4:D:138:ARG:HD3	2.55	0.47
4:D:159:LEU:CG	4:D:391:VAL:HG12	2.45	0.47
4:D:392:PRO:HD3	22:r:60:ARG:HG3	1.96	0.47
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.47
6:F:357:MET:HE1	6:F:363:ILE:HD12	1.95	0.47
6:F:364:VAL:HA	6:F:438:LEU:HD11	1.97	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
7:G:544:MET:HA	7:G:565:PHE:O	2.14	0.47
8:H:129:LEU:O	8:H:133:LEU:HG	2.15	0.47
10:P:40:VAL:O	10:P:42:PRO:HD3	2.15	0.47
10:P:134:TRP:HB3	10:P:312:PRO:CG	2.41	0.47
15:V:6:LYS:HG2	15:V:16:VAL:HG23	1.96	0.47
15:V:44:TYR:O	15:V:48:THR:HG22	2.15	0.47
16:W:28:LEU:O	16:W:32:LYS:HG3	2.15	0.47
16:W:38:LEU:HG	16:W:70:PHE:HZ	1.80	0.47
18:Z:88:ARG:O	18:Z:92:GLU:HG3	2.14	0.47
1:A:72:LEU:HD23	1:A:94:LEU:HD23	1.94	0.47
24:A:201:3PE:H3B2	20:b:26:TRP:CD1	2.50	0.47
2:B:136:THR:HG22	2:B:164:CYS:HB2	1.97	0.47
2:B:146:ARG:NH1	2:B:149:TYR:CD2	2.83	0.47
3:C:168:GLU:HB2	3:C:186:ILE:HG21	1.97	0.47
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.47
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.47
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.47
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.47
7:G:691:ILE:HG12	7:G:695:TYR:CE2	2.50	0.47
8:H:86:TRP:CD2	8:H:233:LEU:HD21	2.50	0.47
8:H:202:GLU:H	8:H:210:GLY:HA3	1.79	0.47
8:H:202:GLU:O	8:H:203:GLY:C	2.58	0.47
10:P:59:PHE:CD2	10:P:152:ILE:HD13	2.49	0.47
14:T:140:CYS:O	14:T:143:GLU:HB2	2.15	0.47
17:X:7:LEU:CD1	18:Z:87:LEU:HD12	2.44	0.47
18:Z:75:PHE:HE2	19:a:47:LEU:HD11	1.79	0.47
19:a:22:SER:O	19:a:23:THR:C	2.57	0.47
3:C:232:PHE:HE1	7:G:244:GLU:HG3	1.80	0.46
5:E:107:PRO:O	5:E:110:ARG:HB3	2.15	0.46
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:382:ARG:NE	7:G:652:ASN:ND2	2.49	0.46
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.46
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.97	0.46
14:T:107:ASP:O	14:T:108:LEU:HB2	2.15	0.46
7:G:30:ASN:O	7:G:45:PRO:HD3	2.15	0.46
7:G:137:CYS:N	11:Q:88:GLN:HE21	2.13	0.46
7:G:671:LEU:CD2	13:S:45:LYS:HG2	2.44	0.46
10:P:73:LEU:CD2	10:P:250:VAL:HG22	2.45	0.46
11:Q:52:LEU:HA	11:Q:52:LEU:HD23	1.73	0.46
12:R:88:HIS:ND1	12:R:89:PRO:O	2.47	0.46
13:S:24:CYS:N	13:S:58:CYS:HB2	2.30	0.46
16:W:124:LYS:O	16:W:125:PHE:C	2.58	0.46
17:X:15:VAL:O	17:X:17:GLU:HG3	2.15	0.46
20:b:63:MET:HB2	20:b:66:VAL:CG1	2.45	0.46
1:A:7:ILE:HD12	24:H:401:3PE:H292	1.96	0.46
3:C:45:THR:OG1	22:r:57:ARG:CD	2.63	0.46
9:I:85:ASN:HB3	9:I:89:GLU:HG3	1.97	0.46
10:P:229:VAL:HG22	10:P:298:TYR:CD2	2.50	0.46
10:P:293:LEU:HB3	10:P:294:PRO:HD2	1.98	0.46
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.46
16:W:22:PRO:HG3	16:W:26:ARG:NH2	2.30	0.46
22:r:8:ILE:HA	22:r:11:LEU:HD12	1.98	0.46
4:D:234:GLN:HE21	9:I:212:ARG:HB3	1.79	0.46
4:D:412:VAL:HG12	15:V:114:TRP:CZ2	2.51	0.46
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.74	0.46
5:E:131:ILE:N	5:E:169:THR:O	2.49	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
5:E:243:GLY:O	5:E:244:VAL:C	2.58	0.46
6:F:212:LEU:HD12	6:F:212:LEU:O	2.15	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
7:G:114:GLU:OE2	22:r:53:TYR:CA	2.51	0.46
7:G:462:PHE:CD1	7:G:465:VAL:HB	2.50	0.46
9:I:155:CYS:HG	25:I:302:SF4:FE3	1.32	0.46
10:P:73:LEU:HD23	10:P:250:VAL:HG22	1.97	0.46
10:P:169:HIS:H	10:P:184:LYS:CE	2.28	0.46
13:S:62:GLN:O	13:S:64:LYS:HG3	2.15	0.46
14:T:98:LEU:O	14:T:99:SER:C	2.57	0.46
16:W:61:GLN:O	16:W:64:ASP:HB2	2.15	0.46
20:b:28:LEU:O	20:b:31:ILE:HG12	2.15	0.46
21:q:17:HIS:CD2	21:q:35:ILE:HD13	2.50	0.46
1:A:73:LEU:HD23	8:H:151:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HA	1:A:87:MET:CE	2.46	0.46
3:C:79:CYS:SG	22:r:64:VAL:HB	2.56	0.46
3:C:155:ILE:O	3:C:156:VAL:C	2.58	0.46
5:E:92:LEU:HG	5:E:92:LEU:O	2.15	0.46
6:F:262:PHE:HA	6:F:265:PHE:HD2	1.81	0.46
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.46
7:G:661:GLU:O	7:G:661:GLU:CG	2.46	0.46
8:H:157:ASN:HD22	8:H:165:LEU:HD11	1.78	0.46
8:H:230:ASN:HA	8:H:233:LEU:HD12	1.97	0.46
15:V:24:LEU:O	15:V:25:THR:C	2.58	0.46
15:V:64:ASP:OD2	15:V:67:LYS:HG2	2.15	0.46
34:a:101:CDL:H711	34:a:101:CDL:H321	1.98	0.46
21:q:4:VAL:HG23	21:q:5:GLU:N	2.31	0.46
21:q:60:ARG:HD2	21:q:92:CYS:SG	2.56	0.46
1:A:85:SER:O	1:A:89:ILE:HG13	2.15	0.46
2:B:122:ARG:O	26:B:302:UQ1:O1	2.34	0.46
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.45	0.46
5:E:223:CYS:HB3	6:F:132:ARG:HH11	1.79	0.46
6:F:64:LYS:H	6:F:256:ARG:HH21	1.62	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.84	0.46
9:I:114:ILE:HD13	12:R:106:TYR:CD1	2.51	0.46
11:Q:69:GLU:HA	11:Q:72:ILE:CG2	2.45	0.46
15:V:33:ASP:O	15:V:34:ILE:C	2.59	0.46
18:Z:58:ARG:HG2	20:b:45:ILE:HD11	1.97	0.46
19:a:58:ASN:CB	19:a:60:TYR:CD1	2.89	0.46
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.98	0.46
1:A:49:LEU:N	1:A:49:LEU:CD1	2.78	0.46
6:F:50:ASP:C	6:F:52:ARG:N	2.73	0.46
7:G:665:PHE:O	7:G:666:GLN:C	2.57	0.46
8:H:197:PRO:O	8:H:279:ARG:HA	2.16	0.46
10:P:99:ASP:CG	10:P:100:LEU:H	2.24	0.46
10:P:303:LYS:O	10:P:307:LEU:HG	2.15	0.46
13:S:24:CYS:CA	13:S:58:CYS:HB2	2.46	0.46
34:a:101:CDL:CB6	21:q:6:VAL:HG21	2.46	0.46
2:B:112:TYR:O	2:B:113:ASP:C	2.56	0.46
4:D:238:LEU:O	4:D:238:LEU:HG	2.16	0.46
4:D:409:VAL:HG13	4:D:422:CYS:SG	2.56	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
7:G:35:PHE:O	7:G:101:ASN:HA	2.16	0.46
8:H:19:PHE:CD2	19:a:11:ILE:CG2	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:GLU:OE2	8:H:195:ARG:NH2	2.49	0.46
10:P:220:TYR:CD1	10:P:223:PHE:HE1	2.34	0.46
10:P:229:VAL:C	10:P:231:LEU:N	2.73	0.46
10:P:235:THR:CG2	10:P:323:HIS:O	2.63	0.46
34:a:101:CDL:HB4	22:r:5:THR:OG1	2.15	0.46
2:B:81:LEU:CD1	8:H:53:MET:SD	3.04	0.46
2:B:175:TYR:CE2	4:D:117:HIS:HE1	2.34	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.16	0.46
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.16	0.46
7:G:35:PHE:CE1	7:G:40:SER:CB	2.99	0.46
7:G:182:CYS:SG	25:G:802:SF4:S1	3.14	0.46
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.46
7:G:381:LEU:HD23	13:S:55:ILE:HG12	1.98	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
8:H:65:THR:HG22	8:H:67:SER:H	1.80	0.46
9:I:87:PRO:HG2	9:I:88:PHE:CE2	2.50	0.46
10:P:151:ALA:O	10:P:154:GLN:HB3	2.16	0.46
10:P:276:LEU:CD2	10:P:280:ILE:HD11	2.46	0.46
18:Z:108:GLU:O	18:Z:109:SER:C	2.57	0.46
19:a:4:GLU:C	19:a:7:PRO:HD2	2.40	0.46
21:q:4:VAL:HG23	21:q:5:GLU:H	1.81	0.46
5:E:184:MET:HE2	5:E:184:MET:HB3	1.74	0.46
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.46
7:G:330:LEU:HD12	7:G:544:MET:HE1	1.98	0.46
7:G:330:LEU:CA	7:G:544:MET:HE1	2.46	0.46
7:G:405:THR:O	7:G:407:PRO:HD3	2.16	0.46
7:G:651:PRO:CB	13:S:57:GLU:O	2.62	0.46
8:H:233:LEU:O	8:H:236:ALA:N	2.48	0.46
10:P:354:ARG:HD2	10:P:362:LEU:O	2.16	0.46
15:V:51:ILE:O	15:V:52:THR:C	2.58	0.46
16:W:77:THR:O	16:W:79:PRO:HD3	2.16	0.46
21:q:17:HIS:ND1	21:q:26:VAL:HG21	2.30	0.46
1:A:65:PHE:HA	1:A:68:GLU:CG	2.46	0.45
2:B:207:GLN:HA	2:B:210:ARG:NH2	2.30	0.45
6:F:157:TYR:CG	6:F:212:LEU:HD11	2.51	0.45
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.45
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.98	0.45
7:G:651:PRO:HD2	13:S:56:ARG:HB3	1.96	0.45
10:P:131:GLY:HA3	31:P:401:NDP:O3D	2.15	0.45
14:T:99:SER:HB2	14:T:102:SER:CB	2.33	0.45
15:V:31:THR:C	15:V:33:ASP:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:128:VAL:HG12	20:b:54:PRO:HB2	1.99	0.45
20:b:80:TRP:O	20:b:81:LEU:C	2.59	0.45
4:D:266:ARG:HH11	9:I:66:LEU:HG	1.81	0.45
4:D:345:GLU:CD	18:Z:19:ILE:HG12	2.41	0.45
4:D:348:LEU:HB3	18:Z:16:TYR:CE2	2.52	0.45
4:D:460:GLU:O	4:D:463:ARG:HG2	2.16	0.45
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.31	0.45
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.45
7:G:97:MET:SD	7:G:100:TRP:CZ2	3.09	0.45
7:G:176:CYS:SG	25:G:802:SF4:S1	3.14	0.45
8:H:243:LEU:HB3	8:H:262:GLU:OE1	2.16	0.45
10:P:141:PHE:HD1	10:P:145:PHE:HE2	1.64	0.45
10:P:203:PRO:HG2	31:P:401:NDP:C6N	2.47	0.45
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.16	0.45
15:V:79:GLU:O	15:V:80:VAL:C	2.59	0.45
2:B:174:SER:HB3	4:D:123:LEU:HD11	1.99	0.45
4:D:79:ASN:ND2	4:D:102:SER:HB2	2.32	0.45
4:D:211:PHE:O	4:D:212:GLU:C	2.56	0.45
4:D:326:CYS:CB	4:D:453:THR:HG21	2.47	0.45
5:E:179:CYS:O	5:E:180:VAL:C	2.59	0.45
5:E:241:GLY:O	5:E:244:VAL:HG23	2.17	0.45
6:F:47:GLY:O	6:F:48:ARG:HB3	2.16	0.45
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.46	0.45
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.45
7:G:382:ARG:HA	7:G:385:TYR:CE1	2.51	0.45
9:I:135:ARG:O	9:I:136:ALA:HB3	2.16	0.45
10:P:338:LEU:HD12	10:P:338:LEU:HA	1.73	0.45
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.98	0.45
15:V:43:ALA:O	15:V:44:TYR:C	2.60	0.45
2:B:154:GLU:O	2:B:155:PRO:C	2.57	0.45
3:C:226:ALA:O	11:Q:116:SER:OG	2.31	0.45
4:D:133:LEU:HD11	4:D:148:GLU:HB3	1.98	0.45
4:D:163:PRO:HG2	4:D:168:GLN:NE2	2.32	0.45
6:F:109:ARG:NH2	6:F:232:ASP:O	2.45	0.45
7:G:49:VAL:HB	7:G:91:ALA:HA	1.98	0.45
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.45
8:H:142:TYR:CD1	8:H:289:LEU:HD13	2.51	0.45
10:P:106:LEU:HB2	12:R:50:ASP:OD2	2.16	0.45
10:P:227:PRO:HB3	10:P:291:TYR:CE1	2.51	0.45
16:W:31:ALA:O	16:W:32:LYS:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:36:ARG:O	16:W:40:ARG:HG3	2.16	0.45
4:D:87:GLN:O	4:D:88:HIS:C	2.57	0.45
5:E:180:VAL:HG13	5:E:181:ASN:N	2.31	0.45
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.45
7:G:35:PHE:CD1	7:G:40:SER:HB2	2.51	0.45
7:G:629:ILE:HD11	16:W:122:LEU:HD21	1.98	0.45
8:H:149:ILE:HG21	8:H:185:TRP:HB2	1.98	0.45
8:H:151:LEU:HD23	8:H:151:LEU:C	2.41	0.45
9:I:116:CYS:HB2	9:I:118:LEU:H	1.80	0.45
10:P:188:GLU:HG3	10:P:202:ARG:HH21	1.82	0.45
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.45
14:T:133:ILE:HG13	14:T:137:LYS:NZ	2.30	0.45
15:V:35:LEU:HD22	15:V:48:THR:HG21	1.98	0.45
19:a:7:PRO:HG3	34:a:101:CDL:H152	1.98	0.45
21:q:24:LEU:O	21:q:28:PHE:HB2	2.16	0.45
1:A:24:LEU:HD22	27:B:304:PC1:H352	1.98	0.45
2:B:104:MET:HE3	2:B:104:MET:HB3	1.84	0.45
4:D:137:ASP:OD1	4:D:138:ARG:N	2.50	0.45
4:D:362:LYS:O	4:D:384:LEU:HD21	2.17	0.45
5:E:142:ARG:CB	5:E:182:ALA:HB3	2.46	0.45
5:E:241:GLY:HA2	6:F:63:TYR:CE2	2.51	0.45
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.45
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:157:ASN:HD22	8:H:165:LEU:CD1	2.29	0.45
8:H:200:LEU:HD23	8:H:282:TYR:CD1	2.49	0.45
8:H:206:GLU:HG3	8:H:207:LEU:H	1.79	0.45
11:Q:163:ASN:OD1	11:Q:164:PHE:CG	2.69	0.45
14:T:123:GLU:HA	14:T:128:PHE:O	2.16	0.45
18:Z:69:ILE:HD12	20:b:54:PRO:HD3	1.98	0.45
1:A:13:LEU:HD21	8:H:14:LEU:CD1	2.46	0.45
1:A:24:LEU:HD13	27:B:304:PC1:H3B2	1.99	0.45
2:B:92:PRO:CB	2:B:130:VAL:HG13	2.45	0.45
2:B:137:LEU:HD13	2:B:145:LEU:HD22	1.99	0.45
3:C:229:PHE:CD1	9:I:126:GLN:HG3	2.43	0.45
4:D:80:MET:HE2	4:D:101:LEU:HD12	1.99	0.45
4:D:144:MET:SD	4:D:222:MET:CG	2.98	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
9:I:56:ASN:O	9:I:60:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:81:ILE:HD11	12:R:46:VAL:HG21	1.97	0.45
10:P:128:ASN:HD22	10:P:166:HIS:CD2	2.35	0.45
10:P:168:SER:O	10:P:203:PRO:HD2	2.16	0.45
14:T:140:CYS:O	14:T:141:PRO:C	2.59	0.45
15:V:48:THR:HA	15:V:51:ILE:HD12	1.98	0.45
15:V:65:VAL:O	15:V:66:LYS:C	2.60	0.45
23:s:94:GLN:OE1	23:s:94:GLN:N	2.49	0.45
4:D:232:VAL:HG23	4:D:356:ILE:HD13	1.98	0.45
4:D:256:ASP:OD1	4:D:257:GLU:N	2.50	0.45
5:E:81:VAL:O	5:E:82:LEU:C	2.59	0.45
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.52	0.45
7:G:241:ARG:NH1	9:I:140:ARG:HH22	2.15	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
8:H:142:TYR:CE1	8:H:285:LEU:HD11	2.51	0.45
8:H:148:ILE:HG21	8:H:297:THR:HG22	1.98	0.45
8:H:228:TYR:N	8:H:228:TYR:CD1	2.85	0.45
10:P:315:THR:O	10:P:319:VAL:HG23	2.16	0.45
2:B:153:PRO:O	2:B:156:ARG:HB3	2.16	0.45
3:C:126:GLU:O	3:C:128:VAL:HG23	2.17	0.45
4:D:226:TYR:CZ	4:D:232:VAL:HB	2.52	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.99	0.45
7:G:399:VAL:HG21	7:G:462:PHE:CZ	2.52	0.45
8:H:213:VAL:HG13	8:H:214:GLU:N	2.32	0.45
10:P:88:VAL:O	10:P:91:ILE:HG12	2.17	0.45
10:P:171:ASN:OD1	10:P:171:ASN:O	2.34	0.45
10:P:221:ARG:HD2	10:P:286:ARG:CD	2.43	0.45
10:P:293:LEU:HD12	10:P:298:TYR:OH	2.16	0.45
11:Q:53:ILE:HG22	16:W:20:VAL:O	2.17	0.45
11:Q:112:MET:HG2	11:Q:114:TRP:CE2	2.52	0.45
12:R:44:ARG:HB3	12:R:47:ARG:HH12	1.82	0.45
17:X:27:ALA:HB1	17:X:85:TYR:CD2	2.52	0.45
21:q:37:THR:O	21:q:49:TYR:HA	2.17	0.45
2:B:140:LYS:HD2	4:D:115:LEU:HD23	1.99	0.45
3:C:118:VAL:HB	3:C:121:ARG:HD2	1.98	0.45
4:D:100:GLU:HB2	4:D:107:ARG:HB3	1.99	0.45
4:D:168:GLN:HB3	4:D:310:VAL:HG13	1.99	0.45
4:D:304:LYS:HD3	4:D:318:VAL:CG2	2.47	0.45
5:E:73:HIS:CE1	11:Q:166:TRP:CD2	3.05	0.45
5:E:163:THR:HG23	5:E:168:PHE:O	2.17	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.91	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:381:LEU:HD22	13:S:55:ILE:CD1	2.47	0.45
8:H:227:GLU:C	8:H:228:TYR:HD1	2.25	0.45
10:P:318:LYS:HA	10:P:321:ARG:HG2	1.97	0.45
12:R:46:VAL:O	12:R:47:ARG:C	2.58	0.45
12:R:54:GLU:O	21:q:127:TYR:OH	2.24	0.45
14:T:102:SER:HB2	14:T:107:ASP:CB	2.47	0.45
16:W:31:ALA:C	16:W:33:ARG:N	2.74	0.45
16:W:33:ARG:NH2	16:W:37:GLU:OE2	2.50	0.45
16:W:86:VAL:O	16:W:90:LYS:N	2.41	0.45
17:X:125:LEU:HB2	18:Z:66:GLU:HB3	1.99	0.45
19:a:52:ARG:CG	19:a:57:VAL:O	2.55	0.45
4:D:174:PHE:O	4:D:178:THR:HG23	2.17	0.44
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
16:W:65:LYS:HE3	16:W:69:MET:SD	2.56	0.44
16:W:69:MET:C	16:W:71:MET:H	2.24	0.44
17:X:137:LEU:HD22	17:X:139:GLU:CD	2.42	0.44
20:b:78:LEU:C	20:b:80:TRP:H	2.23	0.44
20:b:80:TRP:CG	20:b:81:LEU:H	2.35	0.44
21:q:48:TYR:OH	21:q:83:PRO:HD2	2.18	0.44
22:r:57:ARG:HG3	22:r:57:ARG:O	2.16	0.44
27:B:303:PC1:H341	27:B:303:PC1:C22	2.45	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
6:F:136:HIS:O	6:F:137:LYS:C	2.59	0.44
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44
7:G:284:GLU:CD	11:Q:84:ARG:NH2	2.75	0.44
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.44
8:H:74:ALA:N	8:H:75:PRO:HD2	2.32	0.44
10:P:92:MET:C	10:P:94:LEU:N	2.74	0.44
10:P:192:ARG:NE	10:P:200:ILE:HD12	2.31	0.44
10:P:294:PRO:HG2	10:P:297:VAL:HG23	1.99	0.44
15:V:31:THR:O	15:V:33:ASP:N	2.50	0.44
15:V:50:GLN:NE2	22:r:94:ALA:H	2.15	0.44
17:X:140:ASN:OD1	17:X:144:SER:N	2.49	0.44
1:A:80:GLN:CA	20:b:46:ASN:ND2	2.61	0.44
2:B:197:THR:O	2:B:200:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:116:LEU:O	4:D:116:LEU:CG	2.62	0.44
4:D:212:GLU:OE1	22:r:27:ARG:NH2	2.50	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.58	0.44
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
10:P:266:THR:CG2	10:P:329:PRO:HB3	2.47	0.44
13:S:20:ARG:CG	13:S:66:TRP:HB2	2.47	0.44
16:W:98:LYS:HD3	16:W:100:TRP:CZ2	2.53	0.44
17:X:139:GLU:O	17:X:140:ASN:C	2.60	0.44
19:a:66:LEU:HD13	19:a:66:LEU:O	2.17	0.44
1:A:24:LEU:O	1:A:25:PRO:C	2.56	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:309:ASN:OD1	7:G:310:GLU:N	2.51	0.44
7:G:388:ASN:N	7:G:514:ASN:CB	2.69	0.44
10:P:370:LYS:HD3	10:P:371:PRO:O	2.16	0.44
13:S:59:SER:O	13:S:60:GLU:C	2.59	0.44
15:V:56:LEU:O	15:V:60:LYS:HG2	2.18	0.44
21:q:43:LYS:HG3	21:q:44:TYR:CD2	2.53	0.44
2:B:79:ASP:OD1	2:B:80:ASP:N	2.51	0.44
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.52	0.44
3:C:153:ASP:OD1	3:C:153:ASP:N	2.50	0.44
4:D:142:VAL:HG11	4:D:185:MET:CB	2.48	0.44
4:D:325:ASP:O	4:D:326:CYS:C	2.58	0.44
5:E:79:LEU:HB2	5:E:80:PRO:HD3	2.00	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
6:F:119:GLU:HB3	6:F:124:THR:HG22	2.00	0.44
7:G:75:CYS:SG	28:G:803:FES:S2	3.15	0.44
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.44
7:G:308:ARG:NH1	7:G:578:PRO:O	2.50	0.44
7:G:629:ILE:HD11	16:W:122:LEU:HD11	2.00	0.44
8:H:62:ARG:HD2	8:H:68:MET:HB2	2.00	0.44
8:H:187:ILE:HD11	9:I:63:TRP:CH2	2.53	0.44
8:H:193:THR:O	8:H:194:ASN:C	2.58	0.44
9:I:98:ARG:NH1	9:I:155:CYS:O	2.50	0.44
10:P:331:ASP:O	10:P:332:LEU:HD23	2.18	0.44
14:T:103:HIS:O	14:T:107:ASP:N	2.51	0.44
15:V:62:GLU:HA	15:V:63:PRO:HD3	1.82	0.44
4:D:113:ILE:CG2	4:D:432:LEU:HD21	2.48	0.44
4:D:256:ASP:C	4:D:259:GLU:HB3	2.43	0.44
4:D:259:GLU:HG2	18:Z:25:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:259:GLU:CD	4:D:263:THR:HG1	2.26	0.44
4:D:378:LEU:HD22	7:G:126:LEU:HB2	1.99	0.44
5:E:247:GLY:HA2	6:F:257:ARG:O	2.17	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.44
8:H:195:ARG:HH12	8:H:274:ARG:HB2	1.82	0.44
10:P:114:ASP:O	10:P:118:LYS:HG2	2.18	0.44
10:P:265:PHE:CD2	10:P:335:LEU:HD21	2.52	0.44
14:T:99:SER:C	14:T:101:ASN:N	2.75	0.44
15:V:39:PRO:O	15:V:40:LYS:C	2.60	0.44
16:W:104:THR:HG22	16:W:108:ARG:HE	1.82	0.44
2:B:154:GLU:O	10:P:89:TYR:OH	2.27	0.44
2:B:192:PRO:HD3	9:I:176:SER:HA	1.98	0.44
3:C:183:LEU:HD22	16:W:91:MET:HE1	1.99	0.44
4:D:133:LEU:O	4:D:134:PRO:C	2.59	0.44
4:D:150:ALA:O	4:D:151:TYR:C	2.57	0.44
4:D:292:MET:HA	4:D:329:ARG:HD3	1.98	0.44
4:D:319:PRO:HG3	4:D:336:GLU:HG3	2.00	0.44
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.96	0.44
5:E:228:GLY:H	6:F:284:HIS:CG	2.35	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.98	0.44
10:P:97:MET:HE2	10:P:97:MET:HB3	1.83	0.44
17:X:49:GLU:CG	17:X:50:GLU:H	2.30	0.44
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.44
6:F:261:TRP:HZ3	6:F:262:PHE:CE2	2.35	0.44
8:H:84:SER:O	8:H:87:VAL:HG13	2.18	0.44
8:H:112:SER:O	8:H:113:VAL:C	2.59	0.44
9:I:152:CYS:SG	25:I:302:SF4:S2	3.16	0.44
10:P:263:PHE:CE1	10:P:333:PRO:HB2	2.51	0.44
10:P:270:ARG:O	10:P:375:VAL:N	2.37	0.44
10:P:321:ARG:HA	10:P:325:SER:HB2	2.00	0.44
15:V:82:LEU:HG	15:V:86:LYS:HE2	2.00	0.44
17:X:73:GLN:O	17:X:77:HIS:N	2.51	0.44
21:q:9:ARG:O	21:q:13:GLN:HG3	2.18	0.44
21:q:41:GLU:HG3	21:q:47:LYS:HD3	2.00	0.44
1:A:102:LEU:HD12	1:A:111:LEU:HD21	1.99	0.44
2:B:153:PRO:CG	8:H:58:LYS:HE3	2.47	0.44
2:B:202:LEU:HD21	9:I:86:TYR:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:LEU:HD21	11:Q:64:LEU:HD21	1.86	0.44
3:C:229:PHE:CE1	9:I:126:GLN:CG	2.71	0.44
4:D:326:CYS:HB3	4:D:453:THR:HG21	1.99	0.44
5:E:133:VAL:HG22	5:E:185:VAL:HG12	2.00	0.44
5:E:240:PRO:CB	6:F:60:GLY:HA3	2.46	0.44
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.44
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.44
7:G:662:THR:HB	13:S:25:GLN:NE2	2.33	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
8:H:201:THR:C	8:H:203:GLY:N	2.70	0.44
10:P:146:VAL:O	10:P:147:ASN:C	2.60	0.44
10:P:275:HIS:CE1	10:P:373:LYS:HE2	2.53	0.44
4:D:126:TYR:HA	4:D:418:ARG:HH11	1.83	0.43
6:F:231:ALA:O	6:F:239:PRO:HA	2.18	0.43
6:F:257:ARG:HB3	6:F:262:PHE:HE1	1.82	0.43
6:F:299:LEU:CD1	6:F:300:ILE:N	2.67	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:422:TRP:HZ2	7:G:441:ARG:HB3	1.82	0.43
8:H:91:MET:HE1	8:H:259:PHE:CE1	2.53	0.43
8:H:184:MET:CG	8:H:293:PHE:CE2	2.87	0.43
24:H:401:3PE:H2A1	24:H:401:3PE:H2D2	1.80	0.43
10:P:223:PHE:CZ	10:P:227:PRO:HG3	2.53	0.43
17:X:137:LEU:HD23	17:X:138:PRO:N	2.33	0.43
19:a:57:VAL:O	19:a:57:VAL:HG22	2.18	0.43
1:A:58:VAL:HG21	1:A:113:TRP:CZ2	2.53	0.43
4:D:138:ARG:HG2	4:D:223:HIS:CE1	2.53	0.43
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.43
6:F:382:CYS:SG	25:F:502:SF4:S1	3.13	0.43
6:F:412:LEU:CD2	6:F:435:VAL:HG13	2.48	0.43
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.58	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.43
7:G:466:LEU:HD13	7:G:500:ILE:CG1	2.48	0.43
7:G:611:THR:CG2	11:Q:104:ARG:C	2.91	0.43
8:H:97:ASN:O	24:H:401:3PE:H111	2.17	0.43
8:H:138:GLN:HG3	8:H:285:LEU:HD21	1.99	0.43
8:H:277:TYR:OH	9:I:66:LEU:O	2.29	0.43
10:P:81:ILE:HG12	12:R:46:VAL:HG11	1.99	0.43
10:P:231:LEU:HB2	10:P:233:PHE:HD1	1.82	0.43
10:P:304:LEU:HA	10:P:307:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:55:VAL:HG22	16:W:20:VAL:HG21	1.99	0.43
11:Q:59:LEU:N	11:Q:59:LEU:CD1	2.78	0.43
13:S:85:ASP:OD1	13:S:86:GLU:N	2.51	0.43
18:Z:101:VAL:CB	18:Z:102:PRO:HD2	2.45	0.43
18:Z:128:ARG:O	18:Z:129:THR:C	2.61	0.43
20:b:37:PRO:O	20:b:40:LYS:NZ	2.51	0.43
1:A:72:LEU:O	8:H:151:LEU:HD11	2.19	0.43
27:B:304:PC1:H241	10:P:310:PHE:CE1	2.53	0.43
3:C:117:ASP:OD1	3:C:124:ARG:HB2	2.18	0.43
4:D:129:TYR:CE2	4:D:391:VAL:HG22	2.54	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
8:H:124:ASN:HD22	8:H:124:ASN:HA	1.63	0.43
8:H:318:MET:HB2	8:H:318:MET:HE3	1.92	0.43
9:I:57:ALA:O	9:I:61:LEU:HB2	2.18	0.43
11:Q:75:ARG:NH1	11:Q:102:ASP:OD1	2.51	0.43
16:W:45:GLU:O	16:W:46:VAL:C	2.59	0.43
1:A:79:ILE:HG13	1:A:87:MET:HE1	2.01	0.43
1:A:87:MET:O	1:A:88:MET:C	2.60	0.43
4:D:137:ASP:HB2	4:D:223:HIS:HA	1.99	0.43
4:D:142:VAL:HG12	4:D:182:ASN:HA	2.01	0.43
5:E:196:THR:O	5:E:199:ASP:N	2.51	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
7:G:462:PHE:CZ	7:G:466:LEU:HD21	2.54	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.61	0.43
10:P:232:GLY:O	10:P:273:LEU:HB3	2.18	0.43
21:q:26:VAL:HG13	21:q:30:ALA:HB3	2.00	0.43
21:q:68:MET:HE2	21:q:71:LYS:HD3	1.99	0.43
1:A:33:LYS:NZ	2:B:154:GLU:HB2	2.33	0.43
2:B:108:ALA:N	2:B:114:MET:HE3	2.33	0.43
2:B:170:TYR:CD2	4:D:135:TYR:CE1	3.06	0.43
2:B:224:ARG:HG3	10:P:136:THR:HG21	2.00	0.43
4:D:172:VAL:HG21	4:D:310:VAL:CG2	2.49	0.43
4:D:211:PHE:HD1	4:D:221:ARG:O	2.01	0.43
5:E:63:GLU:O	5:E:64:ALA:C	2.61	0.43
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.41	0.43
5:E:162:THR:HG21	5:E:166:LYS:HA	2.01	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:36:LYS:CB	6:F:38:GLU:HG2	2.42	0.43
6:F:119:GLU:H	6:F:159:ARG:HD2	1.83	0.43
7:G:291:ARG:HD2	7:G:292:PHE:CE2	2.54	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
7:G:617:ARG:HH22	16:W:128:GLY:H	1.64	0.43
10:P:111:ARG:NH1	10:P:138:ASN:HB3	2.33	0.43
10:P:283:MET:HG2	10:P:353:LEU:HD12	1.99	0.43
15:V:56:LEU:HG	15:V:60:LYS:HE3	2.01	0.43
19:a:18:ILE:O	19:a:22:SER:HB3	2.18	0.43
1:A:96:THR:O	1:A:97:ILE:C	2.61	0.43
4:D:188:THR:O	4:D:192:LEU:HD13	2.18	0.43
4:D:265:ASN:O	4:D:266:ARG:C	2.61	0.43
6:F:398:ARG:HH21	7:G:155:GLU:HG3	1.83	0.43
10:P:187:GLY:O	10:P:188:GLU:C	2.62	0.43
10:P:276:LEU:CD2	10:P:280:ILE:CD1	2.95	0.43
13:S:44:LEU:CD2	13:S:91:MET:HG2	2.48	0.43
21:q:66:THR:HG23	21:q:74:PHE:HD1	1.83	0.43
2:B:74:VAL:O	2:B:78:LEU:HG	2.19	0.43
2:B:199:GLU:O	2:B:200:ALA:C	2.60	0.43
6:F:157:TYR:CG	6:F:212:LEU:CD1	3.01	0.43
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.43
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.43
7:G:184:ARG:O	7:G:185:PHE:C	2.60	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
7:G:651:PRO:HG2	13:S:57:GLU:O	2.19	0.43
8:H:61:MET:O	8:H:63:PRO:HD3	2.18	0.43
8:H:231:ILE:O	8:H:231:ILE:HG22	2.19	0.43
16:W:87:ILE:O	16:W:88:LYS:C	2.61	0.43
19:a:49:GLU:O	19:a:50:ARG:C	2.60	0.43
21:q:41:GLU:HG2	21:q:42:ASP:H	1.84	0.43
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.43
7:G:61:PRO:HB3	7:G:146:PHE:CD2	2.53	0.43
7:G:114:GLU:CD	22:r:53:TYR:HD1	2.26	0.43
7:G:165:ILE:CG2	7:G:169:VAL:HB	2.48	0.43
8:H:142:TYR:CD2	8:H:289:LEU:HD12	2.54	0.43
10:P:134:TRP:CZ2	10:P:311:GLU:HG2	2.54	0.43
10:P:226:VAL:HG21	10:P:277:VAL:CG1	2.49	0.43
14:T:147:TYR:O	14:T:148:ILE:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:42:TRP:CE2	33:W:201:EHZ:O1	2.71	0.43
17:X:131:VAL:HG23	17:X:131:VAL:O	2.19	0.43
18:Z:87:LEU:HA	18:Z:90:ASN:HB2	2.01	0.43
18:Z:120:LEU:O	18:Z:121:ILE:C	2.61	0.43
19:a:37:ARG:NH1	19:a:59:ARG:HD2	2.34	0.43
3:C:53:THR:O	3:C:54:HIS:C	2.60	0.43
3:C:120:THR:CG2	3:C:121:ARG:H	2.32	0.43
5:E:145:ASP:O	5:E:146:SER:C	2.62	0.43
7:G:246:ARG:NH1	11:Q:106:ARG:HE	2.17	0.43
7:G:571:HIS:HD2	7:G:572:HIS:NE2	2.09	0.43
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
7:G:651:PRO:O	7:G:654:VAL:HG12	2.19	0.43
7:G:664:TYR:OH	13:S:23:LEU:HD11	2.18	0.43
8:H:283:ASP:N	8:H:283:ASP:OD1	2.52	0.43
9:I:71:GLY:O	22:r:15:ALA:HB1	2.19	0.43
10:P:92:MET:C	10:P:94:LEU:H	2.26	0.43
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.43
15:V:31:THR:O	15:V:32:LEU:C	2.61	0.43
17:X:48:TRP:CD2	20:b:55:VAL:HG22	2.54	0.43
22:r:5:THR:CG2	22:r:7:VAL:HG12	2.46	0.43
1:A:34:ALA:O	1:A:35:ASN:C	2.59	0.43
2:B:171:TYR:CE1	4:D:135:TYR:CD1	3.06	0.43
3:C:127:ILE:H	3:C:127:ILE:HD12	1.83	0.43
3:C:219:VAL:HG21	16:W:113:THR:HG21	2.01	0.43
5:E:138:PRO:HG3	6:F:355:ILE:HD13	1.99	0.43
5:E:144:SER:O	5:E:147:ILE:HB	2.19	0.43
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.34	0.43
6:F:88:ARG:HA	6:F:88:ARG:HD3	1.85	0.43
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.43
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.43
11:Q:132:GLU:H	11:Q:132:GLU:CD	2.27	0.43
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.43
16:W:104:THR:HG22	16:W:108:ARG:NE	2.34	0.43
17:X:18:VAL:CG1	17:X:20:VAL:HG22	2.44	0.43
17:X:130:LYS:HE2	17:X:130:LYS:HB3	1.79	0.43
19:a:18:ILE:H	19:a:19:PRO:HD3	1.84	0.43
19:a:48:MET:HG3	19:a:59:ARG:CD	2.48	0.43
21:q:14:VAL:HG13	21:q:23:LEU:HG	2.01	0.43
3:C:184:ARG:NH2	4:D:112:HIS:HE2	2.17	0.42
4:D:218:SER:OG	4:D:219:GLY:N	2.51	0.42
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.42
6:F:45:LEU:HG	6:F:46:TYR:CE1	2.54	0.42
6:F:410:ASP:OD1	6:F:410:ASP:C	2.62	0.42
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.42
7:G:117:MET:SD	7:G:143:SER:HB2	2.58	0.42
7:G:304:GLU:CG	7:G:305:PRO:HD2	2.47	0.42
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.42
8:H:102:ILE:HG22	8:H:150:LEU:HD11	2.00	0.42
8:H:249:ILE:HG12	17:X:99:HIS:CE1	2.54	0.42
8:H:307:LEU:HD23	8:H:310:PHE:HZ	1.84	0.42
8:H:309:ILE:HG22	20:b:39:THR:HG23	2.01	0.42
10:P:72:HIS:O	10:P:73:LEU:C	2.61	0.42
16:W:98:LYS:HD3	16:W:100:TRP:CE2	2.53	0.42
2:B:108:ALA:HB2	2:B:114:MET:HE3	2.01	0.42
2:B:122:ARG:HB3	26:B:302:UQ1:H72	1.98	0.42
4:D:159:LEU:HG	4:D:391:VAL:HG12	2.01	0.42
5:E:78:VAL:HG21	6:F:218:GLY:O	2.20	0.42
6:F:291:GLU:OE2	6:F:292:MET:N	2.53	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:304:GLU:HB3	7:G:316:TYR:HD1	1.83	0.42
7:G:480:ALA:O	7:G:481:LEU:C	2.63	0.42
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.18	0.42
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.54	0.42
8:H:231:ILE:HG23	8:H:270:PHE:CD2	2.54	0.42
10:P:271:TYR:CA	10:P:375:VAL:HG22	2.50	0.42
10:P:309:PRO:HG2	10:P:310:PHE:CD2	2.54	0.42
11:Q:69:GLU:O	11:Q:72:ILE:CG2	2.62	0.42
14:T:105:MET:HE1	14:T:115:GLN:HG3	1.99	0.42
17:X:119:ARG:NH1	18:Z:63:GLU:OE2	2.52	0.42
20:b:31:ILE:O	20:b:35:ILE:HG22	2.18	0.42
4:D:96:ARG:HB2	4:D:112:HIS:HB2	2.01	0.42
4:D:97:LEU:O	4:D:97:LEU:CG	2.52	0.42
4:D:141:TYR:HB2	4:D:222:MET:CE	2.49	0.42
4:D:236:LEU:HD22	4:D:240:LEU:CD2	2.41	0.42
6:F:41:ILE:HD13	6:F:250:VAL:HG12	2.02	0.42
6:F:296:LEU:HD22	6:F:337:MET:HE1	2.01	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
6:F:363:ILE:HG23	6:F:364:VAL:N	2.33	0.42
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.42
8:H:45:ILE:CD1	19:a:11:ILE:CD1	2.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:85:LEU:CD2	8:H:108:THR:HB	2.49	0.42
8:H:179:TRP:NE1	18:Z:43:LEU:HD12	2.34	0.42
8:H:195:ARG:HG3	8:H:196:ALA:N	2.34	0.42
8:H:303:TRP:HA	20:b:29:ALA:HB2	2.01	0.42
9:I:135:ARG:HD2	12:R:61:ILE:CG1	2.49	0.42
10:P:144:VAL:HG23	10:P:145:PHE:CD2	2.54	0.42
11:Q:130:ALA:O	11:Q:131:LYS:C	2.62	0.42
16:W:23:ILE:HD12	16:W:80:ARG:O	2.19	0.42
16:W:69:MET:O	16:W:71:MET:N	2.53	0.42
16:W:87:ILE:CG2	16:W:91:MET:HE3	2.45	0.42
18:Z:143:TYR:O	18:Z:144:THR:HB	2.14	0.42
19:a:14:VAL:HA	19:a:17:VAL:HG22	2.00	0.42
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.66	0.42
3:C:227:GLN:NE2	9:I:129:THR:HG21	2.34	0.42
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.84	0.42
4:D:234:GLN:NE2	9:I:212:ARG:HB3	2.35	0.42
4:D:261:MET:CE	9:I:73:THR:CG2	2.90	0.42
5:E:73:HIS:HE1	11:Q:166:TRP:CG	2.38	0.42
6:F:126:LYS:HE2	6:F:274:LYS:HZ3	1.85	0.42
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.42
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.28	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.20	0.42
8:H:84:SER:C	8:H:86:TRP:H	2.27	0.42
8:H:190:LEU:HG	8:H:196:ALA:HB3	2.01	0.42
10:P:140:ASP:O	10:P:141:PHE:C	2.62	0.42
13:S:35:ASP:O	13:S:36:PHE:C	2.60	0.42
18:Z:30:LEU:HD12	18:Z:30:LEU:H	1.84	0.42
4:D:264:ASN:HB2	9:I:65:GLU:OE2	2.19	0.42
4:D:385:TYR:HD2	9:I:122:ILE:CD1	2.31	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.42
6:F:257:ARG:HG2	6:F:258:GLY:H	1.84	0.42
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.42
7:G:65:TYR:HB2	7:G:92:CYS:SG	2.59	0.42
7:G:541:PRO:HB2	7:G:561:PRO:CG	2.50	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
7:G:670:GLU:HB2	13:S:42:VAL:HG23	2.01	0.42
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.01	0.42
10:P:75:ARG:C	10:P:77:GLY:H	2.28	0.42
12:R:43:TYR:C	12:R:45:ARG:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:104:PHE:O	14:T:110:LEU:HB2	2.20	0.42
15:V:62:GLU:OE2	15:V:64:ASP:HB3	2.19	0.42
18:Z:111:PHE:CD1	18:Z:117:VAL:HG21	2.55	0.42
24:A:201:3PE:H252	24:A:201:3PE:H281	1.80	0.42
2:B:87:ARG:HH12	27:B:303:PC1:P	2.43	0.42
2:B:94:THR:H	26:B:302:UQ1:C11	2.19	0.42
2:B:202:LEU:HD21	9:I:86:TYR:CG	2.53	0.42
27:B:303:PC1:H142	21:q:77:VAL:HG12	2.02	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:110:PRO:CB	6:F:152:ARG:HE	2.19	0.42
6:F:126:LYS:HG3	6:F:275:LEU:HB2	2.01	0.42
7:G:480:ALA:O	7:G:483:ARG:HG3	2.20	0.42
11:Q:98:LYS:NZ	11:Q:127:THR:OG1	2.52	0.42
11:Q:99:MET:HB2	11:Q:128:PHE:HE2	1.84	0.42
11:Q:126:LEU:CD1	11:Q:137:PHE:CE2	3.03	0.42
14:T:107:ASP:C	14:T:108:LEU:HD12	2.45	0.42
17:X:41:LYS:HB3	17:X:131:VAL:HG11	2.02	0.42
18:Z:12:PRO:CD	18:Z:16:TYR:CZ	3.02	0.42
19:a:58:ASN:O	19:a:59:ARG:C	2.61	0.42
20:b:69:HIS:H	20:b:72:ASP:CG	2.28	0.42
23:s:87:LEU:CB	23:s:91:ARG:HH12	2.31	0.42
2:B:79:ASP:OD1	2:B:79:ASP:C	2.62	0.42
2:B:92:PRO:CB	2:B:130:VAL:CG1	2.98	0.42
2:B:140:LYS:CD	4:D:115:LEU:HD23	2.49	0.42
2:B:193:GLY:HA2	9:I:154:TYR:CE1	2.55	0.42
2:B:224:ARG:HH21	10:P:85:ARG:NH1	2.17	0.42
4:D:266:ARG:NH2	9:I:59:ARG:O	2.52	0.42
6:F:44:ASN:O	6:F:45:LEU:C	2.62	0.42
6:F:315:LEU:HD22	6:F:363:ILE:HD13	2.02	0.42
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.42
12:R:31:ILE:CG2	12:R:35:GLY:HA2	2.50	0.42
12:R:32:THR:C	12:R:34:THR:N	2.76	0.42
13:S:16:LEU:HD11	13:S:19:ILE:HG12	2.02	0.42
15:V:11:LEU:H	15:V:11:LEU:HD12	1.84	0.42
15:V:24:LEU:HD23	15:V:24:LEU:HA	1.90	0.42
16:W:59:VAL:HG12	16:W:63:ARG:HD2	2.01	0.42
17:X:32:TYR:CE1	17:X:67:ALA:HB2	2.55	0.42
1:A:5:THR:OG1	8:H:2:PHE:HE2	2.02	0.42
1:A:13:LEU:O	1:A:17:LEU:HG	2.19	0.42
5:E:190:ASN:HB3	5:E:192:TYR:CE1	2.55	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.42
8:H:21:THR:HG21	30:H:400:UQ9:H15A	2.02	0.42
8:H:102:ILE:CG1	8:H:162:LEU:HD23	2.50	0.42
8:H:231:ILE:HG23	8:H:270:PHE:HD2	1.83	0.42
9:I:79:ARG:HH21	22:r:20:LEU:CD1	2.33	0.42
9:I:128:ILE:HG22	9:I:130:ILE:HG23	2.01	0.42
9:I:182:GLU:HA	21:q:124:TYR:HD2	1.84	0.42
10:P:110:ALA:HB1	10:P:148:ILE:CD1	2.48	0.42
10:P:220:TYR:HA	10:P:223:PHE:CE1	2.55	0.42
13:S:32:GLY:HA2	13:S:35:ASP:CG	2.44	0.42
14:T:90:TYR:HD2	14:T:93:ILE:CB	2.32	0.42
1:A:52:SER:CB	1:A:55:PHE:CE2	2.88	0.42
4:D:159:LEU:CD2	4:D:391:VAL:HG12	2.48	0.42
4:D:184:ILE:HD12	4:D:210:MET:HE1	2.02	0.42
7:G:114:GLU:OE2	22:r:54:TYR:N	2.51	0.42
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.42
7:G:545:LEU:HD21	7:G:547:LEU:CD2	2.50	0.42
8:H:308:PRO:O	8:H:312:ALA:N	2.53	0.42
10:P:96:LEU:HD12	10:P:97:MET:CA	2.49	0.42
10:P:230:SER:C	10:P:232:GLY:N	2.77	0.42
14:T:85:TYR:CZ	14:T:89:LEU:HD11	2.55	0.42
14:T:90:TYR:OH	14:T:92:LYS:HD3	2.20	0.42
15:V:37:HIS:HB2	15:V:95:LEU:HD11	2.01	0.42
1:A:78:ALA:O	1:A:87:MET:SD	2.78	0.42
2:B:141:MET:CE	4:D:115:LEU:HB3	2.37	0.42
5:E:99:LYS:O	5:E:99:LYS:HD3	2.20	0.42
5:E:129:TYR:HA	5:E:188:ASN:ND2	2.31	0.42
5:E:174:GLU:O	5:E:175:CYS:C	2.63	0.42
6:F:261:TRP:CE3	6:F:262:PHE:CD1	3.05	0.42
8:H:201:THR:O	8:H:202:GLU:C	2.62	0.42
10:P:262:THR:HG22	10:P:263:PHE:N	2.35	0.42
13:S:79:LEU:HA	13:S:82:LEU:CG	2.46	0.42
15:V:20:PRO:HG3	15:V:65:VAL:HG22	2.02	0.42
17:X:131:VAL:HG22	20:b:56:PRO:HB2	2.02	0.42
17:X:132:LYS:CB	20:b:59:ASP:HB3	2.48	0.42
1:A:75:LEU:O	1:A:76:PRO:C	2.60	0.41
6:F:196:PHE:CD1	23:s:91:ARG:NE	2.87	0.41
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.41
7:G:555:ILE:HD13	7:G:560:LEU:HD11	2.01	0.41
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.41
9:I:144:ARG:NH2	11:Q:112:MET:O	2.53	0.41
15:V:13:GLY:O	15:V:14:LEU:C	2.63	0.41
16:W:130:ASP:HB2	16:W:131:PRO:HD2	2.02	0.41
17:X:42:GLU:O	17:X:135:ARG:NH2	2.53	0.41
34:a:101:CDL:HB32	22:r:8:ILE:HG13	2.01	0.41
1:A:79:ILE:CD1	8:H:155:LEU:CD2	2.88	0.41
2:B:110:PRO:O	9:I:83:THR:HG22	2.21	0.41
4:D:128:THR:HG22	4:D:131:GLN:CD	2.45	0.41
4:D:184:ILE:HG23	4:D:203:MET:HB3	2.00	0.41
5:E:78:VAL:HG23	5:E:79:LEU:H	1.84	0.41
7:G:36:VAL:O	7:G:37:ASP:C	2.63	0.41
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.41
7:G:403:VAL:HG13	7:G:476:LEU:CD1	2.50	0.41
10:P:110:ALA:HB1	10:P:148:ILE:HD12	2.02	0.41
12:R:79:CYS:O	12:R:88:HIS:CE1	2.73	0.41
15:V:114:TRP:O	15:V:114:TRP:CE3	2.72	0.41
17:X:40:ASN:OD1	17:X:63:VAL:HG22	2.19	0.41
19:a:34:LYS:O	19:a:35:GLU:C	2.63	0.41
21:q:20:LEU:HD23	21:q:20:LEU:C	2.46	0.41
2:B:179:ARG:NH2	3:C:204:THR:OG1	2.53	0.41
3:C:87:ILE:HG21	3:C:95:THR:HG21	2.02	0.41
3:C:114:THR:OG1	4:D:421:ARG:NH1	2.53	0.41
3:C:127:ILE:HD11	3:C:175:VAL:HG21	2.02	0.41
4:D:140:ASP:OD1	4:D:457:VAL:HG11	2.20	0.41
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.20	0.41
4:D:181:LEU:HD22	4:D:214:TYR:OH	2.21	0.41
5:E:155:LEU:CD1	5:E:204:ILE:HD13	2.50	0.41
6:F:94:PRO:CG	6:F:97:LEU:HD12	2.45	0.41
6:F:262:PHE:HA	6:F:265:PHE:CD2	2.56	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:330:LEU:HD12	7:G:544:MET:CE	2.50	0.41
7:G:652:ASN:HA	7:G:655:ARG:CZ	2.51	0.41
8:H:43:TYR:CD1	19:a:4:GLU:HG2	2.54	0.41
8:H:102:ILE:HG12	8:H:162:LEU:HD23	2.02	0.41
10:P:225:ALA:HB3	10:P:291:TYR:CE2	2.55	0.41
10:P:332:LEU:HA	10:P:333:PRO:HD3	1.82	0.41
11:Q:69:GLU:C	11:Q:72:ILE:HG22	2.45	0.41
12:R:40:GLU:HA	12:R:45:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:90:TYR:CD2	14:T:93:ILE:HG12	2.56	0.41
14:T:112:SER:O	14:T:116:VAL:HG23	2.20	0.41
15:V:114:TRP:O	15:V:116:ILE:N	2.52	0.41
16:W:69:MET:O	16:W:70:PHE:C	2.60	0.41
18:Z:116:TRP:CZ2	18:Z:119:PRO:HD3	2.55	0.41
20:b:72:ASP:HB3	20:b:74:LEU:HD12	2.02	0.41
21:q:25:ARG:HB3	21:q:29:ARG:NH1	2.28	0.41
21:q:75:TRP:CE3	21:q:75:TRP:HA	2.55	0.41
1:A:8:PHE:HB2	24:H:401:3PE:H2D1	2.01	0.41
4:D:181:LEU:HD11	4:D:210:MET:HB3	2.02	0.41
5:E:73:HIS:ND1	11:Q:166:TRP:CE2	2.88	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.41
7:G:82:ILE:HD13	7:G:100:TRP:CZ3	2.55	0.41
7:G:302:LEU:N	7:G:571:HIS:O	2.45	0.41
7:G:308:ARG:HG3	7:G:581:ASP:HA	2.01	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.41
8:H:35:LYS:HE2	9:I:83:THR:OG1	2.20	0.41
8:H:102:ILE:HG12	8:H:162:LEU:CD2	2.51	0.41
8:H:135:ALA:HB2	8:H:201:THR:HB	2.02	0.41
8:H:211:PHE:C	8:H:213:VAL:H	2.27	0.41
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.50	0.41
12:R:84:GLY:O	12:R:85:ALA:CB	2.65	0.41
16:W:53:MET:O	16:W:54:GLN:C	2.62	0.41
17:X:16:GLU:O	17:X:64:ASN:ND2	2.53	0.41
17:X:44:MET:HG3	20:b:53:TYR:CE2	2.56	0.41
19:a:43:TYR:O	19:a:47:LEU:HD13	2.20	0.41
20:b:72:ASP:HB3	20:b:74:LEU:CD1	2.50	0.41
3:C:72:VAL:HG22	3:C:87:ILE:HG22	2.01	0.41
5:E:198:LYS:HA	5:E:201:GLU:HB3	2.02	0.41
6:F:132:ARG:HE	6:F:133:HIS:HE2	1.67	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
10:P:147:ASN:N	10:P:147:ASN:ND2	2.69	0.41
11:Q:78:ARG:O	11:Q:80:PHE:CD1	2.74	0.41
11:Q:126:LEU:CD1	11:Q:137:PHE:HE2	2.33	0.41
11:Q:160:TYR:CE2	11:Q:164:PHE:CE2	3.09	0.41
15:V:5:LEU:O	15:V:6:LYS:C	2.64	0.41
15:V:47:TYR:O	15:V:50:GLN:HB3	2.20	0.41
15:V:81:ILE:O	15:V:84:ALA:N	2.53	0.41
17:X:69:ASN:O	17:X:70:PHE:C	2.63	0.41
3:C:202:PRO:O	3:C:203:LEU:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:240:LEU:HG	4:D:244:ILE:HD11	2.02	0.41
4:D:253:LEU:HD23	4:D:254:ARG:HH22	1.86	0.41
4:D:312:ASP:OD1	4:D:313:GLN:HG3	2.20	0.41
4:D:381:HIS:HE1	9:I:161:ALA:O	2.03	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
6:F:64:LYS:HE3	6:F:67:GLU:OE1	2.21	0.41
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
8:H:248:TYR:O	8:H:249:ILE:C	2.62	0.41
8:H:257:THR:O	8:H:260:MET:HB3	2.20	0.41
9:I:36:TYR:HB3	22:r:104:TRP:HE3	1.85	0.41
11:Q:85:ASN:C	11:Q:87:MET:N	2.77	0.41
11:Q:160:TYR:CE2	11:Q:164:PHE:CZ	3.09	0.41
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.41
17:X:31:HIS:CB	17:X:70:PHE:HZ	2.31	0.41
17:X:75:LYS:O	17:X:79:ALA:HB2	2.20	0.41
20:b:32:MET:N	20:b:33:PRO:CD	2.84	0.41
22:r:4:ALA:O	22:r:5:THR:C	2.63	0.41
2:B:98:ALA:HB2	2:B:135:GLY:HA3	2.01	0.41
4:D:386:THR:HG22	9:I:118:LEU:CD1	2.50	0.41
5:E:48:PRO:HD3	5:E:94:ILE:CG2	2.51	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:296:LEU:HD22	6:F:337:MET:HE3	2.02	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.20	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:51:GLN:HE22	11:Q:158:LYS:HB2	1.85	0.41
7:G:136:GLU:HA	11:Q:88:GLN:HE21	1.85	0.41
7:G:193:ASP:OD1	7:G:193:ASP:N	2.53	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:475:VAL:HG22	7:G:514:ASN:OD1	2.20	0.41
7:G:671:LEU:HD12	13:S:42:VAL:HG23	2.02	0.41
8:H:69:SER:O	8:H:73:ILE:HB	2.21	0.41
10:P:128:ASN:HD21	10:P:149:PRO:HB3	1.84	0.41
16:W:53:MET:O	16:W:103:ARG:HG2	2.20	0.41
16:W:93:LEU:HA	16:W:93:LEU:HD23	1.77	0.41
17:X:21:SER:O	17:X:24:VAL:HG22	2.21	0.41
17:X:49:GLU:OE1	20:b:58:ARG:NH2	2.54	0.41
17:X:89:LEU:HD21	17:X:95:GLN:HB3	2.02	0.41
18:Z:23:ARG:CG	18:Z:25:LEU:HD13	2.51	0.41
18:Z:126:GLY:C	18:Z:128:ARG:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:74:LEU:HD12	20:b:74:LEU:N	2.35	0.41
1:A:34:ALA:HB1	8:H:63:PRO:HA	2.02	0.41
1:A:52:SER:O	1:A:53:MET:C	2.62	0.41
2:B:110:PRO:HA	8:H:34:ARG:HB3	2.02	0.41
27:B:304:PC1:C38	8:H:57:MET:HE2	2.50	0.41
3:C:116:VAL:HG21	4:D:412:VAL:HG21	2.02	0.41
3:C:151:PRO:HG2	16:W:23:ILE:HG23	2.03	0.41
3:C:152:ILE:HD11	3:C:177:PHE:CD2	2.51	0.41
4:D:128:THR:N	4:D:131:GLN:HG2	2.36	0.41
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.56	0.41
4:D:207:ARG:HA	4:D:210:MET:HE3	2.03	0.41
4:D:410:TYR:HB3	4:D:423:LYS:HB3	2.03	0.41
5:E:77:ALA:C	5:E:80:PRO:HD2	2.46	0.41
6:F:70:LEU:O	6:F:71:LYS:C	2.63	0.41
6:F:174:ARG:CB	23:s:87:LEU:HD11	2.49	0.41
6:F:299:LEU:HD12	6:F:300:ILE:HG23	2.01	0.41
6:F:379:CYS:SG	25:F:502:SF4:S2	3.19	0.41
7:G:160:VAL:CG1	7:G:161:GLU:N	2.83	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.20	0.41
9:I:135:ARG:O	9:I:135:ARG:CG	2.69	0.41
13:S:16:LEU:HD21	13:S:19:ILE:CD1	2.50	0.41
14:T:122:MET:HG3	14:T:144:ILE:HG21	2.02	0.41
15:V:51:ILE:H	15:V:51:ILE:HG13	1.77	0.41
17:X:28:ALA:HB3	17:X:71:PHE:HE1	1.86	0.41
1:A:7:ILE:O	1:A:11:ILE:HG13	2.20	0.41
1:A:73:LEU:O	8:H:160:TYR:OH	2.36	0.41
2:B:137:LEU:HD21	2:B:145:LEU:HD23	2.02	0.41
2:B:146:ARG:NH1	2:B:149:TYR:HD2	2.18	0.41
3:C:184:ARG:HH22	4:D:112:HIS:HE2	1.69	0.41
4:D:211:PHE:O	4:D:214:TYR:N	2.53	0.41
4:D:420:TYR:CD2	15:V:114:TRP:HH2	2.38	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
6:F:199:ARG:HD3	23:s:80:PHE:CD2	2.55	0.41
6:F:300:ILE:CD1	6:F:307:VAL:HG23	2.49	0.41
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.41
8:H:17:MET:HG2	8:H:228:TYR:CB	2.50	0.41
8:H:91:MET:C	8:H:93:HIS:N	2.77	0.41
8:H:179:TRP:HE1	18:Z:43:LEU:HB2	1.86	0.41
8:H:277:TYR:HA	8:H:278:PRO:HD2	1.95	0.41
9:I:50:MET:HG2	18:Z:33:TYR:OH	2.21	0.41
9:I:117:LYS:HA	9:I:130:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:I:301:3PE:H3F1	24:I:301:3PE:H3C1	1.96	0.41
10:P:113:LYS:O	10:P:114:ASP:CB	2.69	0.41
10:P:170:LEU:HG	10:P:171:ASN:N	2.36	0.41
10:P:237:LYS:HE2	10:P:322:ILE:O	2.20	0.41
10:P:286:ARG:NH1	10:P:358:THR:HG22	2.36	0.41
10:P:357:ARG:NH2	10:P:364:SER:HB3	2.36	0.41
11:Q:86:ASN:OD1	11:Q:86:ASN:O	2.39	0.41
17:X:130:LYS:HD2	20:b:59:ASP:CG	2.45	0.41
19:a:41:VAL:O	19:a:42:GLN:C	2.64	0.41
3:C:134:LEU:HD12	3:C:134:LEU:H	1.86	0.41
3:C:202:PRO:HD3	11:Q:121:LEU:HD21	2.02	0.41
4:D:220:ALA:HB2	9:I:98:ARG:NH2	2.32	0.41
6:F:109:ARG:HH21	6:F:239:PRO:CD	2.34	0.41
6:F:306:GLY:O	6:F:307:VAL:C	2.64	0.41
6:F:427:LEU:HB2	29:F:501:FMN:C7M	2.51	0.41
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.54	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH1	2.48	0.41
7:G:557:ARG:HG3	7:G:579:MET:HB2	2.03	0.41
8:H:89:LEU:HD12	8:H:89:LEU:HA	1.83	0.41
8:H:130:PHE:CE1	8:H:134:ARG:HD2	2.56	0.41
9:I:76:TYR:HE1	9:I:79:ARG:CZ	2.34	0.41
9:I:96:ARG:NH1	9:I:208:ASP:OD1	2.50	0.41
10:P:227:PRO:HB3	10:P:291:TYR:CZ	2.56	0.41
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.35	0.41
19:a:9:LEU:O	19:a:10:ALA:C	2.64	0.41
34:a:101:CDL:C52	21:q:3:LEU:HD13	2.49	0.41
1:A:56:PHE:O	1:A:57:LEU:C	2.63	0.40
2:B:108:ALA:CA	2:B:114:MET:HE3	2.50	0.40
2:B:137:LEU:CD2	2:B:145:LEU:HD23	2.51	0.40
3:C:155:ILE:O	3:C:158:VAL:N	2.54	0.40
3:C:223:VAL:HG23	3:C:225:LEU:HD11	1.93	0.40
4:D:132:ALA:O	4:D:133:LEU:C	2.64	0.40
4:D:151:TYR:O	4:D:152:SER:C	2.63	0.40
6:F:313:ASN:O	6:F:358:ASP:HA	2.21	0.40
6:F:427:LEU:HB2	29:F:501:FMN:HM73	2.03	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
8:H:245:PRO:HG2	8:H:255:TYR:CZ	2.55	0.40
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.21	0.40
9:I:154:TYR:CD1	9:I:154:TYR:N	2.90	0.40
10:P:88:VAL:HG12	10:P:92:MET:HE2	2.03	0.40
10:P:141:PHE:CD1	10:P:145:PHE:HE2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:302:GLY:HA2	10:P:305:PHE:CD2	2.54	0.40
10:P:335:LEU:O	10:P:339:GLY:N	2.54	0.40
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.81	0.40
4:D:81:THR:HA	4:D:99:LEU:O	2.20	0.40
5:E:221:ARG:HB2	5:E:225:GLU:HG2	2.02	0.40
5:E:233:LEU:H	6:F:37:ASP:CG	2.29	0.40
6:F:39:ASP:HA	6:F:261:TRP:CZ2	2.56	0.40
6:F:280:GLY:O	6:F:356:VAL:HB	2.20	0.40
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.40
7:G:50:LEU:HB2	7:G:91:ALA:O	2.21	0.40
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.40
7:G:377:ALA:O	7:G:380:ASP:HB2	2.20	0.40
8:H:84:SER:C	8:H:86:TRP:N	2.75	0.40
8:H:87:VAL:CG2	8:H:88:PRO:HD3	2.49	0.40
8:H:142:TYR:O	8:H:146:MET:HG3	2.22	0.40
8:H:184:MET:CG	8:H:293:PHE:HD2	2.23	0.40
11:Q:112:MET:CE	21:q:126:PRO:HB3	2.51	0.40
13:S:18:GLU:OE2	13:S:68:ARG:NE	2.50	0.40
14:T:105:MET:HE3	14:T:139:MET:HE2	2.03	0.40
17:X:60:GLY:C	18:Z:81:ARG:NH2	2.79	0.40
20:b:66:VAL:HG13	20:b:66:VAL:O	2.20	0.40
21:q:43:LYS:O	21:q:44:TYR:CB	2.70	0.40
1:A:91:ALA:O	1:A:92:PHE:C	2.64	0.40
3:C:208:GLU:HG3	3:C:221:GLU:HG3	2.00	0.40
4:D:201:PHE:CB	8:H:32:GLN:HB3	2.51	0.40
4:D:275:ILE:HG22	4:D:450:ILE:HD11	2.02	0.40
5:E:107:PRO:O	5:E:108:PRO:C	2.64	0.40
6:F:119:GLU:OE1	6:F:119:GLU:HA	2.21	0.40
6:F:128:ARG:HA	6:F:131:MET:CE	2.51	0.40
7:G:161:GLU:OE2	12:R:96:ASP:HB3	2.22	0.40
7:G:381:LEU:HD21	13:S:41:TYR:CZ	2.56	0.40
7:G:403:VAL:O	7:G:476:LEU:HD12	2.21	0.40
7:G:557:ARG:HD3	21:q:144:TYR:CE2	2.56	0.40
7:G:611:THR:HG23	11:Q:104:ARG:O	2.20	0.40
8:H:24:GLU:OE1	8:H:228:TYR:CE2	2.74	0.40
8:H:65:THR:HG22	8:H:67:SER:N	2.37	0.40
8:H:130:PHE:CZ	8:H:134:ARG:HD2	2.56	0.40
8:H:142:TYR:CE2	8:H:289:LEU:HD12	2.57	0.40
8:H:146:MET:CG	8:H:188:SER:HB2	2.52	0.40
8:H:314:VAL:HG23	8:H:314:VAL:O	2.22	0.40
9:I:63:TRP:HZ3	24:I:301:3PE:H322	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:78:PHE:HA	19:a:2:TRP:CD1	2.56	0.40
10:P:83:PRO:C	10:P:108:TRP:CD1	3.00	0.40
11:Q:69:GLU:HG2	11:Q:73:LYS:HG3	2.03	0.40
11:Q:71:HIS:NE2	11:Q:120:PRO:HD2	2.36	0.40
18:Z:10:MET:O	18:Z:11:PRO:C	2.63	0.40
22:r:7:VAL:HG13	22:r:8:ILE:N	2.37	0.40
1:A:88:MET:HE3	1:A:88:MET:HB2	1.80	0.40
1:A:92:PHE:HA	8:H:302:MET:HE2	2.04	0.40
2:B:96:GLY:O	2:B:97:LEU:C	2.63	0.40
2:B:175:TYR:CZ	4:D:117:HIS:HE1	2.39	0.40
3:C:118:VAL:CG1	3:C:120:THR:HG22	2.45	0.40
3:C:164:TRP:CZ2	4:D:111:PRO:HG2	2.57	0.40
4:D:112:HIS:HE1	16:W:100:TRP:NE1	2.18	0.40
4:D:305:THR:OG1	4:D:306:GLN:N	2.54	0.40
6:F:196:PHE:CE1	23:s:91:ARG:CD	2.89	0.40
7:G:49:VAL:HG11	7:G:80:VAL:HG21	2.02	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.10	0.40
7:G:217:GLU:C	7:G:219:SER:N	2.79	0.40
7:G:546:PHE:CD1	7:G:546:PHE:N	2.89	0.40
10:P:132:ARG:NH2	31:P:401:NDP:O2X	2.53	0.40
10:P:175:LYS:HE2	10:P:175:LYS:HB3	1.89	0.40
16:W:58:THR:O	16:W:59:VAL:C	2.62	0.40
17:X:49:GLU:HG3	17:X:50:GLU:N	2.36	0.40
17:X:141:PRO:O	17:X:142:TYR:CB	2.69	0.40
18:Z:10:MET:HE2	18:Z:10:MET:HB2	1.59	0.40
20:b:25:VAL:O	20:b:26:TRP:C	2.62	0.40
20:b:80:TRP:HE3	20:b:84:LEU:HD13	1.87	0.40
21:q:66:THR:O	21:q:67:GLU:HG3	2.21	0.40
22:r:58:ASP:OD1	22:r:58:ASP:O	2.39	0.40
1:A:30:TYR:O	1:A:31:SER:HB2	2.20	0.40
3:C:236:SER:HA	3:C:237:PRO:HD3	1.84	0.40
4:D:113:ILE:HG23	4:D:432:LEU:HD21	2.03	0.40
6:F:102:MET:HE2	6:F:149:MET:HB2	2.03	0.40
6:F:335:VAL:HG12	6:F:336:LEU:N	2.37	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
6:F:413:TRP:CH2	6:F:436:GLN:HG2	2.57	0.40
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.56	0.40
8:H:30:TYR:HB3	9:I:77:LEU:HA	2.03	0.40
9:I:192:ASN:OD1	9:I:193:ASN:N	2.54	0.40
10:P:64:PHE:CE2	10:P:242:VAL:HG22	2.56	0.40
11:Q:55:VAL:HG11	16:W:79:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:35:ASP:HA	13:S:38:VAL:HG22	2.03	0.40
13:S:62:GLN:HA	13:S:63:PRO:HD3	1.98	0.40
14:T:111:ASP:O	14:T:112:SER:C	2.64	0.40
17:X:60:GLY:C	18:Z:81:ARG:HH22	2.30	0.40
22:r:18:GLN:O	22:r:20:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	92/115 (80%)	89 (97%)	3 (3%)	0	100	100
2	B	153/224 (68%)	141 (92%)	11 (7%)	1 (1%)	18	49
3	C	196/263 (74%)	189 (96%)	7 (4%)	0	100	100
4	D	383/463 (83%)	360 (94%)	22 (6%)	1 (0%)	36	65
5	E	208/248 (84%)	194 (93%)	14 (7%)	0	100	100
6	F	424/464 (91%)	404 (95%)	20 (5%)	0	100	100
7	G	685/727 (94%)	635 (93%)	50 (7%)	0	100	100
8	H	313/318 (98%)	281 (90%)	31 (10%)	1 (0%)	36	65
9	I	168/212 (79%)	152 (90%)	16 (10%)	0	100	100
10	P	337/377 (89%)	309 (92%)	28 (8%)	0	100	100
11	Q	114/175 (65%)	100 (88%)	14 (12%)	0	100	100
12	R	81/116 (70%)	72 (89%)	9 (11%)	0	100	100
13	S	81/99 (82%)	74 (91%)	7 (9%)	0	100	100
14	T	73/156 (47%)	69 (94%)	4 (6%)	0	100	100
15	V	110/116 (95%)	99 (90%)	11 (10%)	0	100	100
16	W	112/131 (86%)	103 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	140/172 (81%)	125 (89%)	15 (11%)	0	100	100
18	Z	136/144 (94%)	129 (95%)	5 (4%)	2 (2%)	8	32
19	a	65/70 (93%)	59 (91%)	6 (9%)	0	100	100
20	b	78/84 (93%)	69 (88%)	9 (12%)	0	100	100
21	q	119/145 (82%)	110 (92%)	9 (8%)	0	100	100
22	r	78/113 (69%)	75 (96%)	3 (4%)	0	100	100
23	s	21/104 (20%)	20 (95%)	1 (5%)	0	100	100
All	All	4167/5036 (83%)	3858 (93%)	304 (7%)	5 (0%)	49	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	324	GLY
8	H	196	ALA
18	Z	129	THR
2	B	195	PRO
18	Z	18	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	89/104 (86%)	88 (99%)	1 (1%)	65	76
2	B	131/185 (71%)	129 (98%)	2 (2%)	57	72
3	C	181/227 (80%)	181 (100%)	0	100	100
4	D	332/395 (84%)	330 (99%)	2 (1%)	78	81
5	E	182/206 (88%)	180 (99%)	2 (1%)	65	76
6	F	341/370 (92%)	340 (100%)	1 (0%)	86	86
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	88
8	H	279/280 (100%)	277 (99%)	2 (1%)	76	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	146/178 (82%)	146 (100%)	0	100	100
10	P	296/325 (91%)	295 (100%)	1 (0%)	86	86
11	Q	103/153 (67%)	101 (98%)	2 (2%)	50	68
12	R	70/96 (73%)	70 (100%)	0	100	100
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	73
14	T	69/135 (51%)	69 (100%)	0	100	100
15	V	100/102 (98%)	98 (98%)	2 (2%)	48	68
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	129 (100%)	0	100	100
18	Z	119/123 (97%)	119 (100%)	0	100	100
19	a	57/60 (95%)	57 (100%)	0	100	100
20	b	71/73 (97%)	71 (100%)	0	100	100
21	q	110/131 (84%)	110 (100%)	0	100	100
22	r	76/96 (79%)	75 (99%)	1 (1%)	61	74
23	s	23/95 (24%)	23 (100%)	0	100	100
All	All	3665/4292 (85%)	3647 (100%)	18 (0%)	78	83

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
2	B	82	ILE
2	B	177	VAL
4	D	94	VAL
4	D	127	LYS
5	E	99	LYS
5	E	200	ILE
6	F	137	LYS
7	G	271	MET
8	H	87	VAL
8	H	144	VAL
10	P	318	LYS
11	Q	125	VAL
11	Q	135	ILE
13	S	48	HIS
15	V	51	ILE
15	V	93	LYS

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Mol	Chain	Res	Type
22	r	91	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	106	HIS
2	B	207	GLN
2	B	209	GLN
3	C	88	HIS
3	C	102	HIS
3	C	130	ASN
3	C	163	ASN
3	C	195	HIS
4	D	79	ASN
4	D	92	HIS
4	D	117	HIS
4	D	147	ASN
4	D	149	GLN
4	D	168	GLN
4	D	182	ASN
4	D	234	GLN
4	D	270	ASN
4	D	285	ASN
4	D	313	GLN
4	D	381	HIS
4	D	454	GLN
5	E	132	GLN
5	E	152	GLN
5	E	245	GLN
6	F	116	ASN
6	F	168	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	277	ASN
6	F	346	GLN
7	G	51	GLN
7	G	74	ASN
7	G	101	ASN
7	G	140	GLN
7	G	205	GLN
7	G	384	ASN

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Mol	Chain	Res	Type
7	G	388	ASN
7	G	444	HIS
7	G	495	ASN
7	G	498	GLN
7	G	571	HIS
7	G	572	HIS
7	G	605	GLN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	124	ASN
8	H	171	HIS
8	H	284	GLN
8	H	287	HIS
8	H	292	ASN
9	I	180	HIS
10	P	79	GLN
10	P	128	ASN
10	P	251	ASN
10	P	285	HIS
11	Q	86	ASN
11	Q	88	GLN
13	S	22	HIS
13	S	48	HIS
13	S	81	ASN
13	S	92	GLN
14	T	103	HIS
15	V	50	GLN
15	V	110	ASN
16	W	54	GLN
16	W	61	GLN
16	W	102	GLN
16	W	105	HIS
16	W	129	HIS
17	X	64	ASN
17	X	99	HIS
18	Z	24	ASN
18	Z	90	ASN
20	b	46	ASN
21	q	17	HIS
21	q	91	HIS
21	q	135	HIS

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Mol	Chain	Res	Type
22	r	18	GLN
22	r	21	GLN
22	r	29	GLN
23	s	76	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\# Z > 2$
25	SF4	I	303	9	0,12,12	-	-	-		
34	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.20	6 (9%)
31	NDP	P	401	-	49,52,52	1.20	6 (12%)	66,80,80	1.67	12 (18%)
28	FES	G	803	7	0,4,4	-	-	-		
25	SF4	G	802	7	0,12,12	-	-	-		
25	SF4	G	801	7	0,12,12	-	-	-		
25	SF4	B	301	2	0,12,12	-	-	-		
24	3PE	I	301	-	50,50,50	0.91	2 (4%)	53,55,55	1.03	2 (3%)
24	3PE	A	201	-	41,41,50	1.01	2 (4%)	44,46,55	1.09	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	FES	E	301	5	0,4,4	-	-	-		
27	PC1	B	303	-	34,34,53	1.14	2 (5%)	40,42,61	1.11	3 (7%)
27	PC1	B	304	-	42,42,53	1.04	2 (4%)	48,50,61	1.01	3 (6%)
25	SF4	I	302	9	0,12,12	-	-	-		
26	UQ1	B	302	-	18,18,18	1.96	2 (11%)	22,25,25	1.25	4 (18%)
24	3PE	H	401	-	47,47,50	0.93	2 (4%)	50,52,55	1.11	3 (6%)
29	FMN	F	501	-	33,33,33	1.41	5 (15%)	48,50,50	1.19	6 (12%)
33	EHZ	W	201	-	27,31,37	1.73	5 (18%)	37,41,47	1.55	5 (13%)
25	SF4	F	502	6	0,12,12	-	-	-		
30	UQ9	H	400	-	35,35,58	0.80	2 (5%)	42,45,73	0.47	0

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
25	SF4	I	303	9	-	-	0/6/5/5
34	CDL	a	101	-	-	18/67/67/110	-
31	NDP	P	401	-	-	6/34/77/77	0/5/5/5
28	FES	G	803	7	-	-	0/1/1/1
25	SF4	G	802	7	-	-	0/6/5/5
25	SF4	G	801	7	-	-	0/6/5/5
25	SF4	B	301	2	-	-	0/6/5/5
24	3PE	I	301	-	-	17/54/54/54	-
24	3PE	A	201	-	-	12/45/45/54	-
28	FES	E	301	5	-	-	0/1/1/1
27	PC1	B	303	-	-	13/38/38/57	-
27	PC1	B	304	-	-	14/46/46/57	-
25	SF4	I	302	9	-	-	0/6/5/5
26	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
24	3PE	H	401	-	-	13/51/51/54	-
29	FMN	F	501	-	-	4/18/18/18	0/3/3/3
33	EHZ	W	201	-	-	12/39/39/45	-
25	SF4	F	502	6	-	-	0/6/5/5
30	UQ9	H	400	-	-	16/30/54/81	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	302	UQ1	C6-C5	7.34	1.48	1.35
33	W	201	EHZ	C15-N2	5.16	1.44	1.33
33	W	201	EHZ	C12-N1	5.03	1.44	1.33
29	F	501	FMN	C9A-C5A	4.84	1.49	1.41
34	a	101	CDL	OA8-CA7	4.31	1.45	1.33
24	A	201	3PE	O31-C31	4.28	1.45	1.33
27	B	303	PC1	O31-C31	4.20	1.45	1.33
27	B	304	PC1	O31-C31	4.16	1.45	1.33
34	a	101	CDL	OB8-CB7	4.16	1.45	1.33
27	B	304	PC1	O21-C21	4.16	1.46	1.34
24	I	301	3PE	O31-C31	4.15	1.45	1.33
31	P	401	NDP	C5A-C4A	4.12	1.46	1.39
24	H	401	3PE	O31-C31	4.12	1.45	1.33
24	I	301	3PE	O21-C21	4.08	1.45	1.34
24	H	401	3PE	O21-C21	4.06	1.45	1.34
24	A	201	3PE	O21-C21	4.06	1.45	1.34
34	a	101	CDL	OA6-CA5	4.04	1.45	1.34
27	B	303	PC1	O21-C21	3.94	1.45	1.34
34	a	101	CDL	OB6-CB5	3.93	1.45	1.34
31	P	401	NDP	C6N-C5N	3.25	1.39	1.33
29	F	501	FMN	C8-C7	3.11	1.48	1.40
26	B	302	UQ1	C3-C2	3.09	1.48	1.36
29	F	501	FMN	C4-N3	-2.76	1.33	1.38
30	H	400	UQ9	C3-C2	-2.66	1.41	1.48
30	H	400	UQ9	C4-C5	-2.53	1.41	1.48
33	W	201	EHZ	O4-C15	-2.44	1.18	1.23
31	P	401	NDP	C5A-N7A	-2.43	1.34	1.39
31	P	401	NDP	C5A-C6A	2.43	1.47	1.41
29	F	501	FMN	C5A-N5	-2.38	1.34	1.39
33	W	201	EHZ	O3-C12	-2.37	1.18	1.23
31	P	401	NDP	C8A-N7A	2.36	1.36	1.31
33	W	201	EHZ	C9-S1	2.23	1.81	1.76
31	P	401	NDP	C4A-N9A	-2.07	1.33	1.37
29	F	501	FMN	C4A-N5	2.06	1.34	1.30

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	W	201	EHZ	C8-C9-S1	6.03	121.09	113.63
31	P	401	NDP	C5A-C4A-N3A	-6.01	118.91	126.75
31	P	401	NDP	N3A-C4A-N9A	4.71	134.85	127.08
34	a	101	CDL	OA6-CA5-C11	4.21	120.58	111.50
24	I	301	3PE	O21-C21-C22	4.10	120.34	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	401	3PE	O21-C21-C22	4.05	120.22	111.50
31	P	401	NDP	PN-O3-PA	-4.05	118.94	132.83
27	B	304	PC1	O21-C21-C22	3.96	120.03	111.50
24	A	201	3PE	O21-C21-C22	3.92	119.96	111.50
31	P	401	NDP	C2A-N3A-C4A	3.81	120.75	111.75
27	B	303	PC1	O21-C21-C22	3.67	119.42	111.50
34	a	101	CDL	OB6-CB5-C51	3.53	119.11	111.50
31	P	401	NDP	N3A-C2A-N1A	-3.19	123.61	128.60
31	P	401	NDP	C4A-C5A-N7A	-3.12	106.81	110.62
24	H	401	3PE	O31-C31-C32	2.88	120.94	111.91
31	P	401	NDP	C4A-N9A-C8A	2.83	108.79	105.73
26	B	302	UQ1	CM5-C5-C6	-2.82	119.80	124.40
27	B	303	PC1	O31-C31-C32	2.81	120.73	111.91
34	a	101	CDL	OA8-CA7-C31	2.80	120.68	111.91
31	P	401	NDP	C5A-N7A-C8A	2.67	107.30	103.51
24	A	201	3PE	O31-C31-C32	2.65	120.23	111.91
27	B	303	PC1	C2-O21-C21	-2.64	111.29	117.79
33	W	201	EHZ	C10-S1-C9	2.62	110.03	101.87
24	I	301	3PE	O31-C31-C32	2.50	119.76	111.91
29	F	501	FMN	C4A-C10-N1	-2.50	118.92	124.73
29	F	501	FMN	O4-C4-C4A	-2.48	120.02	126.60
33	W	201	EHZ	C13-C12-N1	2.48	120.59	116.42
34	a	101	CDL	OB8-CB7-C71	2.45	119.60	111.91
33	W	201	EHZ	C14-N2-C15	-2.44	118.24	122.59
26	B	302	UQ1	C11-C9-C10	2.41	119.92	114.60
27	B	304	PC1	O31-C31-C32	2.36	119.33	111.91
33	W	201	EHZ	O2-C9-S1	-2.34	119.58	122.61
31	P	401	NDP	C2B-C1B-N9A	-2.32	109.62	113.53
29	F	501	FMN	C4-C4A-N5	2.31	121.53	118.23
31	P	401	NDP	N9A-C8A-N7A	-2.24	110.85	113.91
34	a	101	CDL	CB4-OB6-CB5	-2.16	112.47	117.79
27	B	304	PC1	C2-O21-C21	-2.13	112.53	117.79
26	B	302	UQ1	C7-C8-C9	-2.13	120.60	127.26
31	P	401	NDP	C6A-C5A-N7A	2.12	135.98	132.02
34	a	101	CDL	CA4-OA6-CA5	-2.10	112.63	117.79
31	P	401	NDP	C3D-C2D-C1D	2.09	105.39	101.43
29	F	501	FMN	C4A-C10-N10	2.04	119.46	116.48
26	B	302	UQ1	C8-C7-C6	-2.03	106.57	112.05
29	F	501	FMN	C4A-C4-N3	2.03	118.34	113.19
29	F	501	FMN	C10-N1-C2	2.02	120.94	116.90
24	H	401	3PE	O21-C21-O22	-2.00	118.86	123.70

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	201	3PE	C1-O11-P-O14
24	A	201	3PE	C11-O13-P-O11
24	A	201	3PE	C11-O13-P-O14
24	A	201	3PE	C22-C21-O21-C2
24	H	401	3PE	C1-O11-P-O14
24	H	401	3PE	C11-O13-P-O14
24	H	401	3PE	O22-C21-O21-C2
24	H	401	3PE	C22-C21-O21-C2
24	I	301	3PE	C1-O11-P-O14
24	I	301	3PE	C11-O13-P-O12
27	B	303	PC1	C11-O13-P-O14
27	B	303	PC1	C22-C21-O21-C2
27	B	304	PC1	C1-O11-P-O14
27	B	304	PC1	C22-C21-O21-C2
29	F	501	FMN	C5'-O5'-P-O2P
29	F	501	FMN	C5'-O5'-P-O3P
30	H	400	UQ9	C22-C23-C24-C26
30	H	400	UQ9	C22-C23-C24-C25
30	H	400	UQ9	C20-C19-C21-C22
30	H	400	UQ9	C18-C19-C21-C22
30	H	400	UQ9	C15-C14-C16-C17
30	H	400	UQ9	C13-C14-C16-C17
30	H	400	UQ9	C12-C13-C14-C16
30	H	400	UQ9	C12-C13-C14-C15
30	H	400	UQ9	C11-C12-C13-C14
31	P	401	NDP	C5D-O5D-PN-O1N
33	W	201	EHZ	O1-C7-C8-C9
33	W	201	EHZ	C6-C7-C8-C9
33	W	201	EHZ	C16-C17-C20-O6
33	W	201	EHZ	O2-C9-S1-C10
33	W	201	EHZ	C8-C9-S1-C10
34	a	101	CDL	CA2-OA2-PA1-OA4
34	a	101	CDL	OA7-CA5-OA6-CA4
34	a	101	CDL	C11-CA5-OA6-CA4
34	a	101	CDL	CB2-OB2-PB2-OB3
27	B	304	PC1	O32-C31-O31-C3
24	A	201	3PE	O22-C21-O21-C2
27	B	303	PC1	O22-C21-O21-C2
27	B	304	PC1	O22-C21-O21-C2
27	B	304	PC1	C32-C31-O31-C3
24	I	301	3PE	C32-C31-O31-C3
24	H	401	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
24	I	301	3PE	O32-C31-O31-C3
24	H	401	3PE	C32-C31-O31-C3
34	a	101	CDL	C31-CA7-OA8-CA6
24	I	301	3PE	C22-C21-O21-C2
34	a	101	CDL	OA9-CA7-OA8-CA6
30	H	400	UQ9	C9-C11-C12-C13
30	H	400	UQ9	C17-C18-C19-C20
24	I	301	3PE	O22-C21-O21-C2
30	H	400	UQ9	C17-C18-C19-C21
27	B	303	PC1	C11-C12-N-C13
30	H	400	UQ9	C19-C21-C22-C23
24	I	301	3PE	C1-O11-P-O13
24	I	301	3PE	C11-O13-P-O11
27	B	303	PC1	C11-O13-P-O11
27	B	303	PC1	C1-O11-P-O13
34	a	101	CDL	CA2-OA2-PA1-OA5
27	B	303	PC1	C11-C12-N-C14
24	I	301	3PE	C32-C33-C34-C35
33	W	201	EHZ	C18-C17-C20-O6
33	W	201	EHZ	C19-C17-C20-O6
27	B	303	PC1	C11-C12-N-C15
34	a	101	CDL	C13-C14-C15-C16
27	B	304	PC1	C1-O11-P-O13
34	a	101	CDL	C14-C15-C16-C17
33	W	201	EHZ	C3-C4-C5-C6
33	W	201	EHZ	C5-C6-C7-O1
24	H	401	3PE	C3-C2-O21-C21
24	H	401	3PE	C2-C1-O11-P
29	F	501	FMN	C5'-O5'-P-O1P
24	I	301	3PE	C3B-C3C-C3D-C3E
33	W	201	EHZ	C5-C6-C7-C8
30	H	400	UQ9	C14-C16-C17-C18
27	B	303	PC1	C2-C1-O11-P
24	A	201	3PE	C1-C2-C3-O31
24	H	401	3PE	C2B-C2C-C2D-C2E
27	B	304	PC1	C38-C39-C3A-C3B
24	H	401	3PE	C2C-C2D-C2E-C2F
31	P	401	NDP	C2B-O2B-P2B-O1X
27	B	303	PC1	C31-C32-C33-C34
31	P	401	NDP	PN-O3-PA-O2A
31	P	401	NDP	O4D-C1D-N1N-C6N
34	a	101	CDL	CB4-CB3-OB5-PB2

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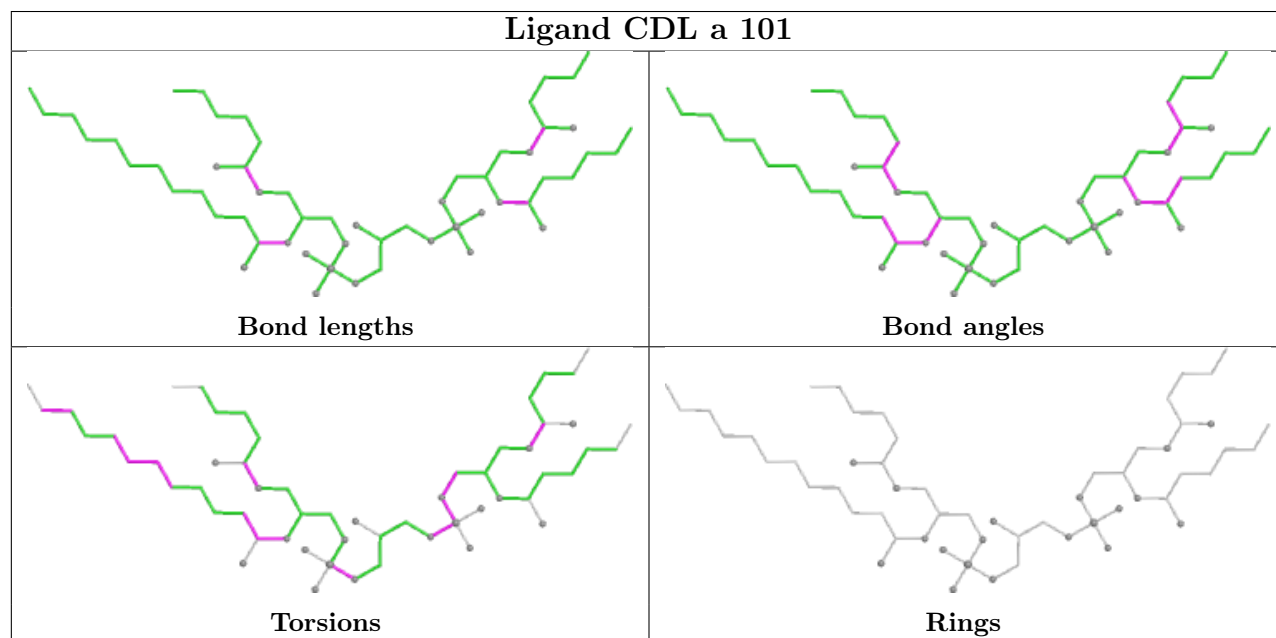
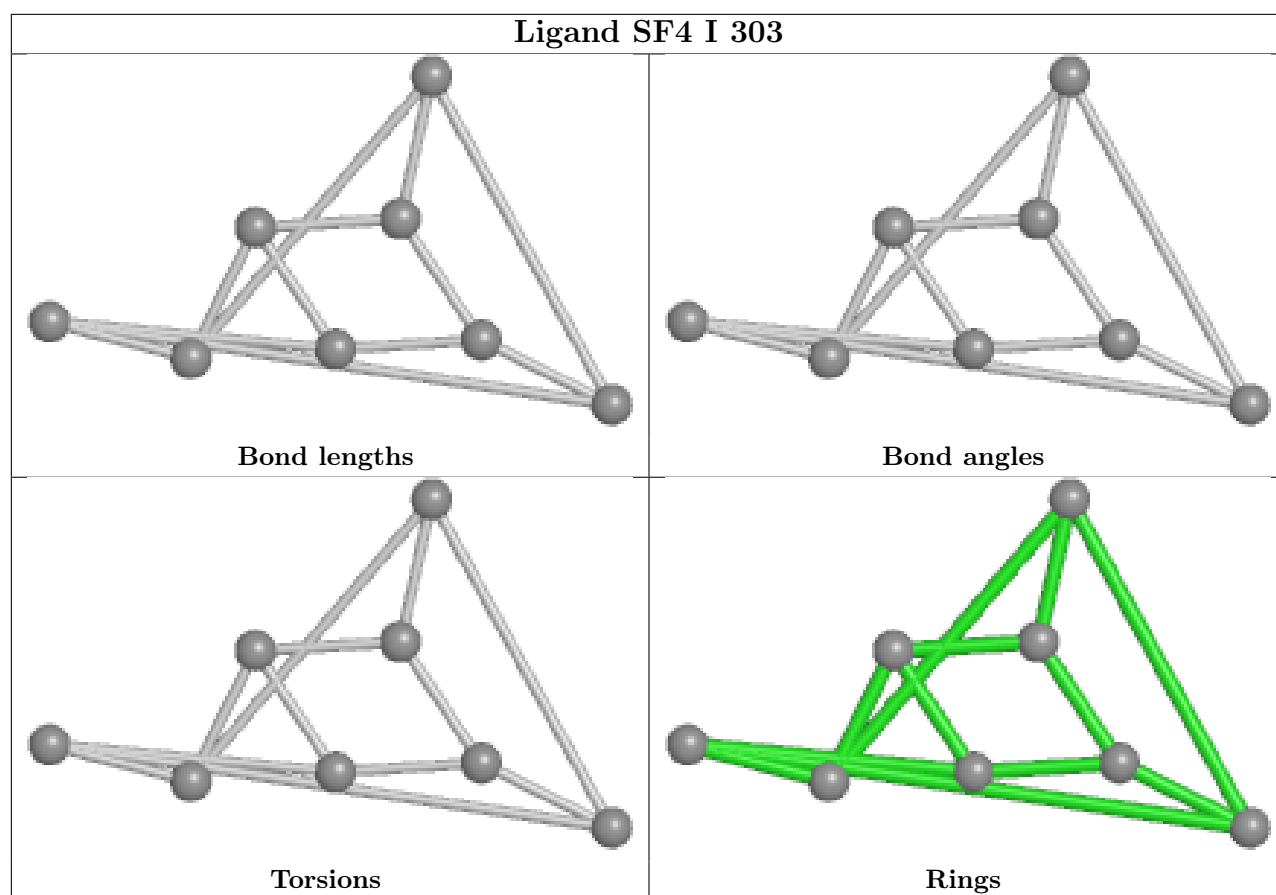
Mol	Chain	Res	Type	Atoms
24	I	301	3PE	C1-O11-P-O12
24	I	301	3PE	C11-O13-P-O14
27	B	303	PC1	C11-O13-P-O12
27	B	303	PC1	C1-O11-P-O14
27	B	304	PC1	C1-O11-P-O12
29	F	501	FMN	N10-C1'-C2'-O2'
33	W	201	EHZ	C2-C3-C4-C5
27	B	304	PC1	C11-C12-N-C14
30	H	400	UQ9	C12-C11-C9-C10
33	W	201	EHZ	O4-C15-C16-O5
24	A	201	3PE	O21-C2-C3-O31
24	A	201	3PE	C1-O11-P-O13
24	H	401	3PE	C11-O13-P-O11
34	a	101	CDL	CB3-OB5-PB2-OB2
34	a	101	CDL	C71-CB7-OB8-CB6
30	H	400	UQ9	C12-C11-C9-C8
27	B	304	PC1	C2-C1-O11-P
24	H	401	3PE	C31-C32-C33-C34
24	A	201	3PE	C23-C24-C25-C26
24	I	301	3PE	O11-C1-C2-C3
34	a	101	CDL	OB9-CB7-OB8-CB6
31	P	401	NDP	PN-O3-PA-O1A
34	a	101	CDL	C15-C16-C17-C18
24	A	201	3PE	C39-C3A-C3B-C3C
27	B	304	PC1	C11-C12-N-C13
24	A	201	3PE	C35-C36-C37-C38
24	I	301	3PE	C31-C32-C33-C34
27	B	304	PC1	C3A-C3B-C3C-C3D
27	B	304	PC1	C11-C12-N-C15
31	P	401	NDP	C5D-O5D-PN-O3
24	H	401	3PE	C37-C38-C39-C3A
34	a	101	CDL	C18-C19-C20-C21
34	a	101	CDL	CB3-OB5-PB2-OB3
24	A	201	3PE	C25-C26-C27-C28
24	I	301	3PE	C12-C11-O13-P
27	B	303	PC1	C33-C34-C35-C36
34	a	101	CDL	C12-C11-CA5-OA7
27	B	304	PC1	C3F-C3G-C3H-C3I
24	I	301	3PE	O31-C31-C32-C33
34	a	101	CDL	C12-C11-CA5-OA6
24	I	301	3PE	O32-C31-C32-C33

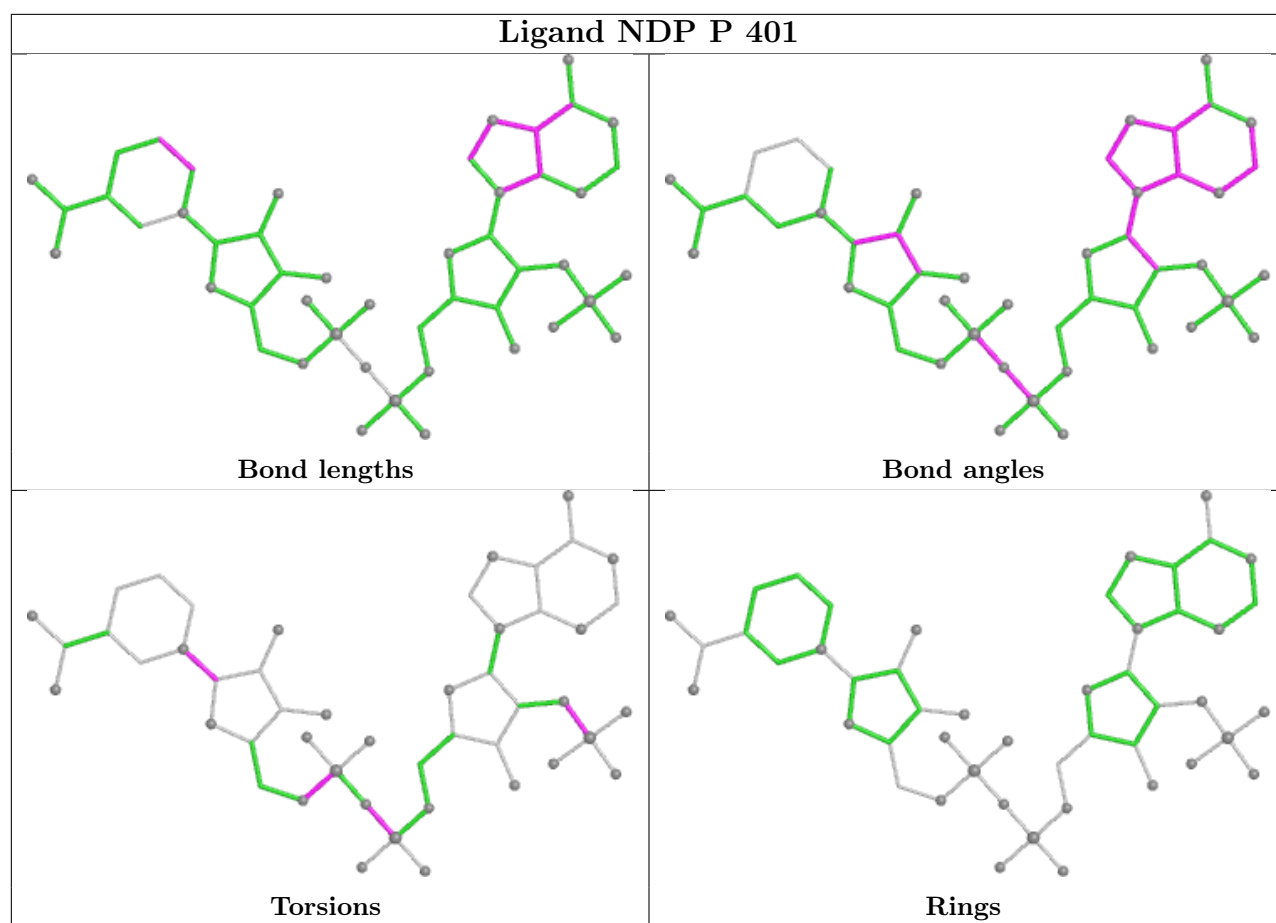
There are no ring outliers.

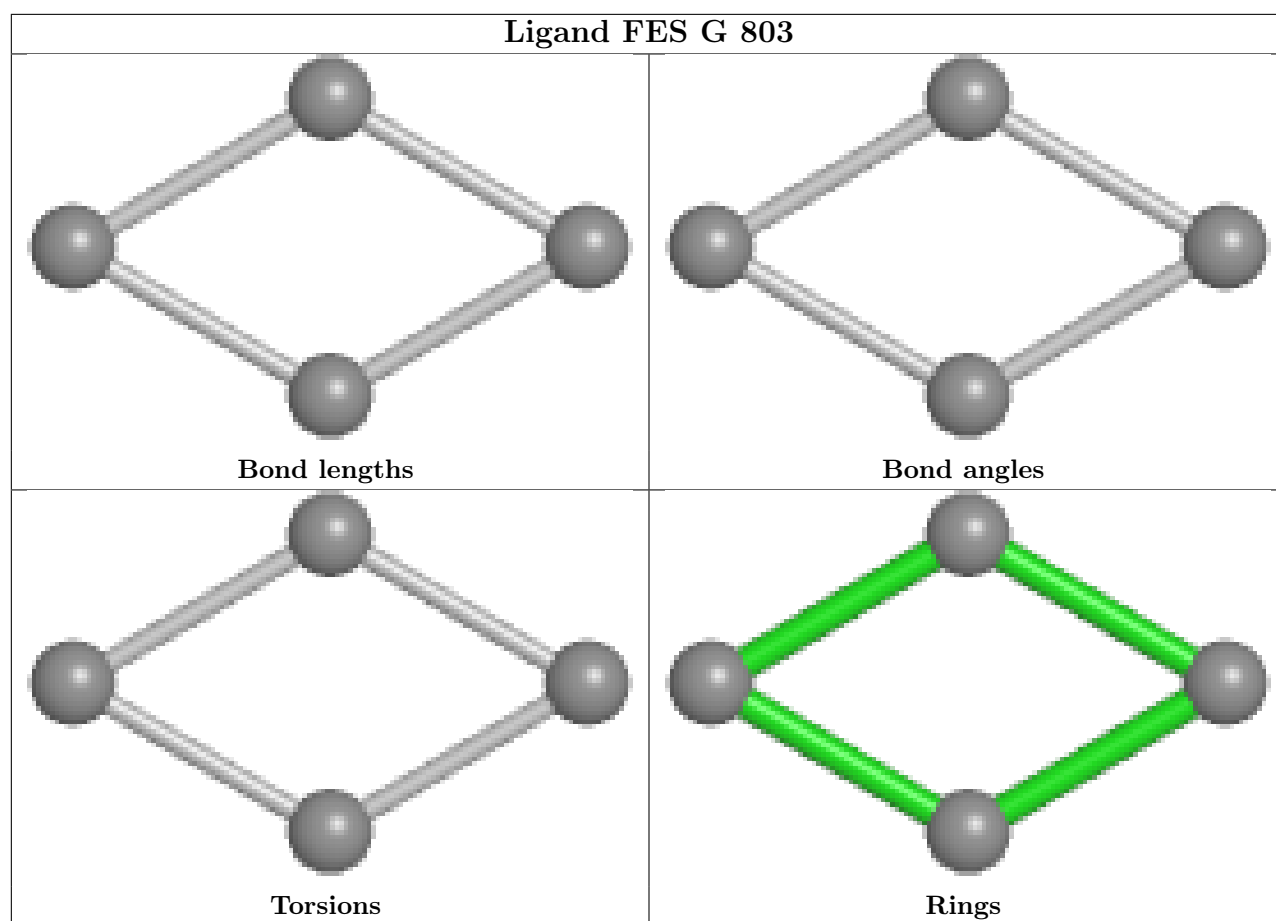
18 monomers are involved in 131 short contacts:

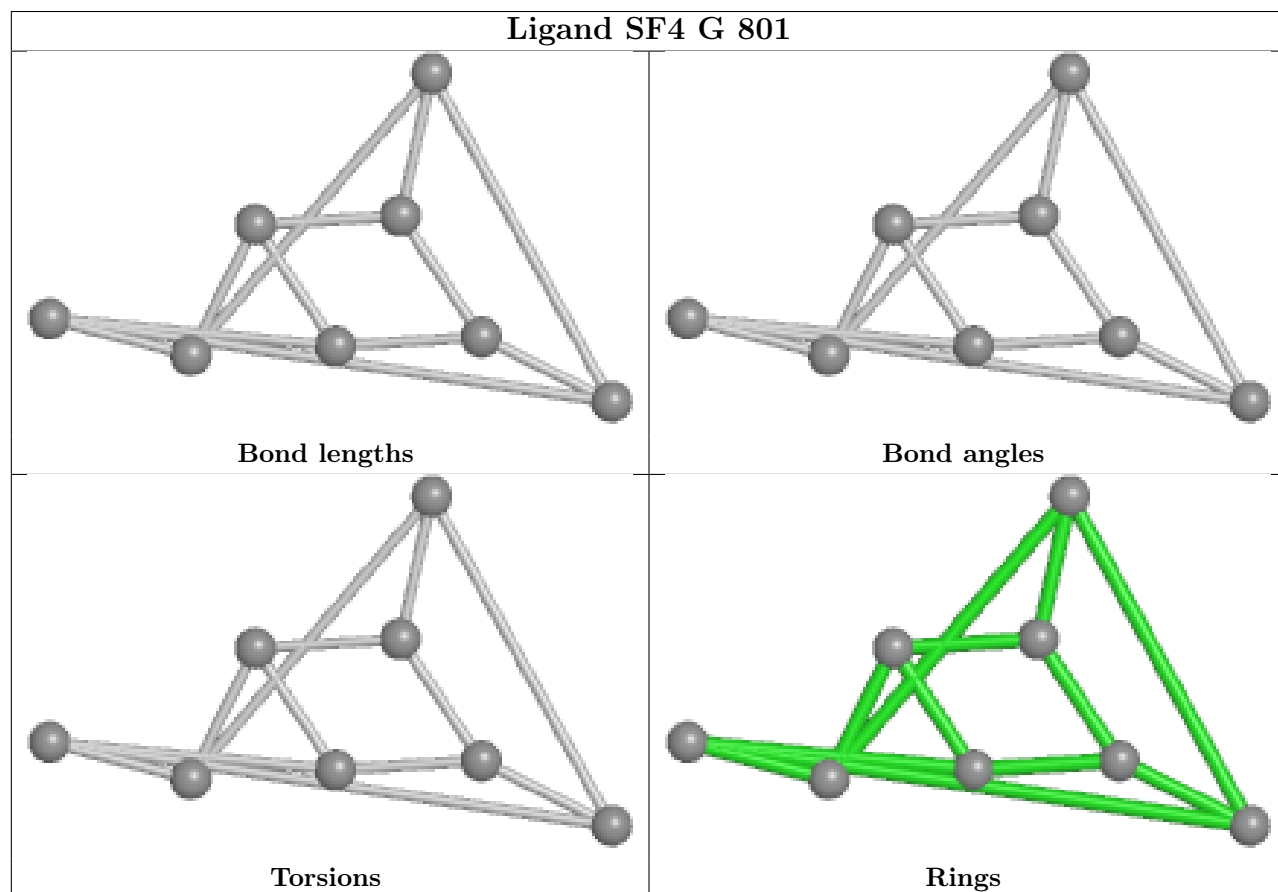
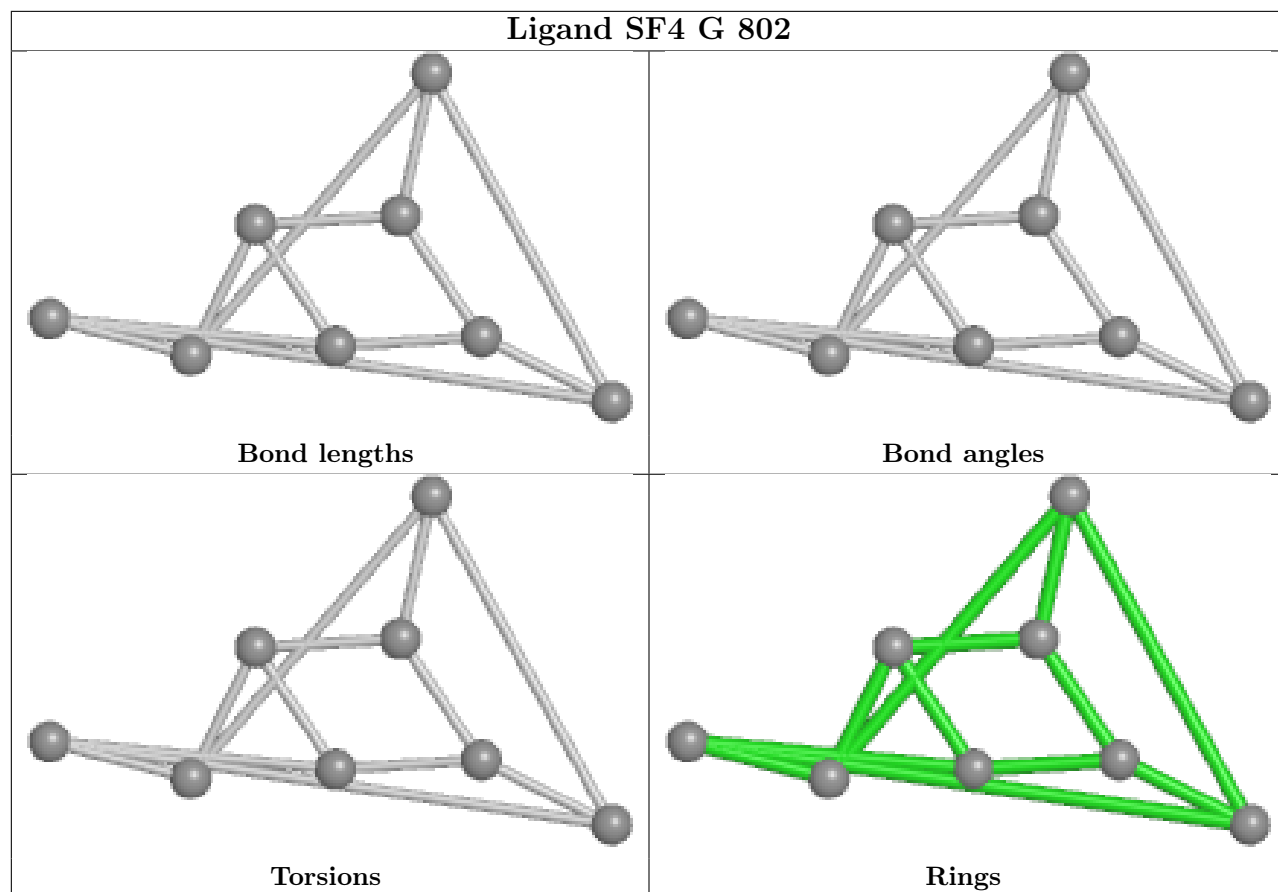
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	I	303	SF4	2	0
34	a	101	CDL	12	0
31	P	401	NDP	7	0
28	G	803	FES	4	0
25	G	802	SF4	8	0
25	B	301	SF4	6	0
24	I	301	3PE	8	0
24	A	201	3PE	8	0
28	E	301	FES	3	0
27	B	303	PC1	9	0
27	B	304	PC1	14	0
25	I	302	SF4	7	0
26	B	302	UQ1	11	0
24	H	401	3PE	12	0
29	F	501	FMN	3	0
33	W	201	EHZ	3	0
25	F	502	SF4	10	0
30	H	400	UQ9	4	0

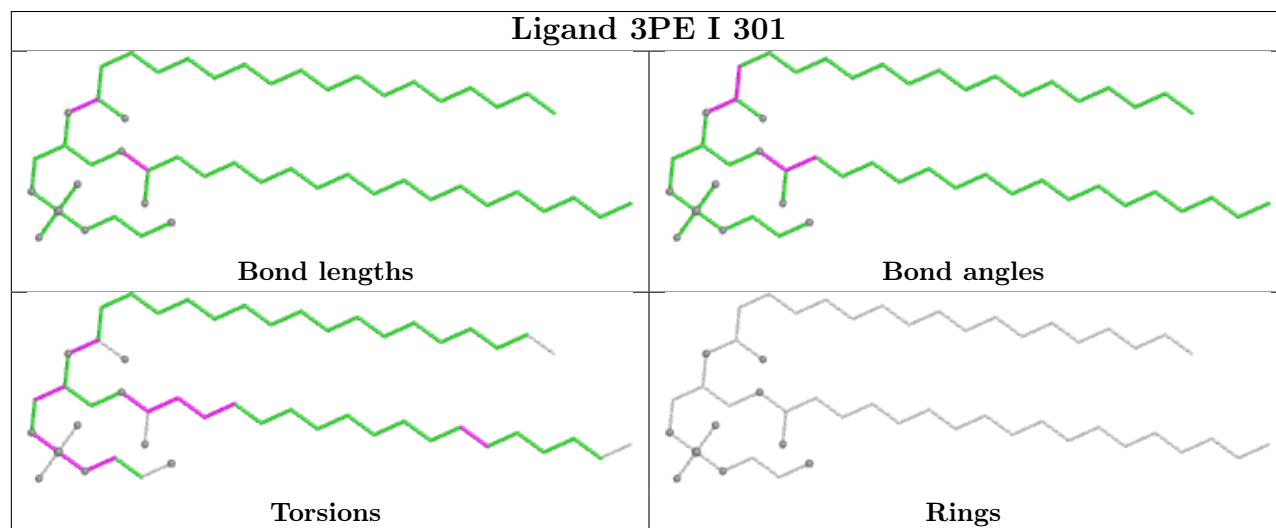
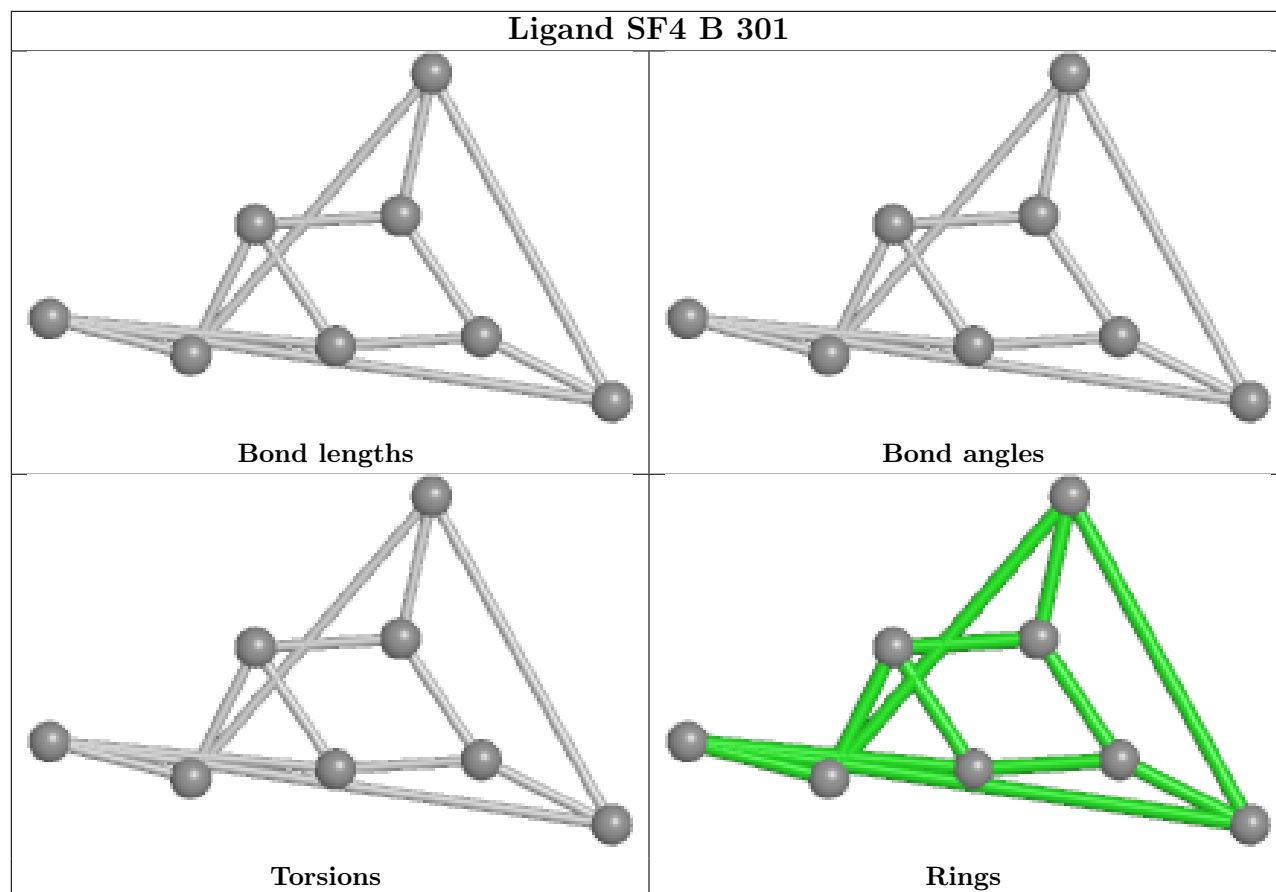
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

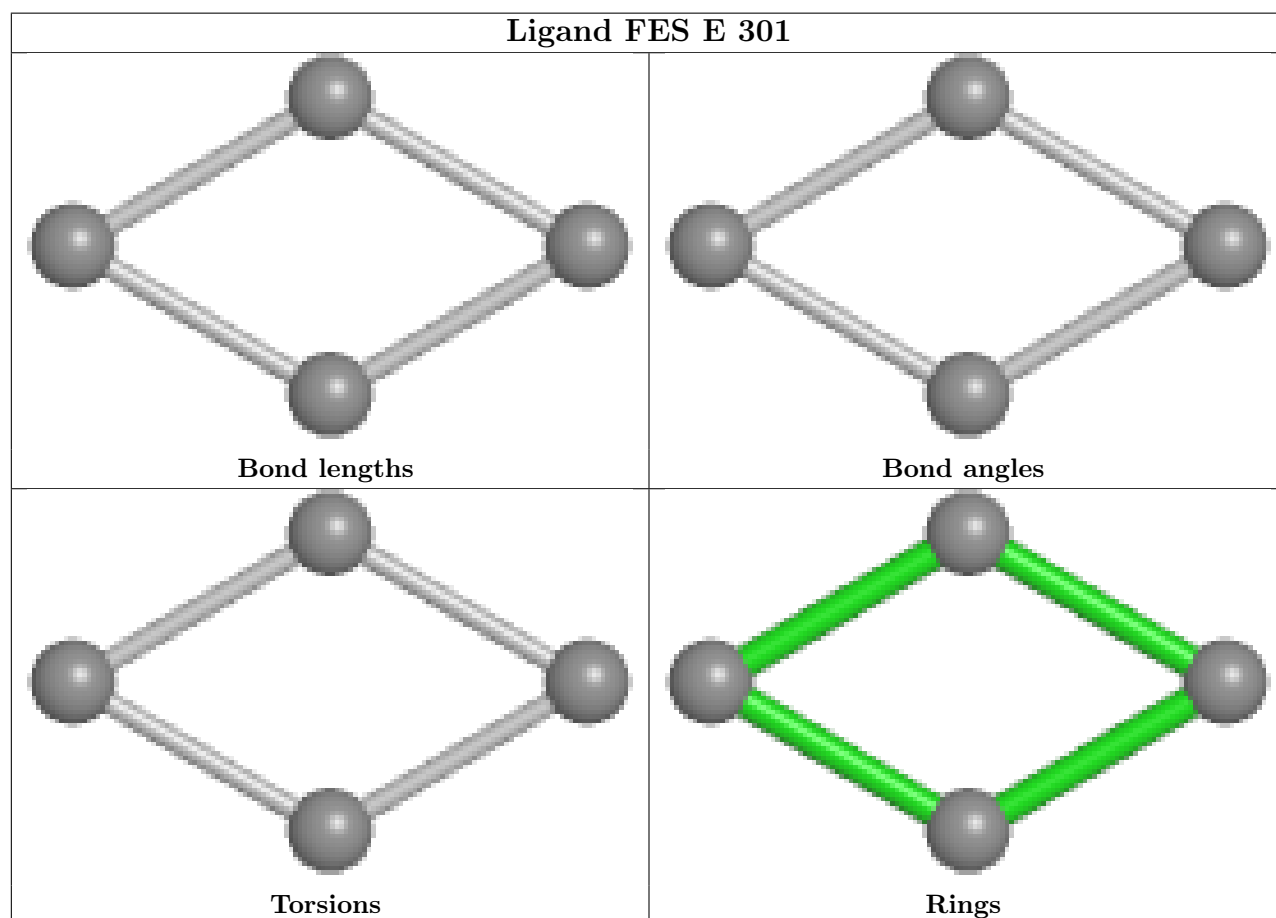
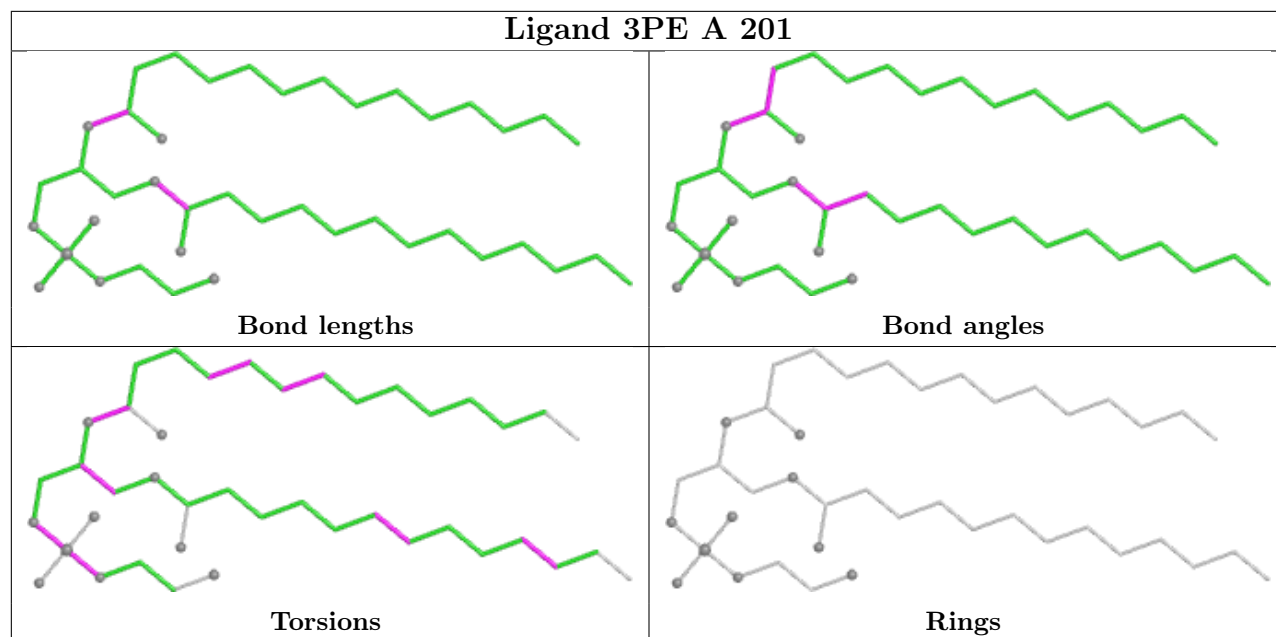


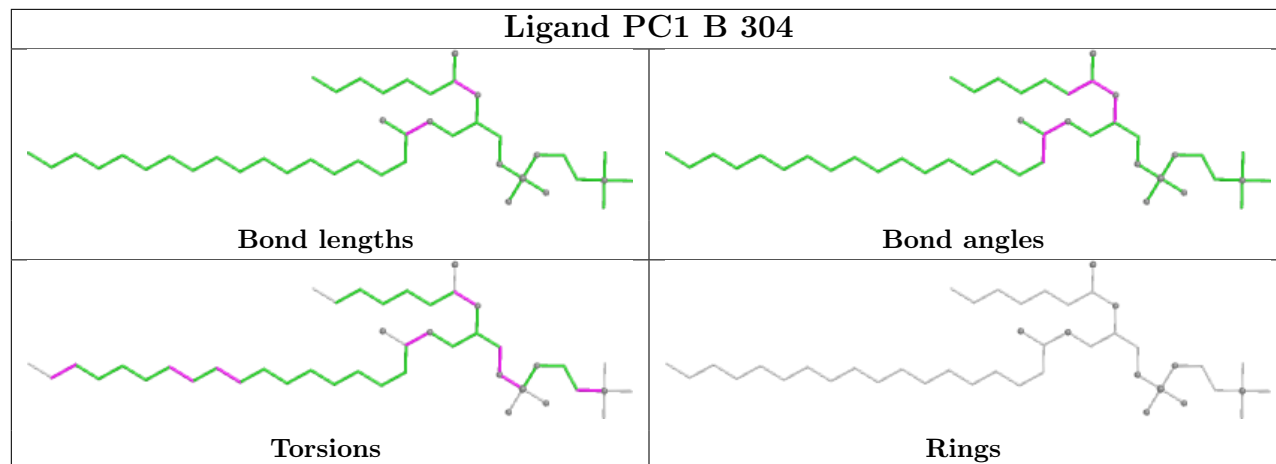
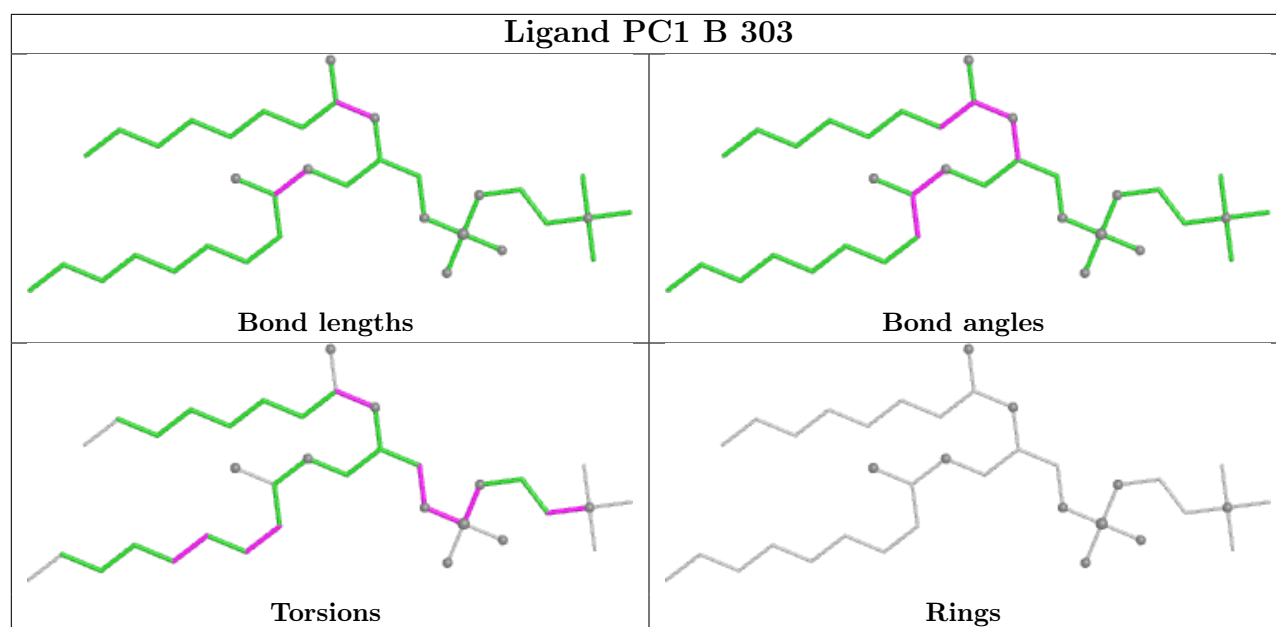


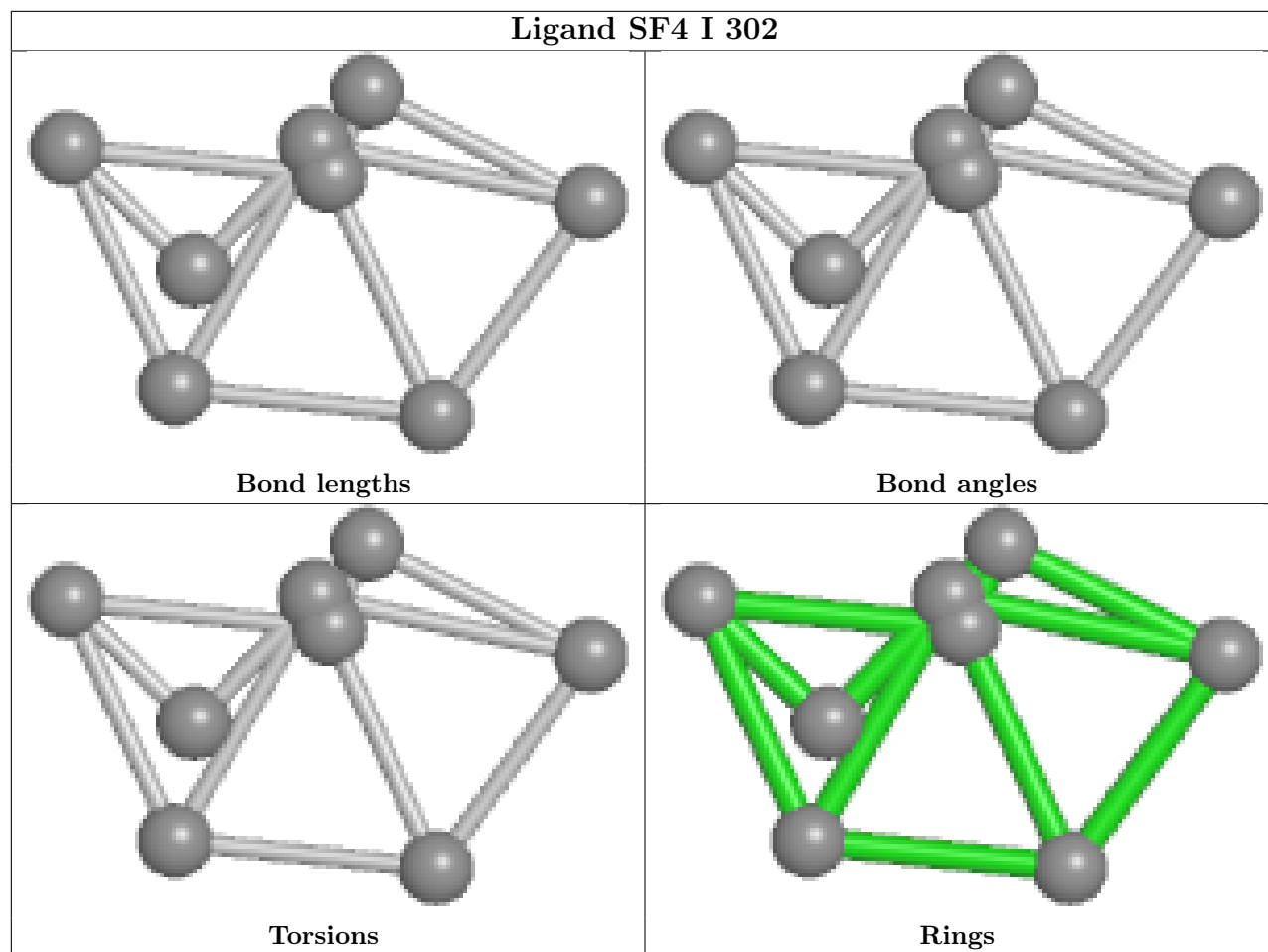




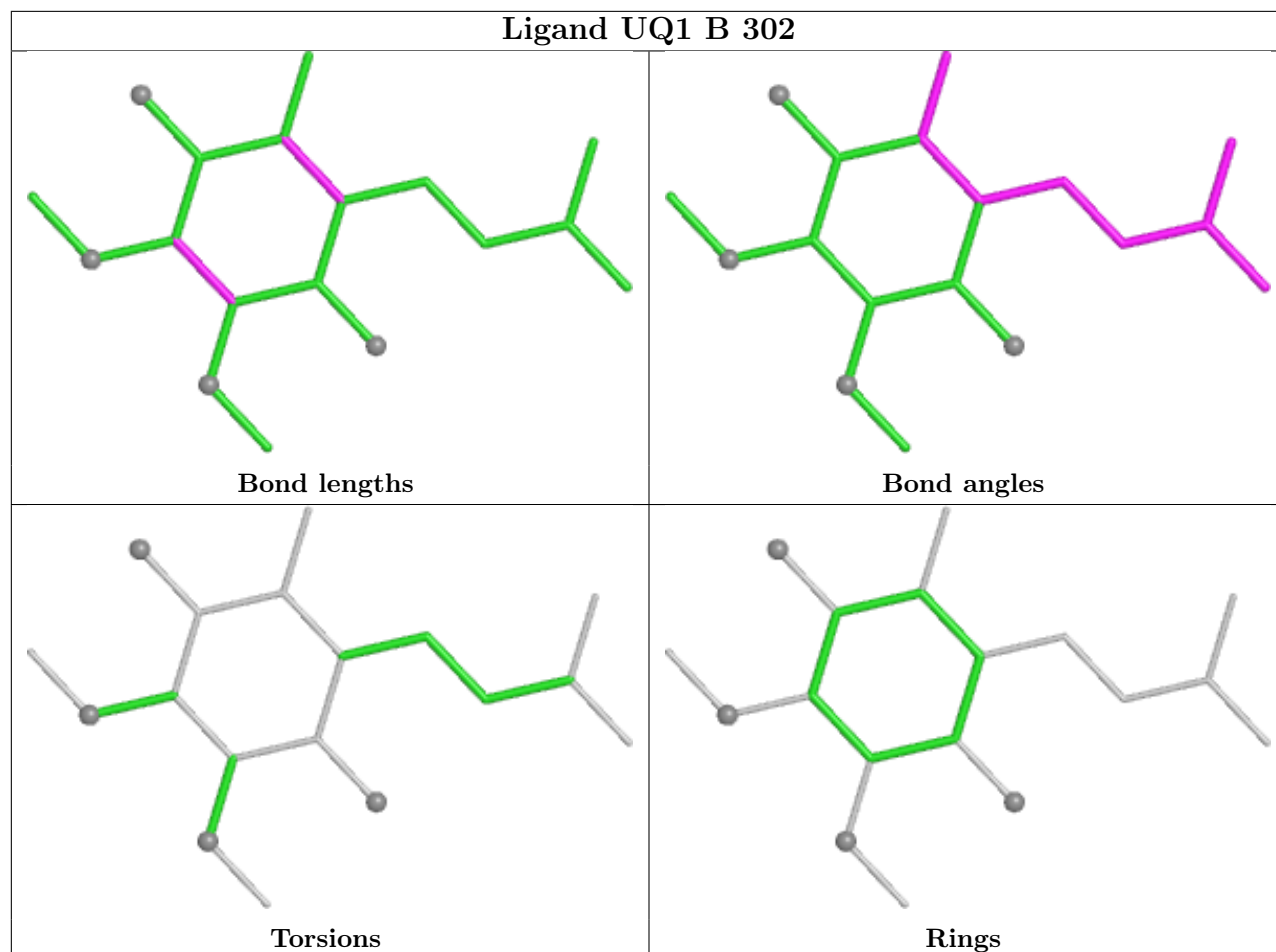




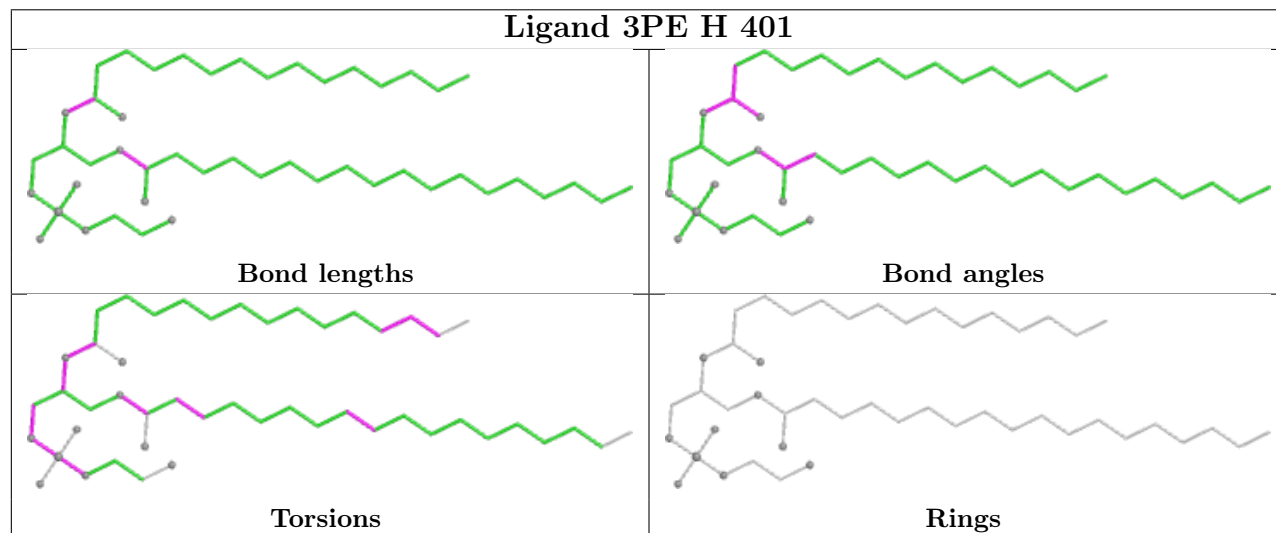


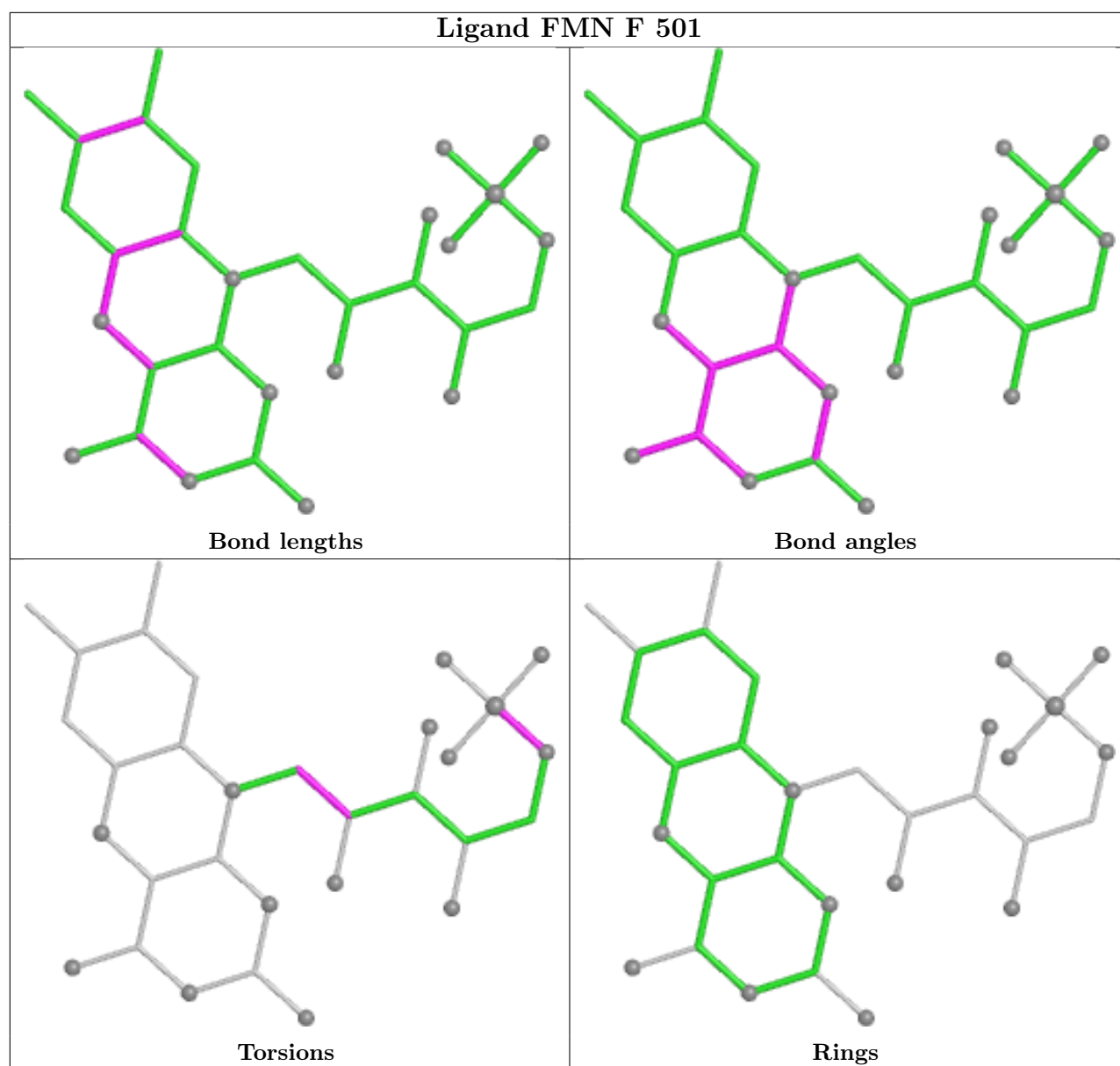


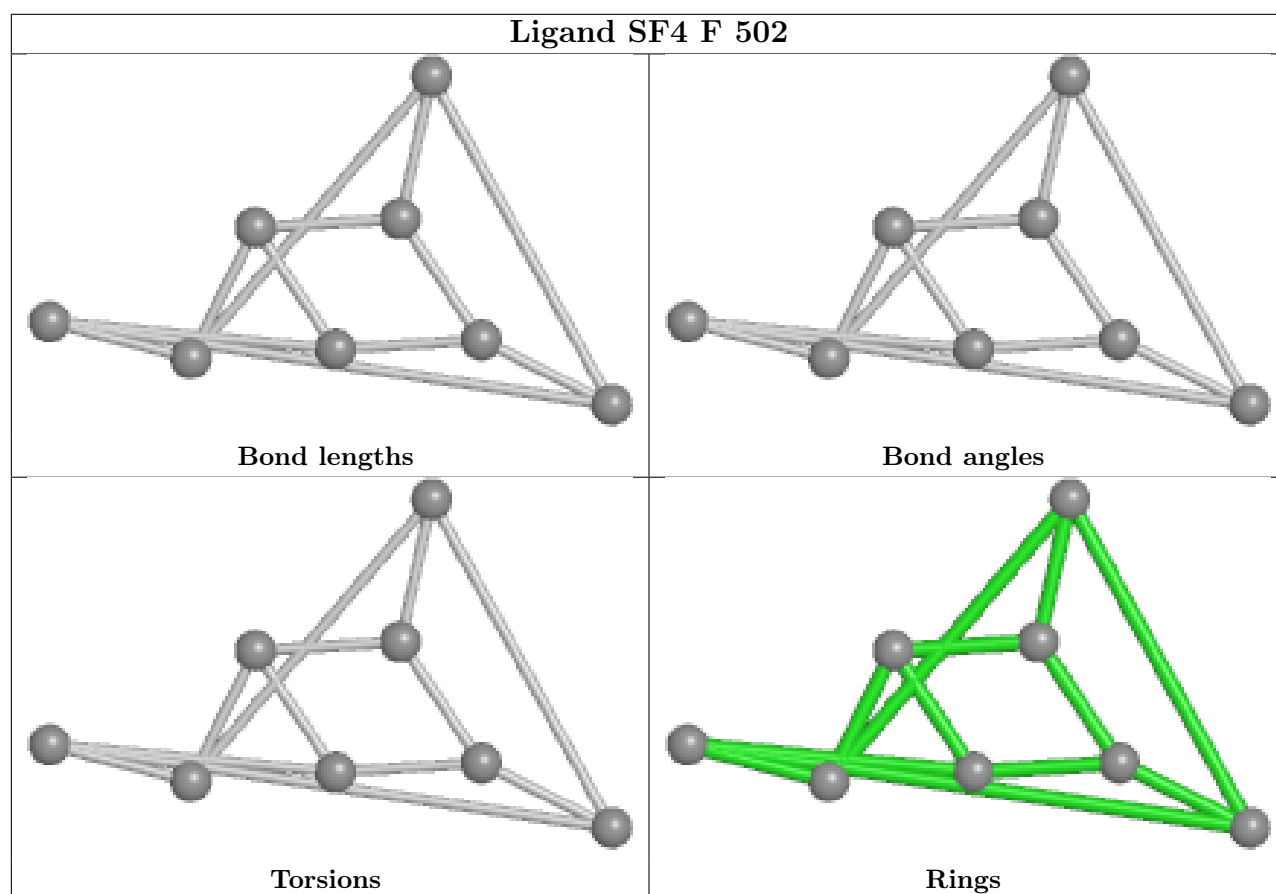
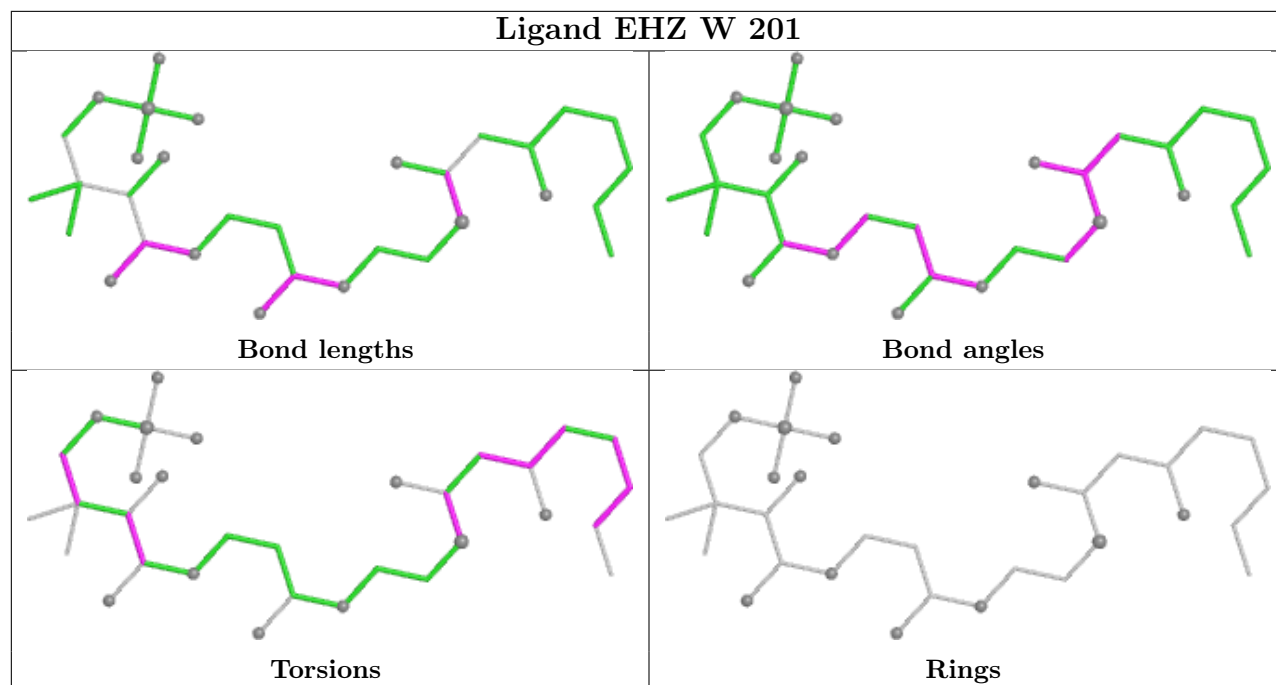
Ligand UQ1 B 302

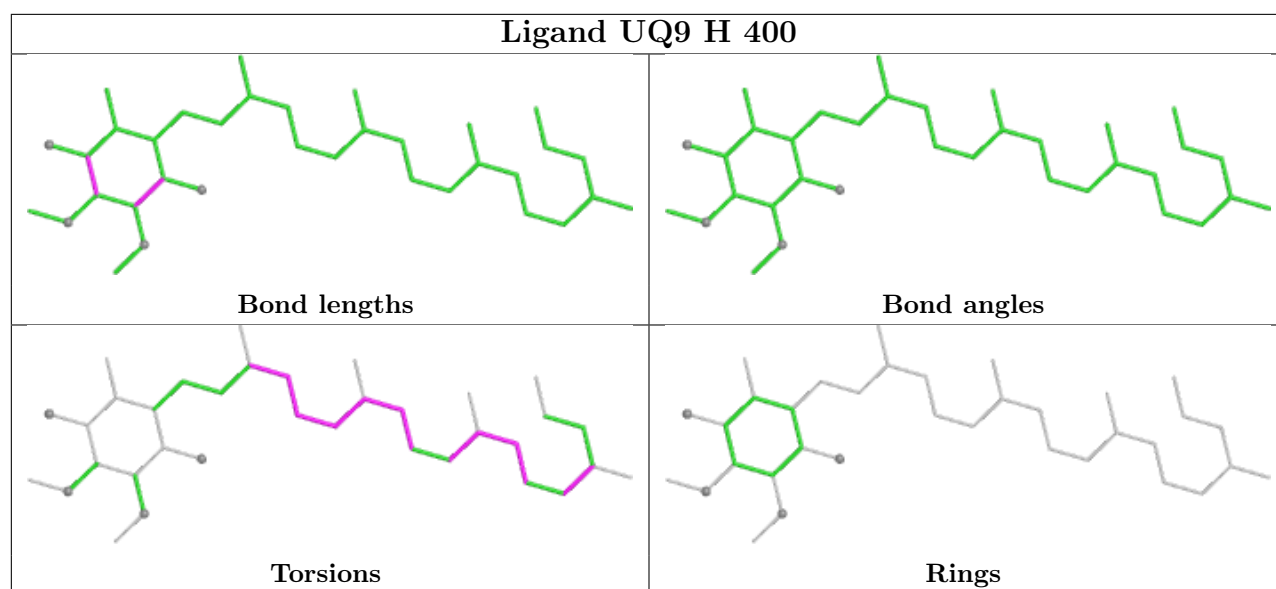


Ligand 3PE H 401









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.

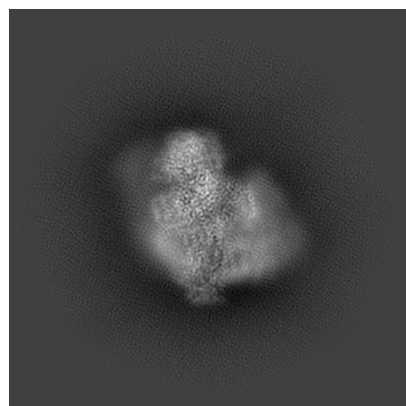
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35341. These allow visual inspection of the internal detail of the map and identification of artifacts.

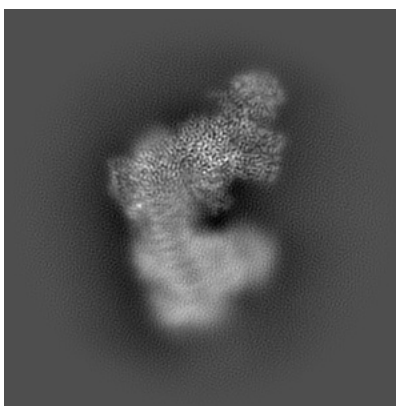
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

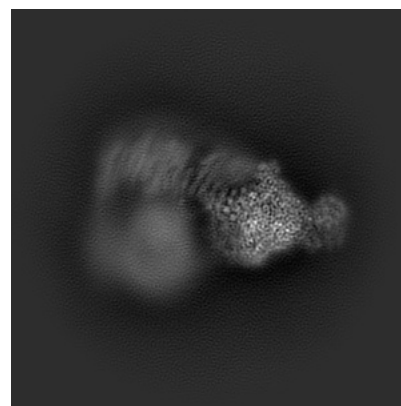
6.1.1 Primary map



X

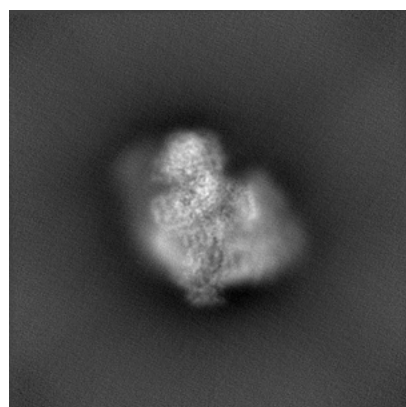


Y

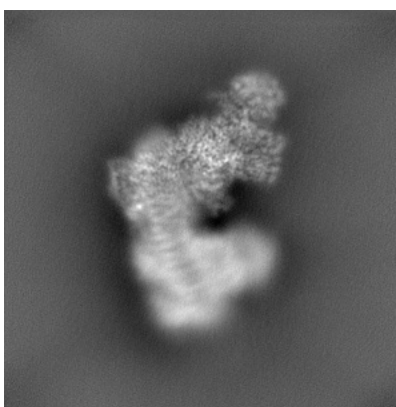


Z

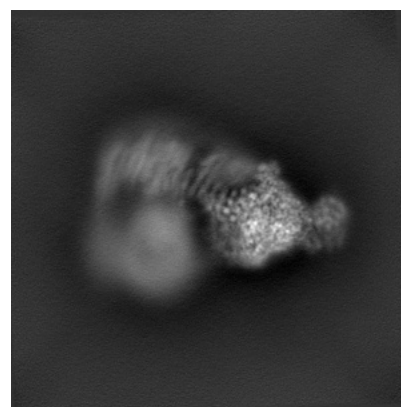
6.1.2 Raw map



X



Y

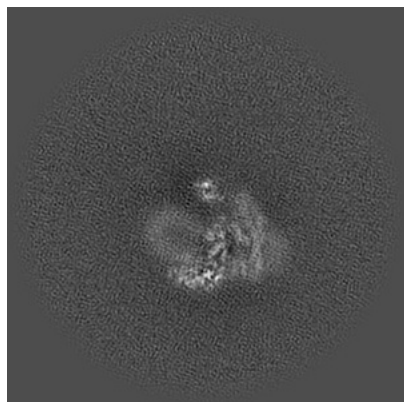


Z

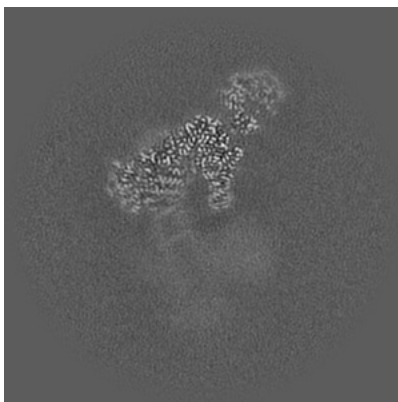
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

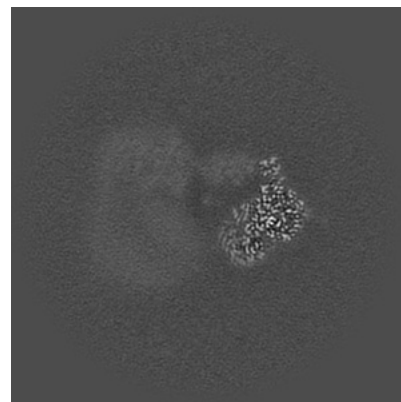
6.2.1 Primary map



X Index: 192

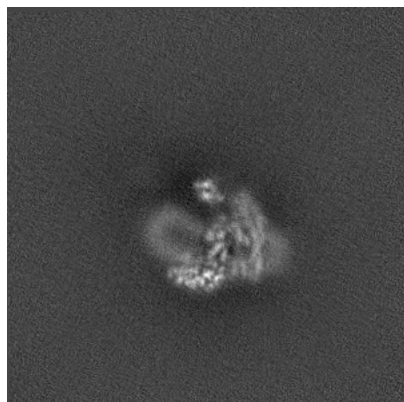


Y Index: 192

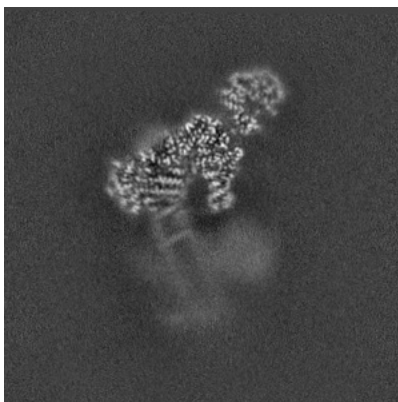


Z Index: 192

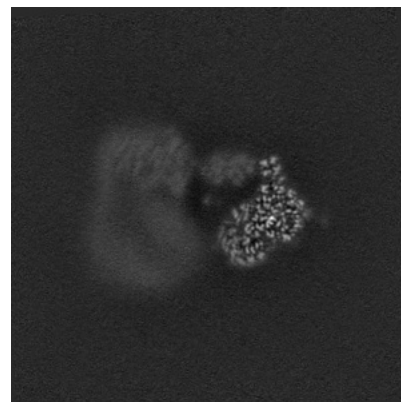
6.2.2 Raw map



X Index: 192



Y Index: 192

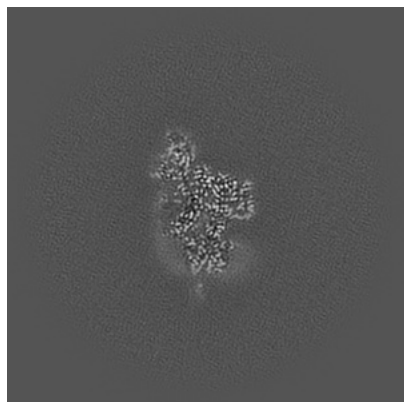


Z Index: 192

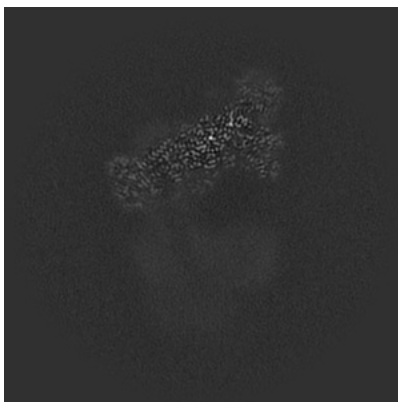
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

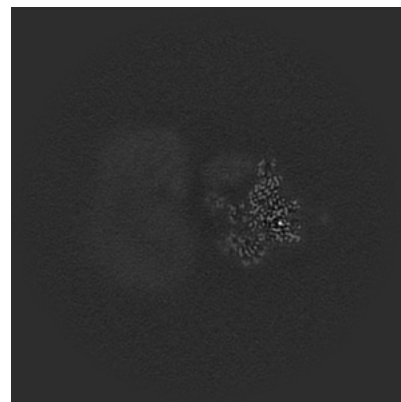
6.3.1 Primary map



X Index: 243

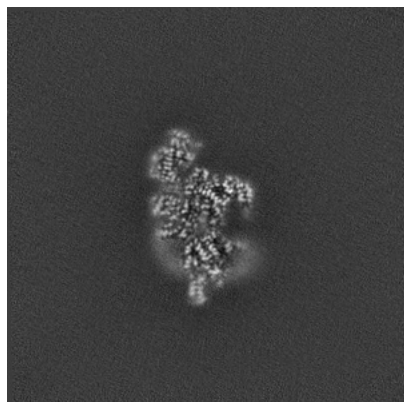


Y Index: 176

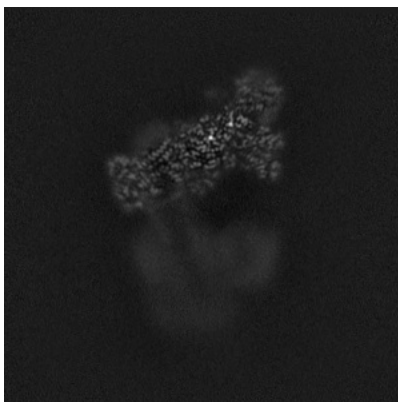


Z Index: 198

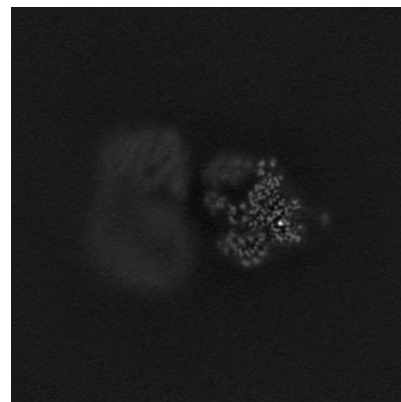
6.3.2 Raw map



X Index: 238



Y Index: 176

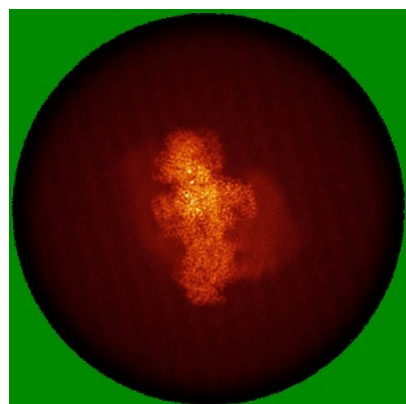


Z Index: 198

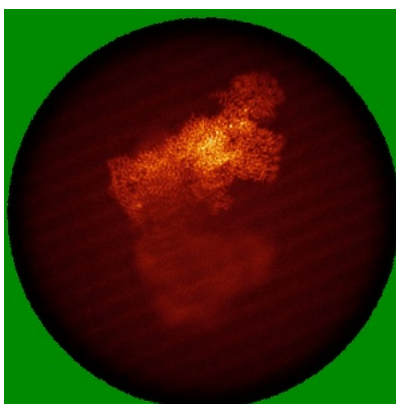
The images above show the largest variance slices of the map in three orthogonal directions.

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

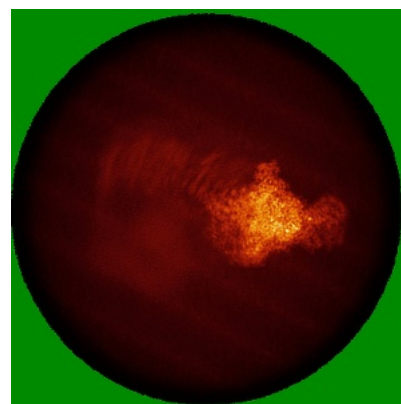
6.4.1 Primary map



X

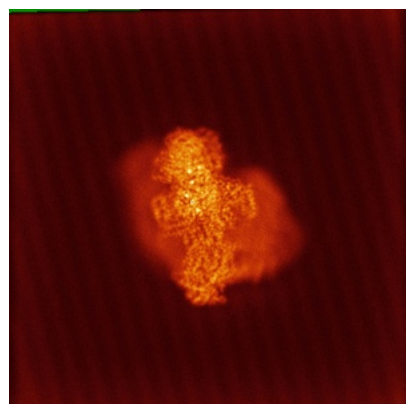


Y

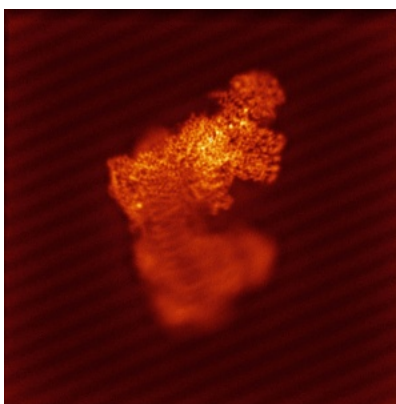


Z

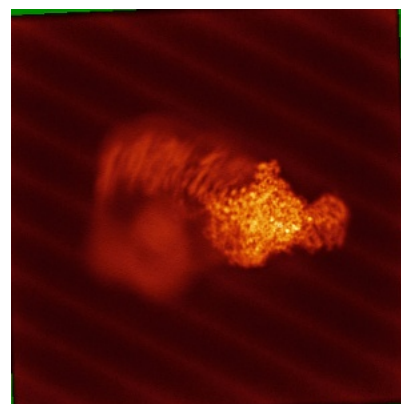
6.4.2 Raw map



X



Y

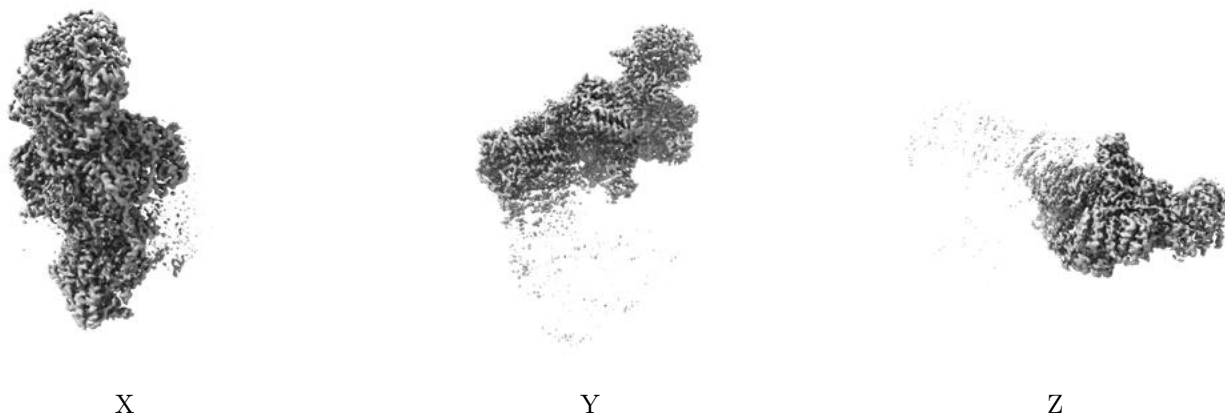


Z

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.

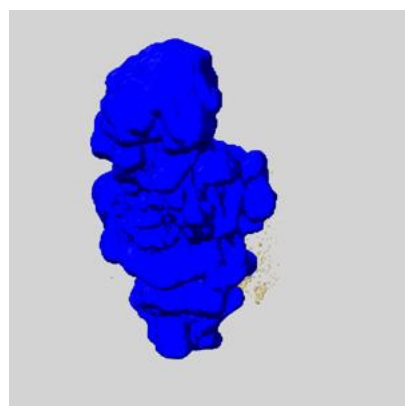
6.6 Mask visualisation [i](#)

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

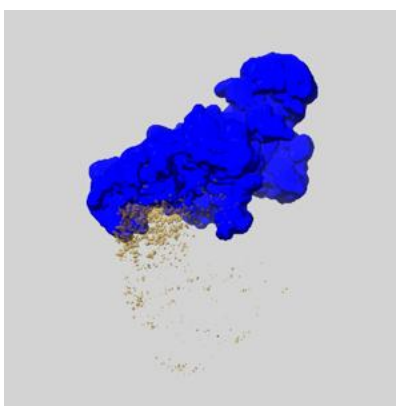
A mask typically either:

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

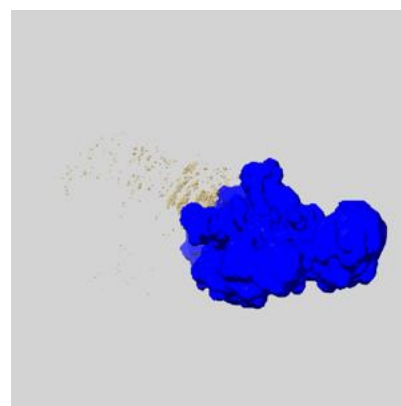
6.6.1 emd_35341_msk_1.map [i](#)



X



Y

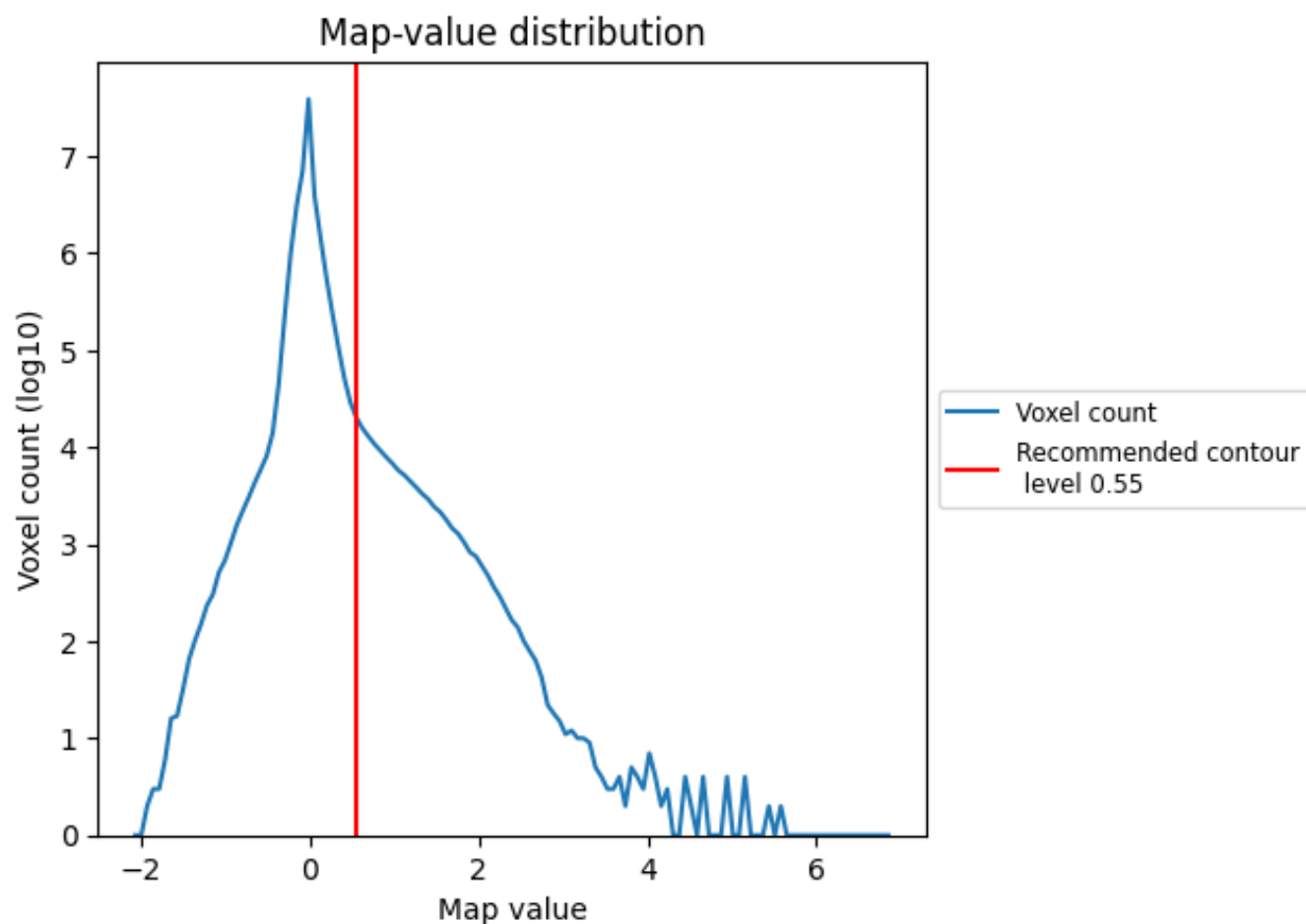


Z

7 Map analysis [i](#)

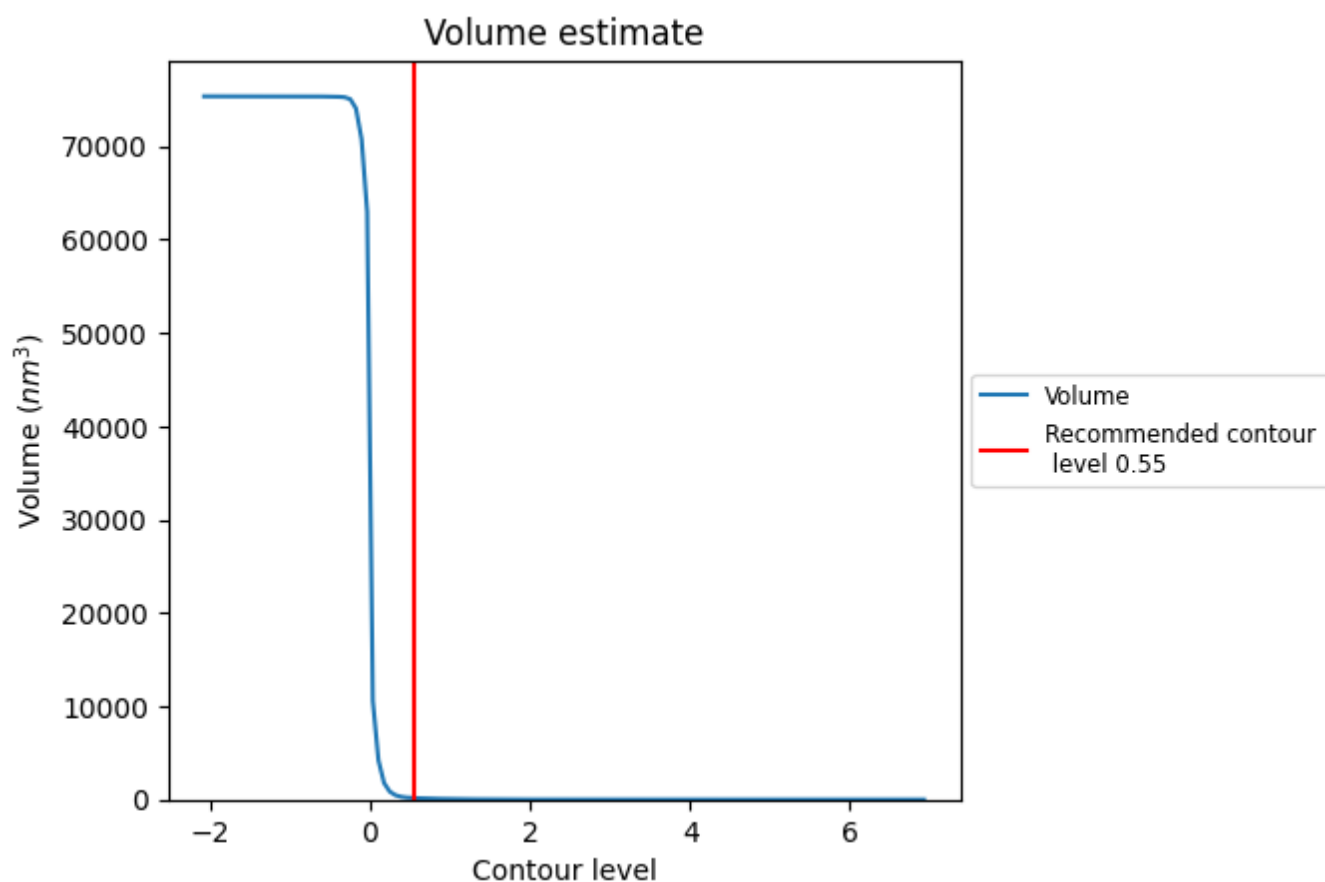
This section contains the results of statistical analysis of the map.

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.

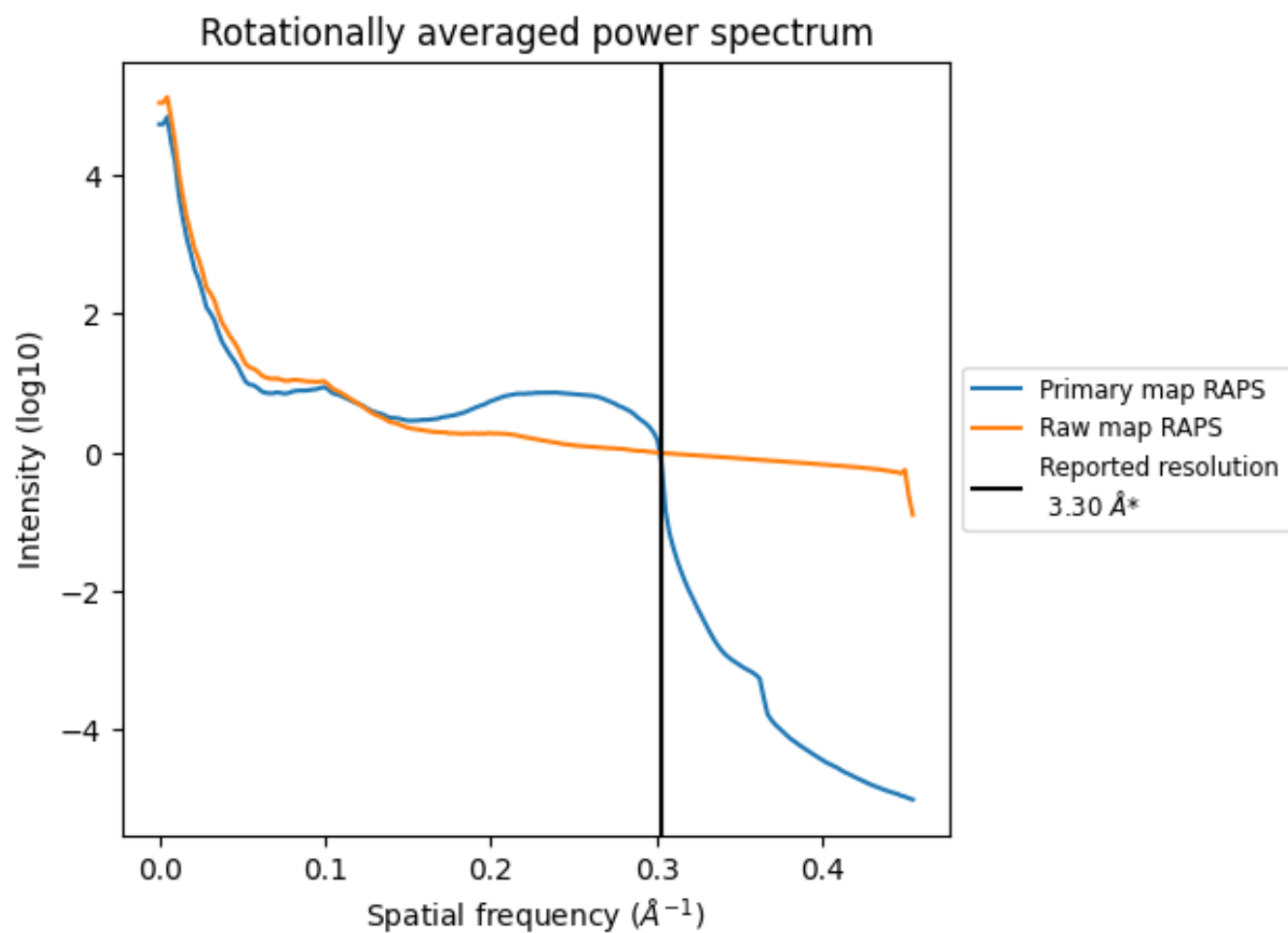
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165 nm^3 ; this corresponds to an approximate mass of 149 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

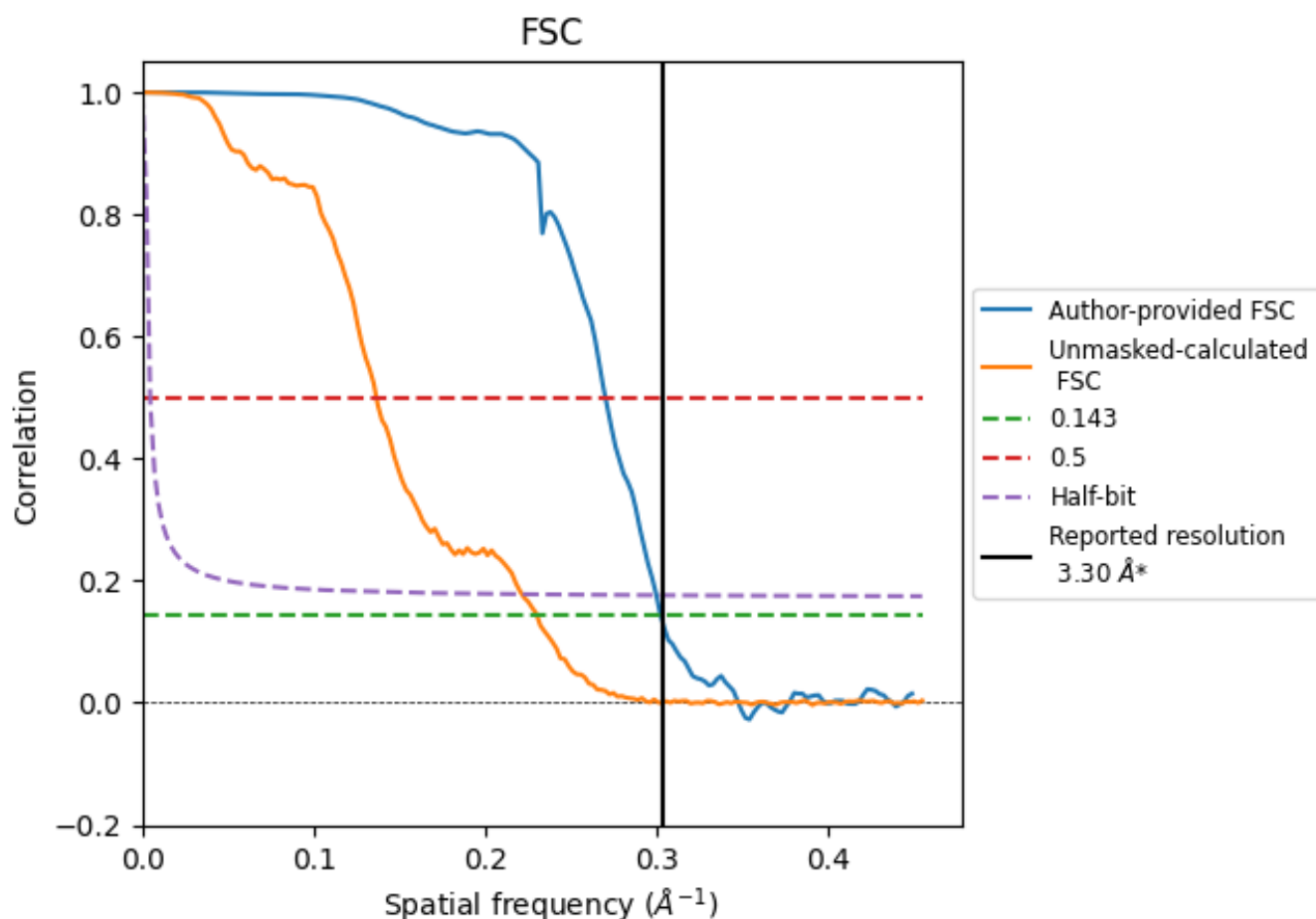


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

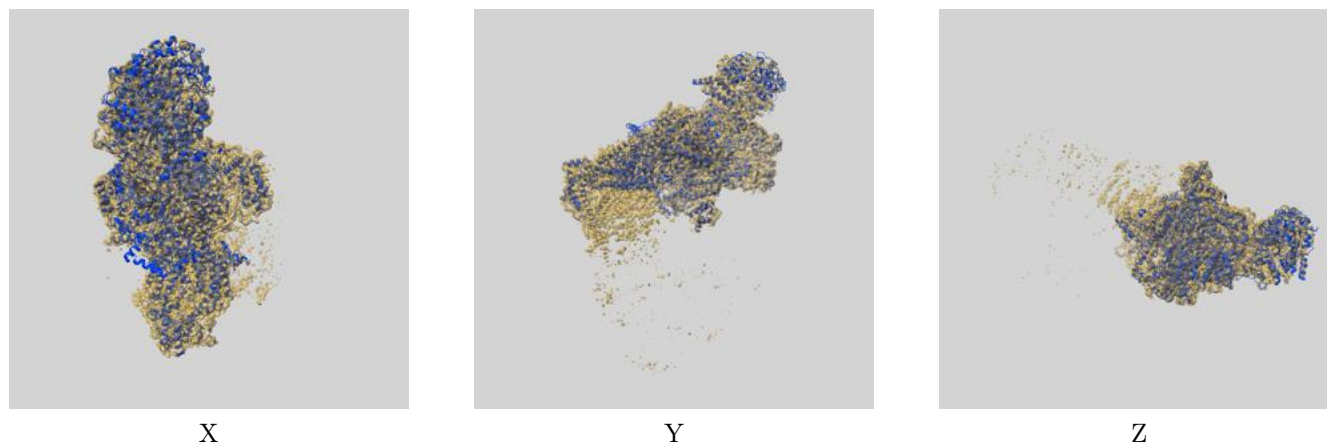
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.71	3.34
Unmasked-calculated*	4.35	7.33	4.52

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

9 Map-model fit [i](#)

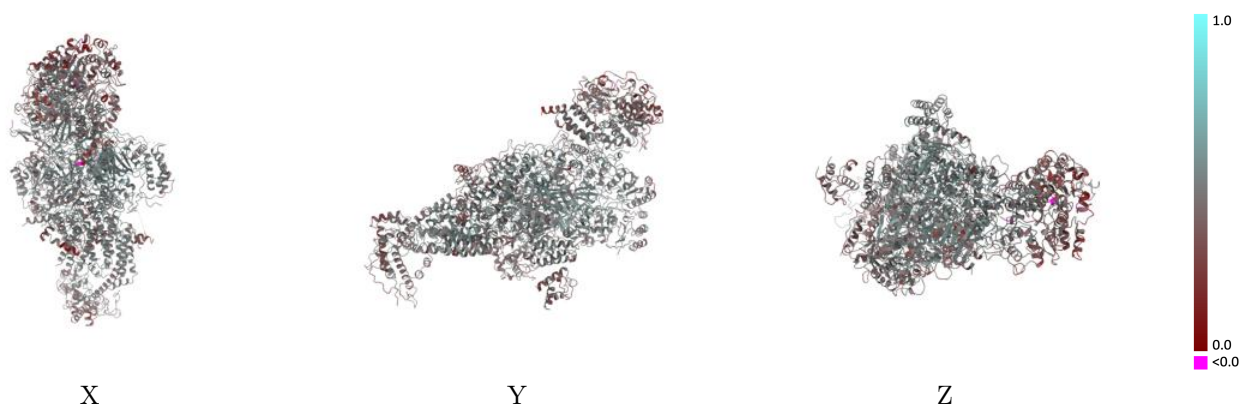
This section contains information regarding the fit between EMDB map EMD-35341 and PDB model 8IBE. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



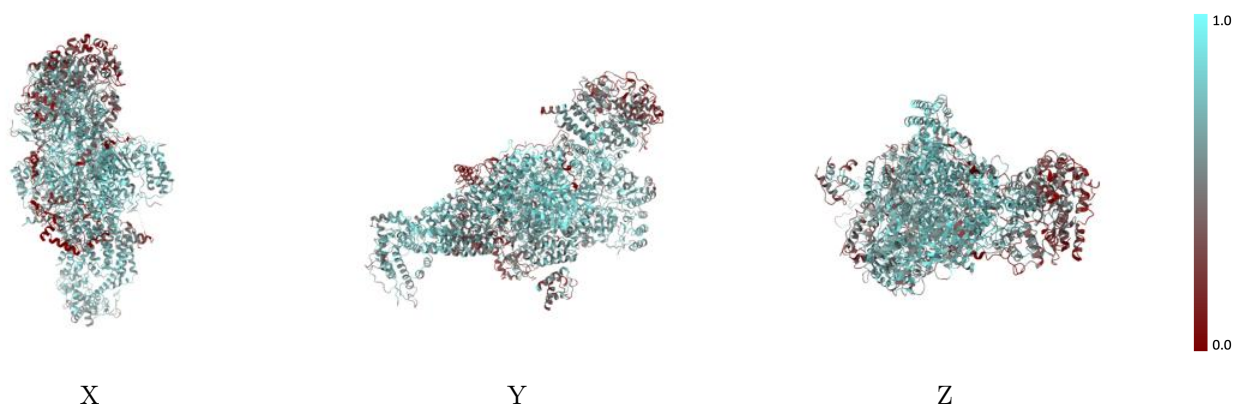
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



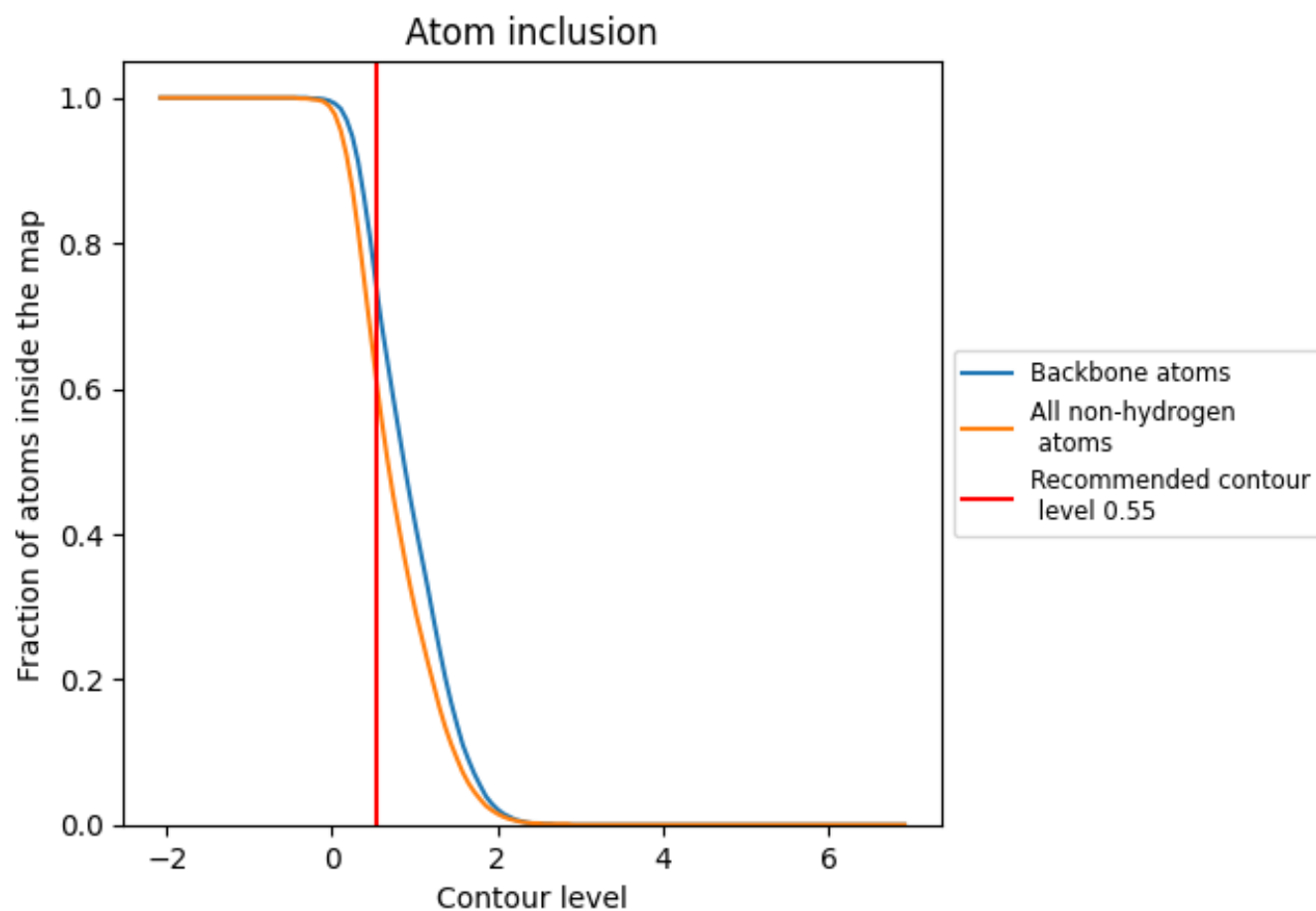
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6000	 0.4580
A	 0.5020	 0.4600
B	 0.7080	 0.5020
C	 0.7680	 0.5310
D	 0.7670	 0.5210
E	 0.3900	 0.3770
F	 0.4690	 0.3940
G	 0.7010	 0.4790
H	 0.6690	 0.4920
I	 0.7660	 0.5030
P	 0.5050	 0.4330
Q	 0.6390	 0.5060
R	 0.2780	 0.4370
S	 0.6670	 0.4530
T	 0.4210	 0.3820
V	 0.7140	 0.4910
W	 0.6230	 0.4830
X	 0.6170	 0.3960
Z	 0.6390	 0.4370
a	 0.6650	 0.4730
b	 0.6070	 0.4310
q	 0.1920	 0.3940
r	 0.2230	 0.3600
s	 0.0740	 0.2940

