



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 09:52 PM JST

PDB ID : 8XNX / pdb_00008xnx
EMDB ID : EMD-38518
Title : Respiratory complex Peripheral Arm of CI, open form A, focus-refined map of type II, Wild type mouse under Cold Acclimation
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-12-30
Resolution : 3.50 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:

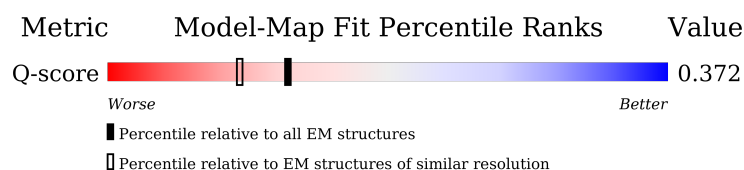
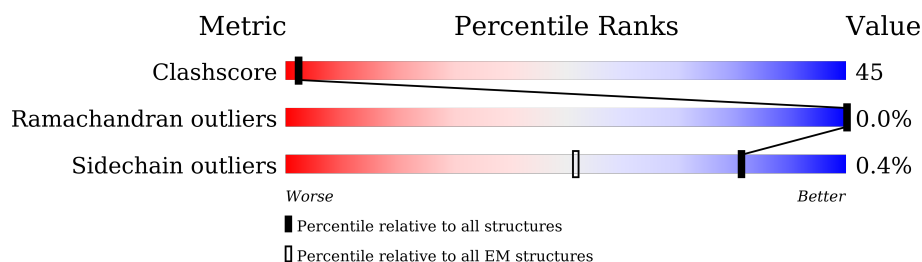
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 3.50 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	13950 (3.00 - 4.00)

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	301	-	-	X	-
25	SF4	I	302	-	-	X	-

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

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 34132 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	90	Total	C	N	O	S	0	0
			735	511	102	117	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	384	Total	C	N	O	S	0	0
			3083	1967	532	561	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	312	Total	C	N	O	S	0	0
			2493	1675	378	418	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		

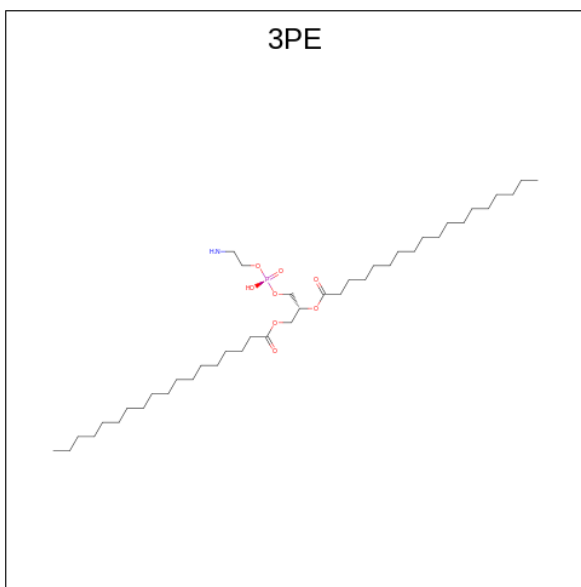
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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.

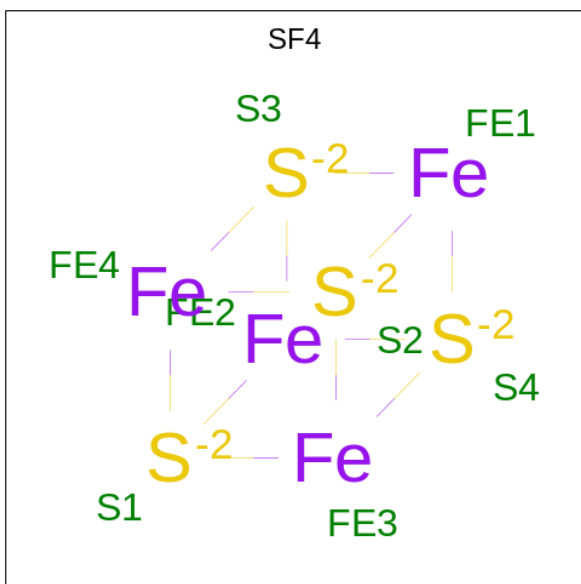
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	23	Total	C	N	O	0	0
			193	126	30	37		

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



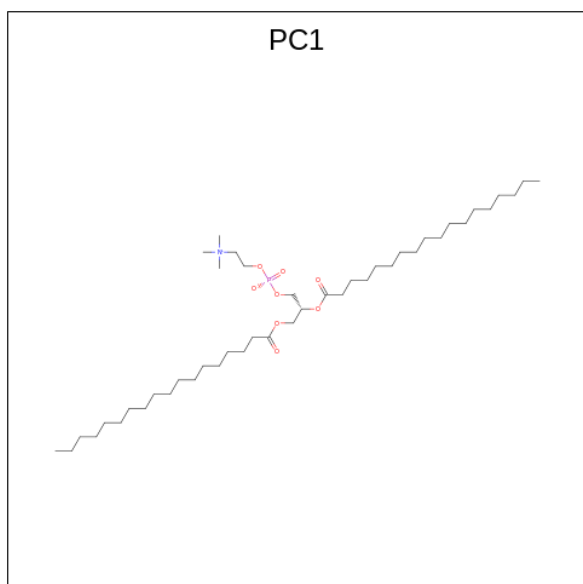
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
24	A	1	Total	C	N	O	P	0
			48	38	1	8	1	
24	H	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



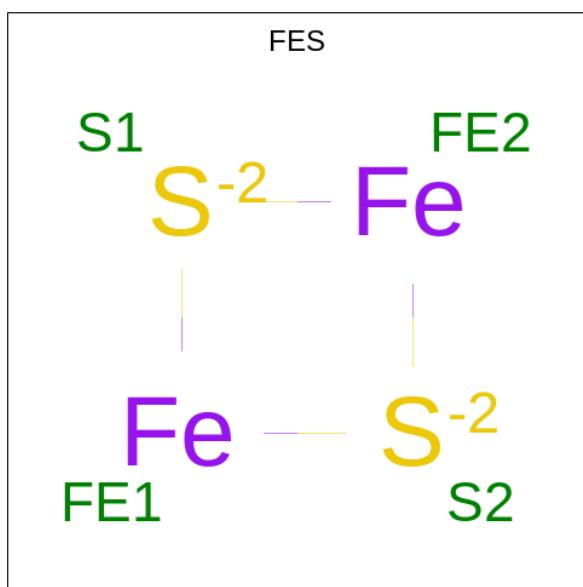
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	Fe	S	0
			8	4	4	
25	F	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	

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



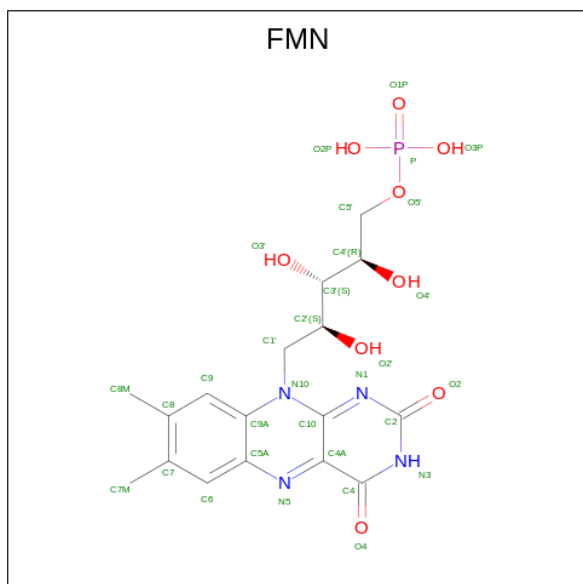
Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
26	B	1	Total	C	N	O	P	0
			43	33	1	8	1	

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



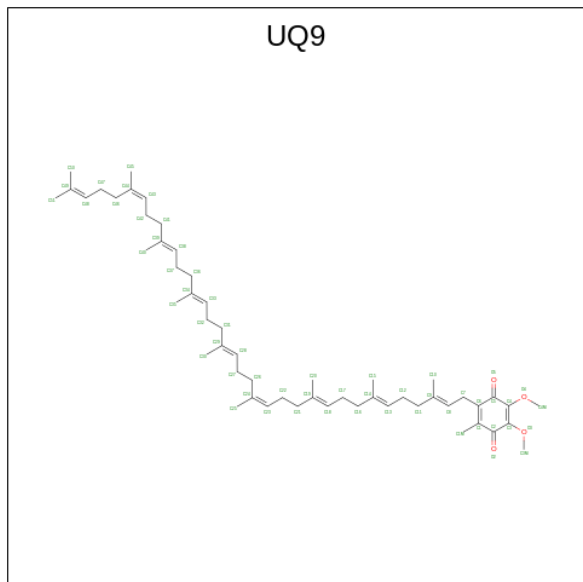
Mol	Chain	Residues	Atoms			AltConf
27	E	1	Total	Fe	S	0
			4	2	2	
27	G	1	Total	Fe	S	0
			4	2	2	

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



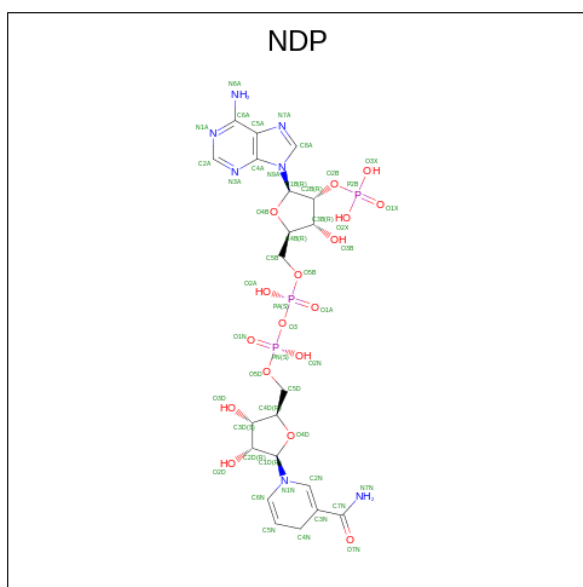
Mol	Chain	Residues	Atoms					AltConf
28	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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



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

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

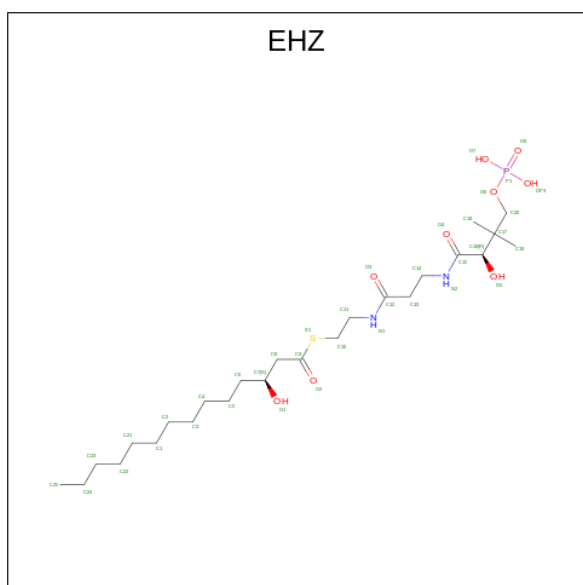


Mol	Chain	Residues	Atoms					AltConf
30	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

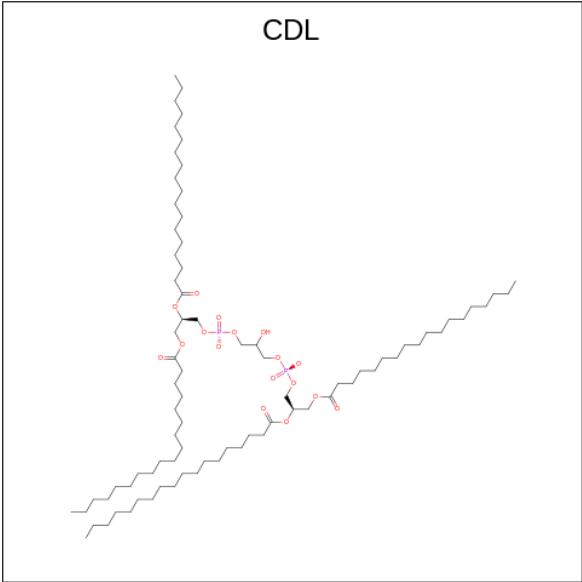
Mol	Chain	Residues	Atoms		AltConf
31	R	1	Total	Zn	0
			1	1	

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

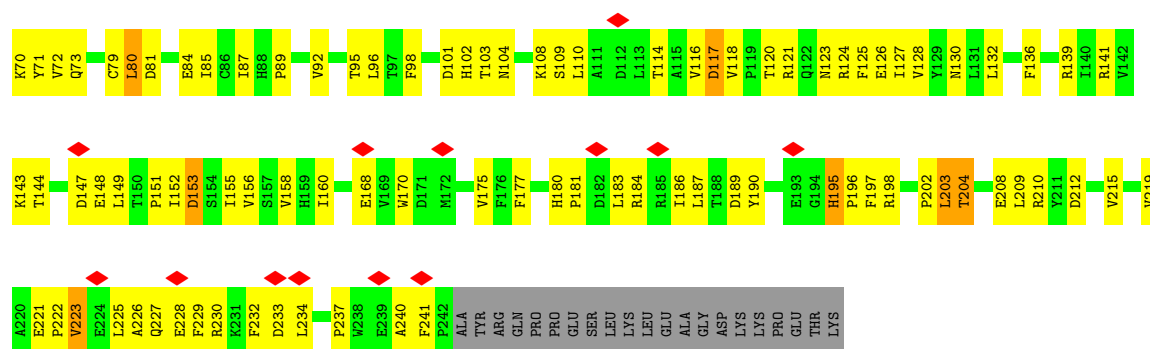


Mol	Chain	Residues	Atoms						AltConf
32	W	1	Total	C	N	O	P	S	0
			35	22	2	9	1	1	

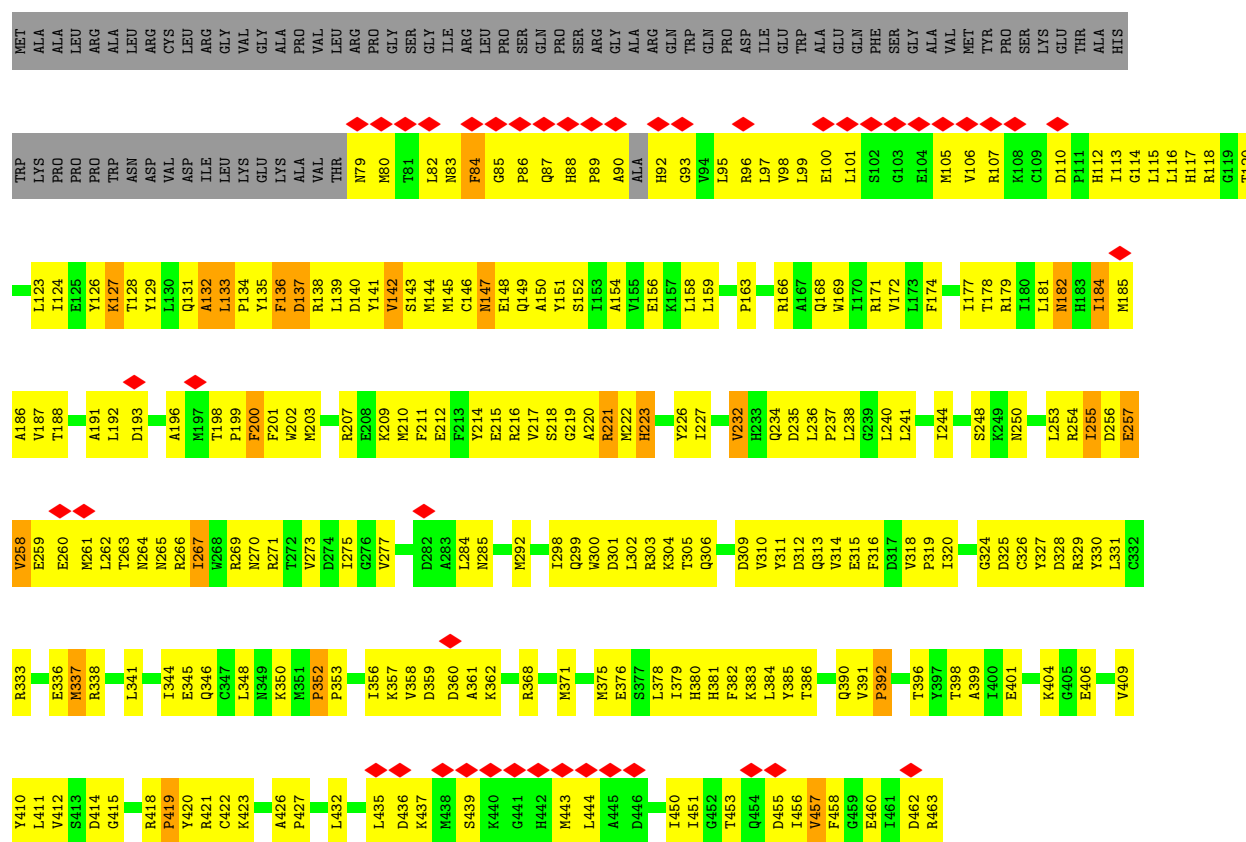
- Molecule 33 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



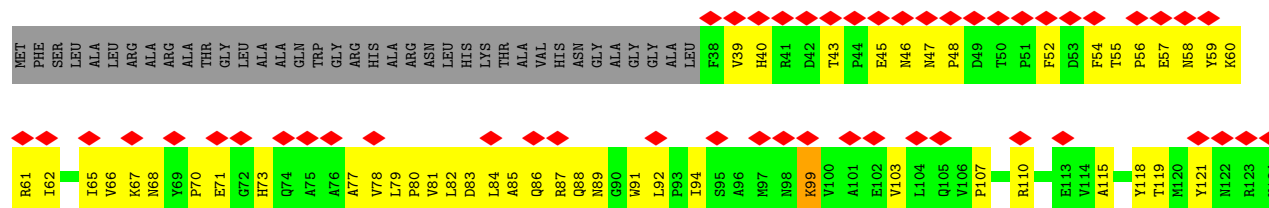
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	q	1	57	38	17	2	0



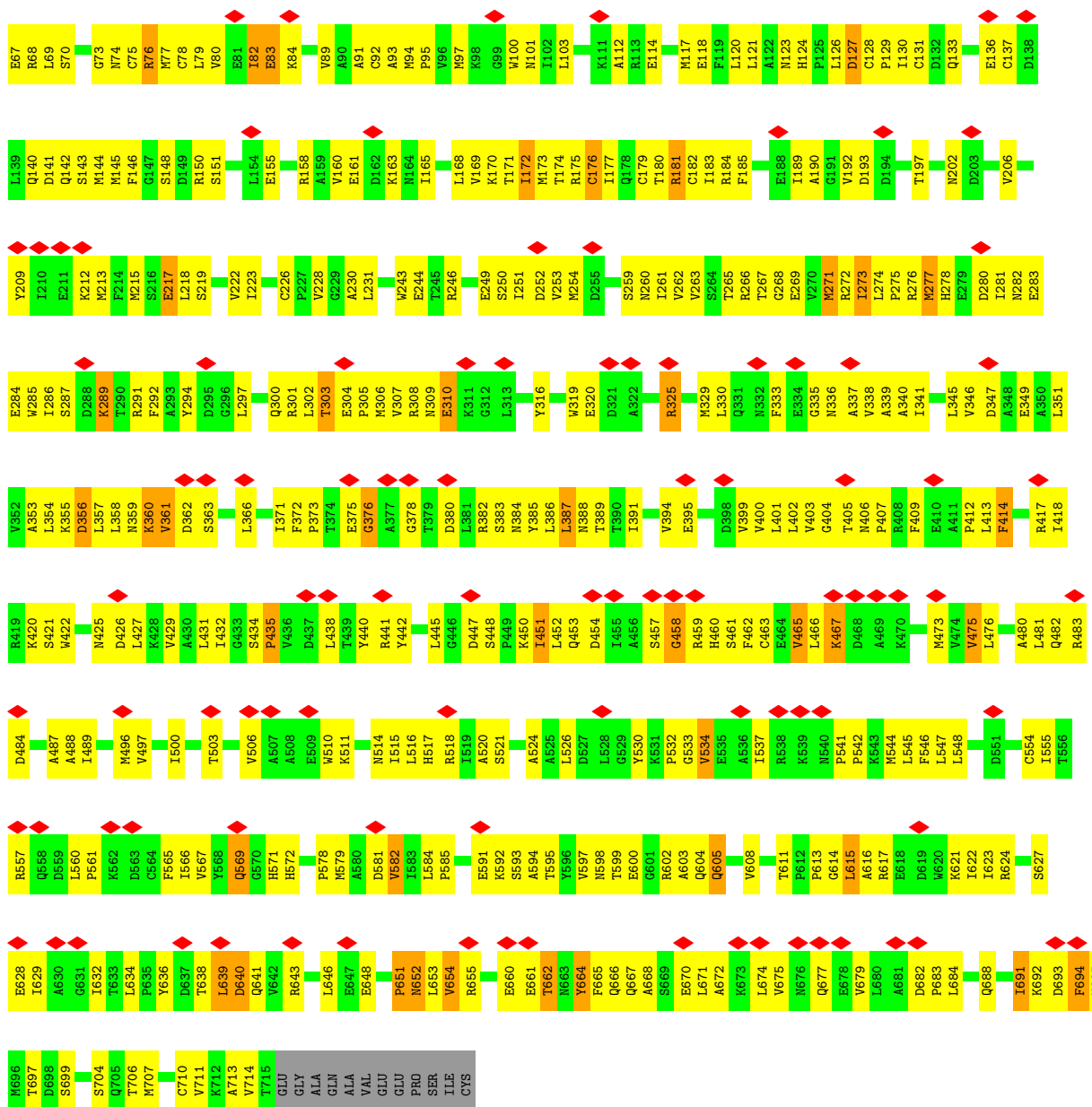
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



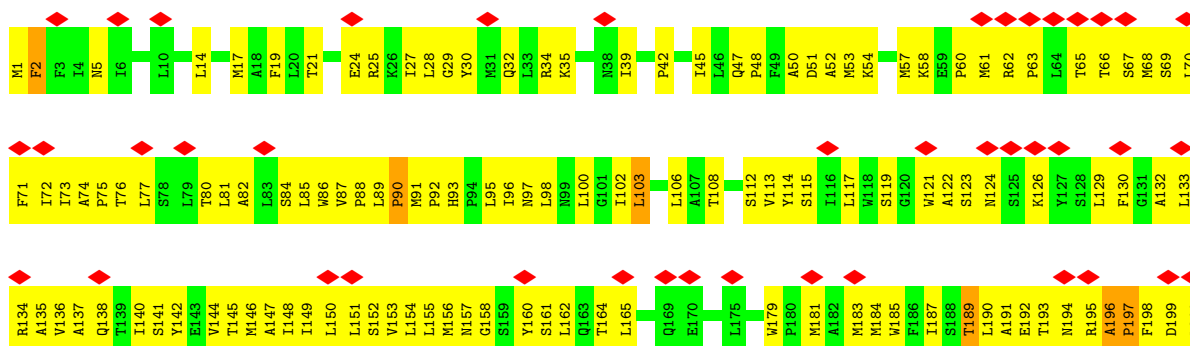
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





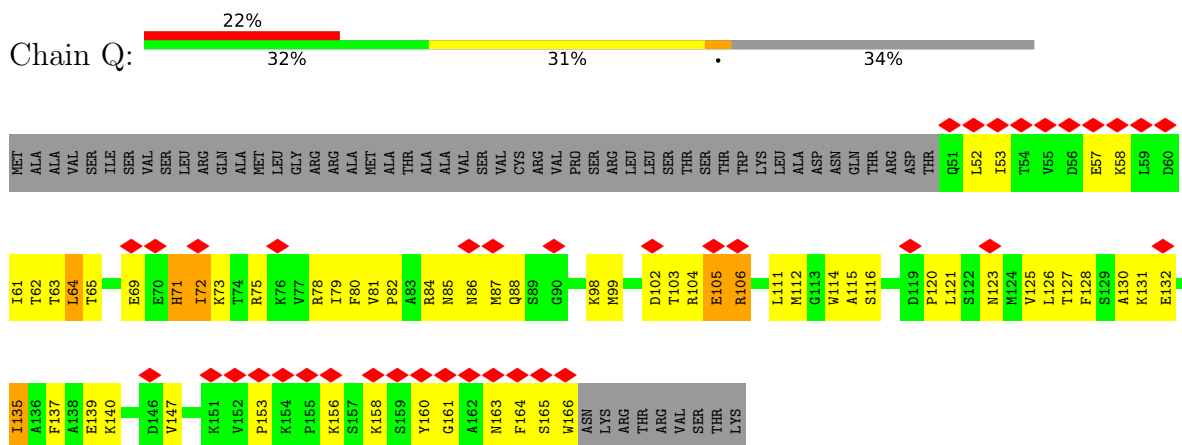


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

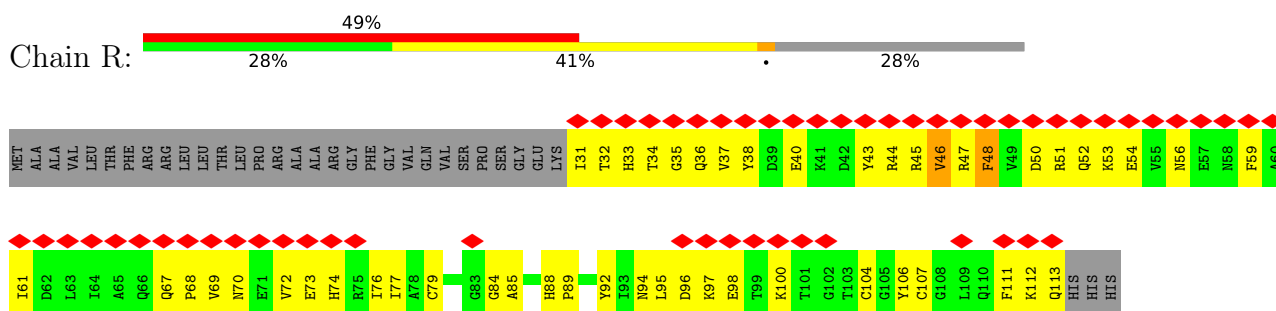




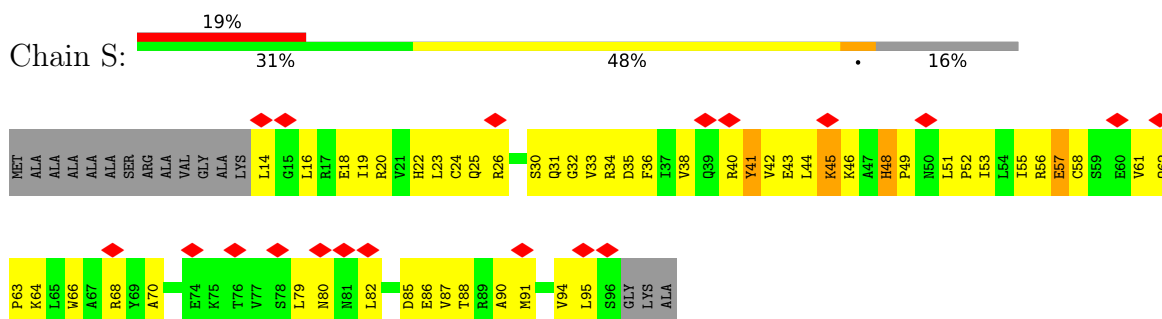
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



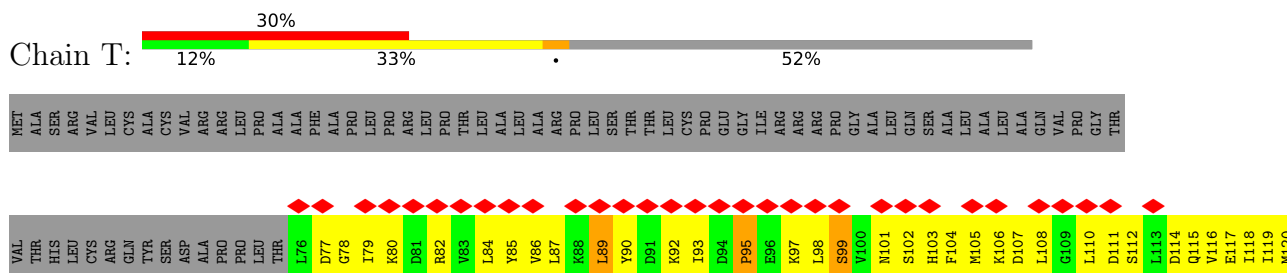
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

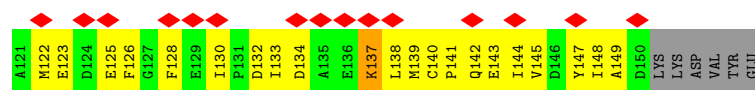


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

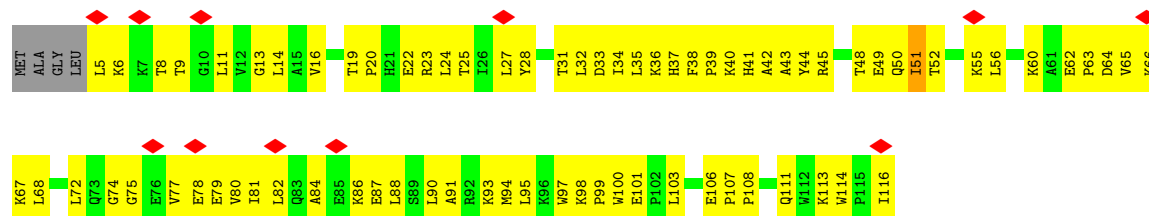


- Molecule 14: Acyl carrier protein, mitochondrial

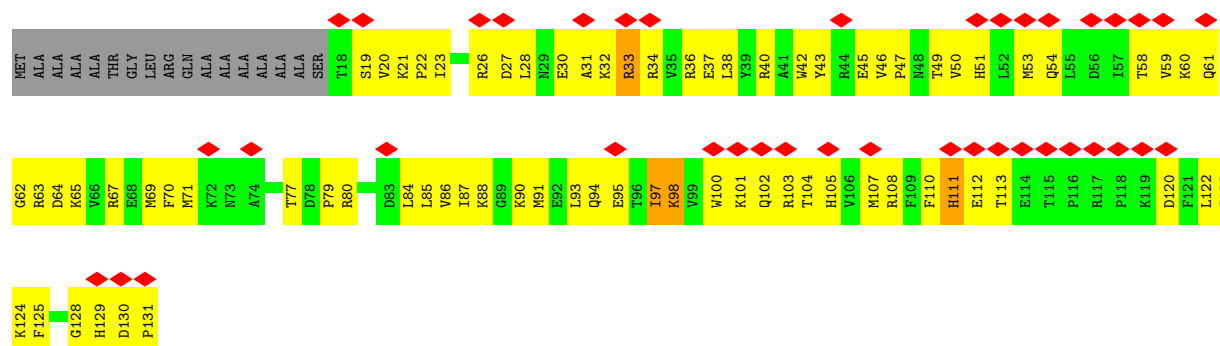




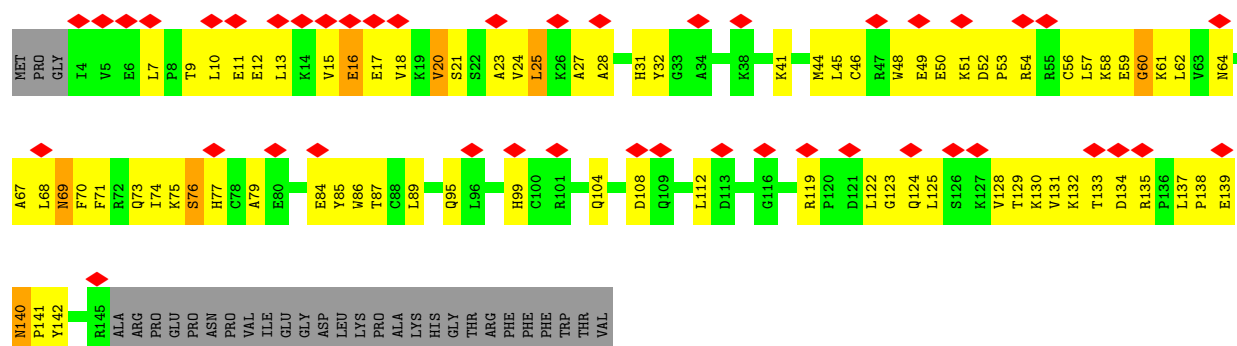
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



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

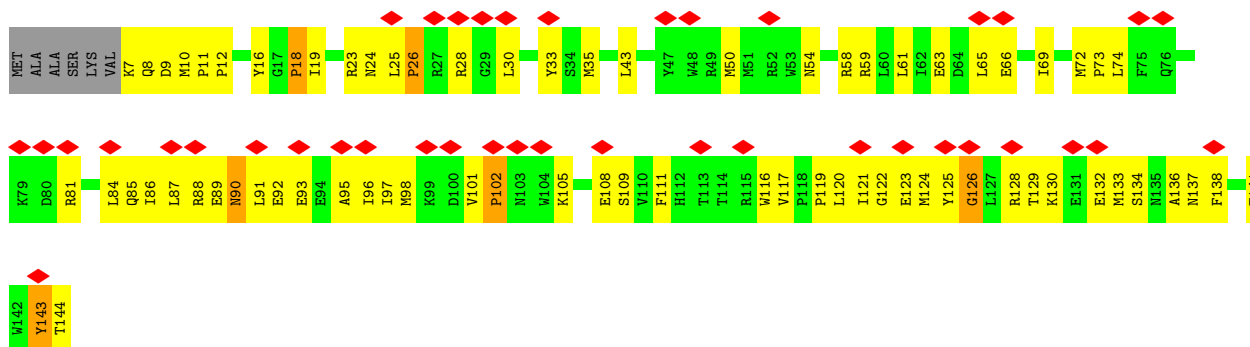


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

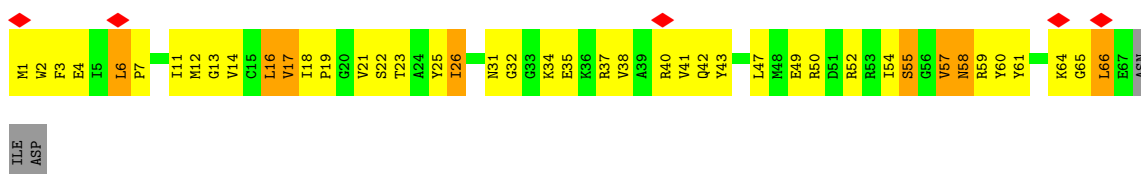


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

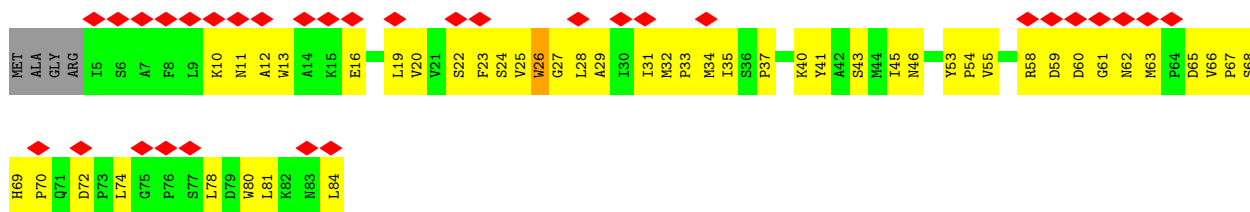




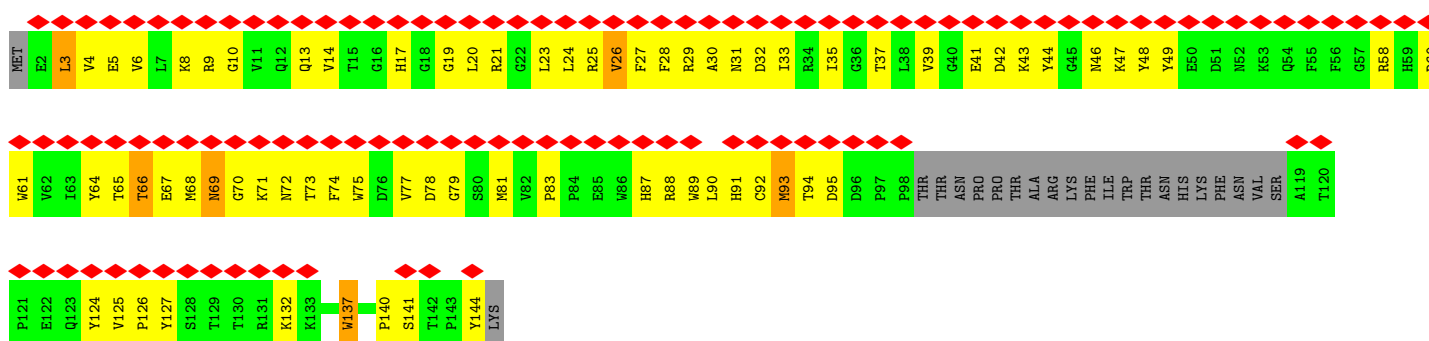
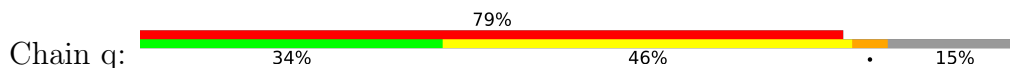
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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

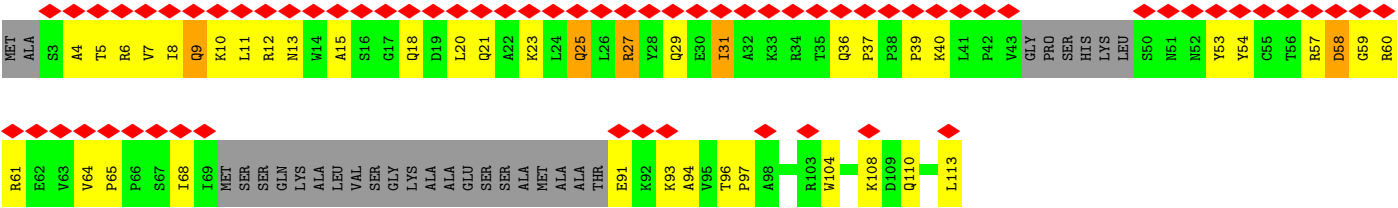


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

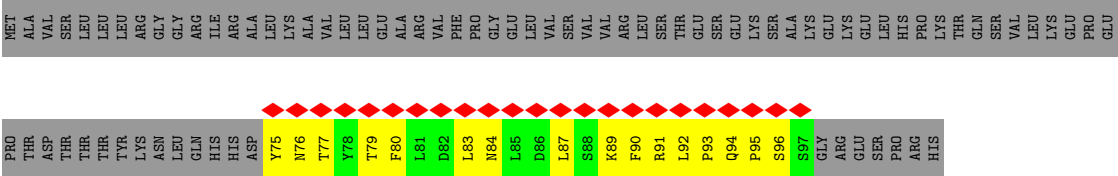


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34219	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	4.446	Depositor
Minimum map value	-1.060	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.075	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: 3PE, EH3, SF4, FMN, CDL, PC1, UQ9, FES, NDP, 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	0.89	0/755	1.26	8/1030 (0.8%)
2	B	1.03	1/1272 (0.1%)	1.42	21/1722 (1.2%)
3	C	1.02	1/1689 (0.1%)	1.39	20/2300 (0.9%)
4	D	0.96	1/3156 (0.0%)	1.44	44/4266 (1.0%)
5	E	0.74	0/1675	1.13	7/2282 (0.3%)
6	F	0.86	0/3363	1.47	58/4543 (1.3%)
7	G	0.91	5/5374 (0.1%)	1.50	86/7281 (1.2%)
8	H	0.89	3/2568 (0.1%)	1.14	18/3509 (0.5%)
9	I	0.74	1/1409 (0.1%)	1.28	22/1904 (1.2%)
10	P	0.75	0/2793	1.18	20/3787 (0.5%)
11	Q	0.91	1/963 (0.1%)	1.30	6/1302 (0.5%)
12	R	0.62	0/671	1.06	4/903 (0.4%)
13	S	0.78	0/678	1.09	4/915 (0.4%)
14	T	0.76	0/613	1.11	7/826 (0.8%)
15	V	0.82	0/937	1.24	4/1270 (0.3%)
16	W	0.80	1/993 (0.1%)	0.94	5/1335 (0.4%)
17	X	0.63	0/1191	1.03	11/1605 (0.7%)
18	Z	0.64	0/1176	1.00	6/1587 (0.4%)
19	a	0.88	0/561	1.41	12/755 (1.6%)
20	b	0.67	0/651	1.00	4/895 (0.4%)
21	q	0.65	1/1059 (0.1%)	1.20	13/1439 (0.9%)
22	r	0.85	0/701	1.48	11/948 (1.2%)
23	s	0.76	0/198	1.10	0/269
All	All	0.85	15/34446 (0.0%)	1.30	391/46673 (0.8%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Q	106	ARG	C-O	8.99	1.34	1.24
9	I	118	LEU	CA-C	8.23	1.64	1.52
7	G	31	LEU	CA-C	-7.25	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	103	LEU	C-O	7.04	1.32	1.24
7	G	127	ASP	CA-C	6.99	1.62	1.53
3	C	203	LEU	CA-C	-6.92	1.43	1.52
7	G	76	ARG	CA-C	6.24	1.61	1.53
7	G	192	VAL	CA-C	-6.09	1.46	1.53
4	D	392	PRO	C-O	-5.81	1.20	1.25
16	W	111	HIS	C-O	5.37	1.30	1.23
7	G	683	PRO	N-CD	-5.31	1.40	1.47
2	B	195	PRO	CA-C	-5.23	1.47	1.52
8	H	90	PRO	CA-C	-5.14	1.48	1.53
21	q	4	VAL	CA-C	5.05	1.58	1.52
8	H	196	ALA	CA-C	-5.02	1.47	1.52

All (391) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	231	ILE	N-CA-C	-19.18	90.98	113.42
7	G	174	THR	N-CA-C	-16.85	89.03	114.64
6	F	125	CYS	N-CA-C	-15.65	93.45	113.17
8	H	197	PRO	N-CA-C	-13.70	96.74	113.86
7	G	77	MET	N-CA-C	-13.08	97.29	113.38
9	I	64	THR	N-CA-C	-12.75	98.37	114.56
10	P	115	SER	N-CA-C	-12.62	97.35	113.12
6	F	171	VAL	N-CA-C	-11.91	99.33	110.53
6	F	449	ARG	N-CA-C	-11.64	98.67	111.36
9	I	118	LEU	N-CA-C	11.45	126.75	113.01
1	A	54	LYS	N-CA-C	-11.09	99.77	113.97
4	D	257	GLU	N-CA-C	-10.83	99.44	111.14
7	G	360	LYS	N-CA-C	-10.78	99.50	111.14
8	H	231	ILE	N-CA-CB	10.57	126.94	112.35
7	G	280	ASP	N-CA-C	10.22	122.42	111.28
9	I	119	CYS	N-CA-C	10.16	126.93	113.72
2	B	80	ASP	N-CA-C	-10.08	100.29	111.28
7	G	414	PHE	N-CA-C	-10.08	101.48	113.88
7	G	325	ARG	N-CA-C	-9.95	100.12	110.97
6	F	144	VAL	N-CA-C	-9.82	101.29	110.53
6	F	178	GLU	N-CA-C	-9.82	99.33	111.11
6	F	141	GLY	N-CA-C	-9.80	101.14	112.50
6	F	103	ASN	N-CA-C	-9.78	101.03	113.16
7	G	35	PHE	N-CA-C	9.66	124.32	108.96
7	G	694	PHE	N-CA-C	9.64	121.39	111.07
6	F	418	GLN	N-CA-C	-9.61	100.76	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	337	ALA	N-CA-C	-9.56	100.83	114.12
22	r	31	ILE	N-CA-C	9.50	121.74	109.30
21	q	3	LEU	N-CA-C	-9.45	100.53	112.90
7	G	692	LYS	N-CA-C	-9.32	100.48	112.23
7	G	640	ASP	N-CA-C	-9.29	101.24	111.36
9	I	95	PRO	N-CA-C	-9.24	102.31	113.86
5	E	85	ALA	N-CA-C	-9.23	101.29	111.36
4	D	223	HIS	N-CA-C	-9.18	98.66	111.52
20	b	26	TRP	N-CA-C	-9.07	101.36	111.07
3	C	180	HIS	N-CA-C	-8.88	95.79	109.64
7	G	212	LYS	N-CA-C	-8.79	94.57	108.90
19	a	66	LEU	N-CA-C	-8.73	102.41	113.23
7	G	133	GLN	N-CA-CB	8.71	121.43	110.45
9	I	62	MET	N-CA-C	-8.70	92.06	107.73
7	G	310	GLU	CB-CA-C	-8.68	106.56	116.54
21	q	66	THR	N-CA-C	-8.66	101.92	111.36
4	D	258	VAL	N-CA-C	-8.45	102.19	110.72
22	r	25	GLN	N-CA-C	-8.36	103.08	113.28
18	Z	90	ASN	N-CA-C	-8.35	103.23	113.41
22	r	29	GLN	N-CA-C	-8.32	102.33	114.39
7	G	452	LEU	N-CA-C	-8.32	102.22	111.28
22	r	58	ASP	N-CA-C	8.31	123.54	108.17
21	q	64	TYR	N-CA-C	8.29	121.03	110.33
6	F	298	GLU	N-CA-C	8.24	120.27	111.28
7	G	387	LEU	N-CA-C	-8.24	97.94	110.30
7	G	691	ILE	N-CA-C	8.23	123.74	111.89
15	V	87	GLU	N-CA-C	-8.23	102.31	111.28
7	G	484	ASP	N-CA-C	8.18	121.12	111.71
10	P	143	ASP	N-CA-C	8.15	119.79	111.07
6	F	191	TYR	N-CA-C	8.12	121.68	110.24
3	C	196	PRO	N-CA-C	8.11	124.80	113.53
7	G	534	VAL	N-CA-C	-8.04	104.75	111.91
7	G	664	TYR	N-CA-C	-8.02	97.59	109.62
4	D	457	VAL	N-CA-C	-8.00	96.92	108.11
22	r	10	LYS	N-CA-C	-7.99	102.98	112.89
7	G	361	VAL	N-CA-C	-7.99	101.34	110.05
6	F	364	VAL	N-CA-C	7.98	118.76	110.62
1	A	61	THR	N-CA-C	-7.96	102.55	111.07
2	B	165	ALA	N-CA-C	-7.87	104.16	114.31
11	Q	72	ILE	N-CA-C	-7.84	105.85	113.53
9	I	118	LEU	CA-C-O	7.82	129.21	119.05
5	E	193	GLU	N-CA-C	7.78	120.55	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	195	PRO	N-CA-C	-7.74	101.26	110.70
7	G	56	VAL	N-CA-C	-7.73	102.91	110.72
11	Q	139	GLU	N-CA-C	-7.72	102.81	111.07
8	H	230	ASN	N-CA-C	-7.72	101.92	112.03
6	F	58	ARG	N-CA-C	-7.70	102.96	111.36
10	P	95	ARG	N-CA-C	7.70	120.56	111.71
4	D	184	ILE	N-CA-C	-7.65	102.81	110.62
4	D	427	PRO	N-CA-C	-7.63	98.52	110.50
10	P	50	SER	N-CA-C	-7.59	98.32	109.63
9	I	190	LEU	N-CA-C	-7.57	104.65	114.04
7	G	569	GLN	N-CA-C	7.57	121.94	108.24
6	F	171	VAL	N-CA-CB	7.57	120.25	110.57
6	F	238	CYS	CA-C-N	-7.55	111.98	119.76
6	F	238	CYS	C-N-CA	-7.55	111.98	119.76
12	R	74	HIS	N-CA-C	7.52	121.10	110.50
7	G	467	LYS	N-CA-C	-7.52	102.24	111.33
15	V	41	HIS	N-CA-CB	-7.51	101.94	110.35
7	G	277	MET	N-CA-C	7.50	120.62	109.59
7	G	497	VAL	N-CA-C	-7.47	103.25	110.42
6	F	430	GLY	N-CA-C	7.46	121.68	112.73
7	G	303	THR	N-CA-C	7.40	123.03	113.18
17	X	69	ASN	N-CA-C	-7.24	102.99	111.03
13	S	57	GLU	N-CA-C	7.22	121.00	109.24
13	S	33	VAL	N-CA-C	-7.21	103.27	110.62
14	T	99	SER	N-CA-C	-7.21	99.22	109.96
4	D	257	GLU	N-CA-CB	7.19	120.50	110.07
18	Z	102	PRO	N-CA-C	7.16	122.45	111.57
7	G	83	GLU	N-CA-C	7.13	120.56	110.50
6	F	73	PRO	N-CA-C	-7.12	103.86	113.40
7	G	465	VAL	N-CA-CB	7.11	118.40	110.51
3	C	195	HIS	CB-CA-C	7.09	117.19	110.17
6	F	81	LYS	N-CA-C	-7.09	103.63	111.36
2	B	194	CYS	N-CA-C	-7.09	102.53	112.17
4	D	303	ARG	N-CA-C	-7.08	104.28	114.12
10	P	97	MET	N-CA-CB	7.08	121.29	110.60
6	F	246	GLU	N-CA-C	-7.07	103.57	111.28
2	B	99	CYS	N-CA-C	7.07	120.02	111.82
7	G	376	GLY	N-CA-C	-7.06	101.34	110.38
7	G	461	SER	N-CA-C	7.06	119.87	111.33
7	G	217	GLU	N-CA-C	-7.06	101.73	110.41
19	a	57	VAL	N-CA-C	-7.02	105.88	112.83
1	A	67	LEU	N-CA-C	-7.01	103.69	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	78	GLY	N-CA-C	-7.00	104.33	112.73
7	G	148	SER	N-CA-C	7.00	120.82	109.40
4	D	193	ASP	N-CA-C	-7.00	103.58	111.07
6	F	169	LEU	N-CA-C	6.98	118.89	111.28
6	F	103	ASN	N-CA-CB	6.97	121.10	110.44
7	G	582	VAL	N-CA-C	6.96	118.50	108.48
6	F	455	GLN	N-CA-C	6.95	118.51	111.07
3	C	80	LEU	N-CA-C	-6.93	104.70	113.02
15	V	74	GLY	N-CA-C	-6.93	104.47	112.79
6	F	428	GLY	N-CA-C	-6.90	103.94	112.77
6	F	418	GLN	N-CA-CB	6.89	120.06	110.07
21	q	137	TRP	N-CA-C	-6.88	99.64	109.96
6	F	148	ALA	N-CA-C	-6.88	103.86	111.36
4	D	255	ILE	N-CA-C	6.88	117.02	110.42
5	E	152	GLN	N-CA-C	-6.88	103.71	111.07
7	G	300	GLN	N-CA-CB	6.87	122.46	112.08
8	H	156	MET	N-CA-C	6.86	118.84	111.36
3	C	233	ASP	CB-CA-C	-6.86	102.21	111.88
7	G	133	GLN	N-CA-C	-6.85	101.16	110.68
8	H	77	LEU	N-CA-C	-6.84	103.51	110.97
7	G	294	TYR	N-CA-C	-6.83	104.76	113.23
2	B	95	PHE	N-CA-C	-6.81	103.88	111.71
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
9	I	119	CYS	N-CA-CB	-6.75	100.73	110.65
17	X	104	GLN	N-CA-C	6.75	118.42	111.14
7	G	268	GLY	N-CA-C	6.74	124.67	115.30
3	C	204	THR	N-CA-C	6.74	120.48	112.93
7	G	434	SER	N-CA-C	-6.74	100.99	110.29
18	Z	126	GLY	N-CA-C	-6.72	103.24	112.25
6	F	344	GLN	N-CA-C	-6.71	103.97	111.28
9	I	86	TYR	CB-CA-C	-6.70	101.30	113.49
3	C	49	ARG	N-CA-C	6.68	120.41	109.85
6	F	206	CYS	N-CA-C	-6.68	104.99	113.01
17	X	57	LEU	N-CA-C	-6.68	104.23	112.38
7	G	640	ASP	N-CA-CB	6.67	120.03	110.16
9	I	49	ASP	N-CA-C	-6.66	99.82	110.14
8	H	311	THR	N-CA-C	-6.64	104.80	113.17
2	B	88	SER	N-CA-C	-6.63	103.98	111.14
7	G	287	SER	N-CA-C	6.62	119.27	110.53
19	a	65	GLY	N-CA-C	-6.61	105.63	114.95
7	G	189	ILE	N-CA-C	-6.56	105.31	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	51	LYS	N-CA-C	-6.56	104.05	111.07
9	I	98	ARG	N-CA-C	6.55	118.96	108.41
1	A	59	ALA	N-CA-C	6.55	118.42	111.28
19	a	16	LEU	CA-C-N	-6.55	112.94	122.69
19	a	16	LEU	C-N-CA	-6.55	112.94	122.69
16	W	98	LYS	N-CA-C	-6.54	102.08	110.19
18	Z	143	TYR	N-CA-C	6.53	118.44	110.41
7	G	435	PRO	N-CA-C	-6.53	100.25	110.50
14	T	95	PRO	N-CA-C	-6.51	106.34	114.68
7	G	605	GLN	N-CA-C	6.51	119.13	108.52
7	G	653	LEU	N-CA-CB	6.50	121.48	110.49
7	G	127	ASP	CA-C-O	6.50	129.06	121.78
6	F	178	GLU	N-CA-CB	6.50	119.62	109.94
19	a	58	ASN	N-CA-C	6.49	119.31	108.73
6	F	234	GLY	N-CA-C	6.48	128.53	113.18
13	S	41	TYR	N-CA-C	-6.46	103.93	110.97
2	B	163	SER	N-CA-C	-6.46	105.36	112.72
7	G	273	ILE	N-CA-C	-6.45	98.34	107.75
10	P	119	ALA	N-CA-C	-6.45	104.18	111.14
7	G	190	ALA	N-CA-C	-6.43	99.16	109.96
4	D	84	PHE	N-CA-C	-6.42	105.51	113.15
10	P	224	LEU	CB-CA-C	-6.40	109.18	116.54
6	F	226	LYS	CA-C-N	-6.40	113.79	120.38
6	F	226	LYS	C-N-CA	-6.40	113.79	120.38
7	G	662	THR	N-CA-C	-6.40	96.47	107.61
6	F	370	LEU	N-CA-C	-6.40	104.39	111.36
5	E	166	LYS	N-CA-C	-6.38	105.91	113.38
7	G	250	SER	N-CA-C	6.36	116.68	108.34
8	H	288	LEU	N-CA-C	-6.36	103.65	111.40
4	D	337	MET	N-CA-C	-6.35	104.36	111.28
22	r	27	ARG	N-CA-C	6.35	118.63	108.41
6	F	144	VAL	N-CA-CB	6.34	118.69	110.57
22	r	37	PRO	CA-C-N	-6.32	115.05	119.66
22	r	37	PRO	C-N-CA	-6.32	115.05	119.66
11	Q	105	GLU	N-CA-C	6.30	119.36	109.96
7	G	176	CYS	N-CA-C	6.28	119.59	110.42
3	C	47	ARG	N-CA-C	6.24	116.77	109.60
2	B	135	GLY	CA-C-O	-6.24	117.96	122.45
3	C	223	VAL	N-CA-C	6.23	117.06	108.84
7	G	451	ILE	N-CA-C	-6.22	104.91	113.00
21	q	5	GLU	N-CA-C	6.22	117.73	111.07
19	a	26	ILE	N-CA-C	-6.22	104.62	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	415	ILE	N-CA-C	-6.21	104.45	110.72
9	I	86	TYR	N-CA-C	6.20	120.92	112.55
6	F	101	PHE	N-CA-C	6.19	118.81	111.33
7	G	389	THR	N-CA-C	-6.18	101.26	110.23
7	G	356	ASP	N-CA-CB	6.18	119.21	110.12
9	I	66	LEU	N-CA-C	-6.17	105.75	113.28
1	A	110	GLY	N-CA-C	-6.17	105.33	112.73
4	D	262	LEU	N-CA-CB	-6.15	102.41	110.59
6	F	192	ASP	N-CA-C	6.15	118.97	109.07
7	G	418	ILE	N-CA-C	-6.14	103.44	112.04
4	D	145	MET	N-CA-C	6.13	123.86	110.80
2	B	194	CYS	N-CA-CB	6.13	116.22	110.39
2	B	80	ASP	N-CA-CB	6.12	119.11	110.12
7	G	325	ARG	N-CA-CB	6.11	118.83	109.91
7	G	420	LYS	N-CA-C	6.10	118.71	111.33
10	P	361	TRP	N-CA-C	-6.09	106.82	114.56
11	Q	71	HIS	N-CA-C	-6.08	105.15	113.30
2	B	100	CYS	N-CA-C	-6.08	105.58	112.87
3	C	101	ASP	CB-CA-C	-6.07	102.92	111.85
10	P	85	ARG	N-CA-C	-6.07	105.46	112.92
21	q	132	LYS	N-CA-CB	-6.06	107.26	114.17
10	P	268	PRO	N-CA-C	6.04	121.92	113.53
21	q	141	SER	N-CA-C	6.04	117.86	111.28
4	D	147	ASN	N-CA-C	-6.03	104.62	111.07
17	X	140	ASN	CA-C-N	-6.03	114.06	120.03
17	X	140	ASN	C-N-CA	-6.03	114.06	120.03
11	Q	64	LEU	N-CA-C	-6.02	106.54	114.31
16	W	33	ARG	N-CA-C	-5.99	104.75	111.28
7	G	638	THR	N-CA-C	-5.95	100.25	109.24
8	H	21	THR	N-CA-C	-5.94	104.88	111.36
7	G	353	ALA	N-CA-C	-5.94	104.75	112.23
6	F	291	GLU	N-CA-C	5.93	118.20	110.43
7	G	651	PRO	N-CA-C	5.93	121.32	114.03
17	X	16	GLU	N-CA-C	-5.93	102.29	110.35
17	X	60	GLY	N-CA-C	-5.92	105.63	112.50
10	P	76	MET	N-CA-C	-5.92	106.11	113.15
6	F	127	ASP	N-CA-C	5.90	118.50	111.71
17	X	76	SER	N-CA-C	-5.89	101.91	111.04
4	D	350	LYS	CB-CA-C	-5.89	103.20	111.85
7	G	639	LEU	N-CA-C	5.87	118.63	111.82
10	P	331	ASP	CB-CA-C	-5.87	103.44	111.95
4	D	455	ASP	CB-CA-C	-5.86	103.57	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	672	ALA	N-CA-C	-5.82	104.94	111.28
9	I	85	ASN	N-CA-C	-5.80	100.79	109.15
19	a	55	SER	N-CA-C	5.80	118.11	108.13
8	H	2	PHE	N-CA-C	-5.80	104.92	112.23
4	D	232	VAL	N-CA-C	-5.79	101.47	109.46
14	T	77	ASP	N-CA-C	-5.78	107.22	114.56
5	E	119	THR	N-CA-C	-5.78	105.72	112.89
6	F	299	LEU	N-CA-C	5.78	118.52	111.82
4	D	114	GLY	N-CA-C	-5.77	99.50	113.18
10	P	44	GLY	N-CA-C	5.77	119.55	110.96
9	I	64	THR	N-CA-CB	-5.77	103.33	111.00
6	F	393	ASN	N-CA-C	-5.75	104.92	111.07
20	b	61	GLY	N-CA-C	-5.74	107.74	115.21
18	Z	26	PRO	N-CA-C	5.74	120.27	110.74
10	P	375	VAL	N-CA-C	5.74	117.94	108.99
4	D	414	ASP	N-CA-C	-5.74	101.47	110.36
16	W	97	ILE	N-CA-C	-5.74	104.91	110.42
7	G	289	LYS	N-CA-C	5.73	117.53	111.28
6	F	102	MET	CB-CA-C	-5.73	101.49	110.94
7	G	181	ARG	N-CA-C	-5.71	104.67	111.69
9	I	65	GLU	N-CA-C	5.71	120.25	113.28
1	A	65	PHE	N-CA-C	-5.70	106.25	113.43
5	E	183	PRO	N-CA-C	-5.70	102.19	110.80
1	A	61	THR	N-CA-CB	5.69	118.27	110.01
9	I	106	TYR	N-CA-C	-5.69	101.93	109.84
6	F	176	ALA	N-CA-C	5.66	118.18	111.33
3	C	117	ASP	CA-C-N	-5.66	116.40	122.85
3	C	117	ASP	C-N-CA	-5.66	116.40	122.85
6	F	416	SER	N-CA-C	5.65	117.89	111.11
7	G	615	LEU	N-CA-C	-5.65	106.16	113.16
6	F	409	ILE	N-CA-C	5.64	116.38	110.62
7	G	59	GLN	N-CA-C	5.64	117.98	107.99
22	r	108	LYS	N-CA-C	5.63	117.42	111.28
7	G	475	VAL	N-CA-C	5.63	115.97	107.75
7	G	530	TYR	N-CA-C	-5.63	101.95	110.28
4	D	143	SER	CB-CA-C	5.62	120.86	111.30
4	D	221	ARG	N-CA-C	-5.62	106.19	113.16
20	b	24	SER	N-CA-C	-5.61	107.08	114.31
6	F	457	HIS	N-CA-CB	-5.61	100.97	110.50
9	I	189	LYS	N-CA-C	-5.61	106.11	113.17
1	A	81	THR	N-CA-C	-5.60	102.19	110.48
4	D	267	ILE	N-CA-C	5.59	120.97	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	103	LEU	O-C-N	5.59	128.13	122.09
2	B	88	SER	N-CA-CB	5.59	118.17	110.07
4	D	137	ASP	N-CA-C	-5.59	106.42	113.18
8	H	103	LEU	CA-C-O	-5.59	114.94	120.70
6	F	304	ALA	CB-CA-C	-5.58	110.12	116.54
8	H	24	GLU	N-CA-C	-5.56	105.22	111.28
2	B	170	TYR	N-CA-C	-5.56	105.60	112.38
4	D	136	PHE	N-CA-C	5.55	119.22	112.23
20	b	25	VAL	N-CA-C	-5.55	106.93	113.42
4	D	186	ALA	N-CA-C	5.55	117.00	111.07
10	P	177	SER	CB-CA-C	-5.53	103.72	111.80
19	a	25	TYR	N-CA-C	-5.53	107.78	114.75
4	D	309	ASP	CB-CA-C	-5.52	109.72	117.23
10	P	110	ALA	N-CA-CB	-5.52	101.72	110.28
14	T	78	GLY	N-CA-C	-5.51	106.11	112.73
4	D	292	MET	N-CA-C	-5.51	105.36	111.36
18	Z	141	THR	N-CA-C	-5.51	105.18	111.07
10	P	141	PHE	N-CA-C	-5.50	104.72	111.75
4	D	182	ASN	N-CA-CB	5.49	118.03	110.07
3	C	153	ASP	N-CA-C	5.48	117.15	110.41
6	F	118	ASP	N-CA-C	-5.48	102.17	110.28
21	q	33	ILE	N-CA-C	-5.45	107.97	113.20
6	F	294	VAL	CA-C-N	-5.45	114.15	119.76
6	F	294	VAL	C-N-CA	-5.45	114.15	119.76
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
8	H	192	GLU	N-CA-C	-5.42	106.67	113.28
10	P	53	GLY	N-CA-C	5.42	121.39	113.48
6	F	411	SER	N-CA-C	-5.42	105.46	111.36
4	D	344	ILE	N-CA-C	-5.42	105.10	110.62
8	H	196	ALA	N-CA-C	5.41	114.36	108.14
7	G	420	LYS	N-CA-CB	-5.39	101.97	110.06
12	R	48	PHE	N-CA-C	5.39	119.60	113.19
22	r	9	GLN	N-CA-C	5.39	118.07	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
3	C	228	GLU	N-CA-C	-5.39	103.38	110.43
4	D	223	HIS	N-CA-CB	-5.39	103.72	111.91
7	G	654	VAL	N-CA-C	-5.37	105.77	113.07
6	F	199	ARG	N-CA-C	5.35	117.46	109.59
2	B	168	GLY	N-CA-C	5.34	125.83	113.18
8	H	227	GLU	N-CA-C	-5.32	107.16	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	652	ASN	CB-CA-C	-5.31	102.19	111.23
4	D	142	VAL	N-CA-C	-5.29	105.68	110.82
17	X	25	LEU	N-CA-C	-5.29	105.51	111.28
6	F	412	LEU	N-CA-C	-5.29	105.69	111.82
4	D	248	SER	N-CA-C	-5.28	105.61	111.36
19	a	17	VAL	CB-CA-C	-5.28	104.66	111.20
7	G	356	ASP	N-CA-C	-5.26	105.55	111.28
7	G	435	PRO	CB-CA-C	-5.26	105.83	111.56
7	G	682	ASP	CA-C-N	-5.26	114.34	119.76
7	G	682	ASP	C-N-CA	-5.26	114.34	119.76
2	B	155	PRO	N-CA-C	-5.25	101.66	112.47
2	B	141	MET	N-CA-C	-5.24	106.89	113.28
14	T	137	LYS	N-CA-C	5.24	117.90	111.82
7	G	277	MET	N-CA-CB	-5.24	101.65	109.71
10	P	96	LEU	CB-CA-C	-5.23	99.68	109.72
4	D	132	ALA	N-CA-C	-5.23	107.92	114.56
21	q	93	MET	N-CA-C	-5.22	105.76	111.82
3	C	240	ALA	N-CA-CB	-5.22	102.18	110.06
9	I	96	ARG	N-CA-C	5.22	119.49	113.18
4	D	426	ALA	CA-C-N	-5.22	113.81	120.23
4	D	426	ALA	C-N-CA	-5.22	113.81	120.23
2	B	76	THR	N-CA-C	-5.21	105.04	111.40
6	F	300	ILE	N-CA-CB	5.21	119.26	110.56
21	q	26	VAL	N-CA-CB	5.21	119.82	111.23
6	F	131	MET	N-CA-C	-5.20	105.77	112.68
17	X	20	VAL	N-CA-C	-5.19	100.73	108.46
4	D	133	LEU	CA-C-N	-5.18	113.46	119.47
4	D	133	LEU	C-N-CA	-5.18	113.46	119.47
4	D	439	SER	CB-CA-C	-5.18	104.35	112.12
8	H	189	THR	N-CA-C	-5.18	106.98	113.72
13	S	45	LYS	N-CA-C	-5.17	105.53	111.07
21	q	8	LYS	N-CA-C	-5.17	105.55	111.14
7	G	63	PHE	CA-C-O	-5.16	115.08	121.06
7	G	569	GLN	CB-CA-C	-5.15	104.22	112.05
7	G	458	GLY	N-CA-C	-5.15	108.22	115.32
2	B	194	CYS	CA-C-N	-5.14	115.08	120.38
2	B	194	CYS	C-N-CA	-5.14	115.08	120.38
7	G	172	ILE	N-CA-C	-5.14	98.64	109.34
21	q	87	HIS	N-CA-C	-5.14	105.75	111.36
3	C	109	SER	N-CA-C	5.14	118.19	109.76
4	D	352	PRO	N-CA-C	5.12	116.94	110.70
7	G	713	ALA	N-CA-C	-5.12	105.59	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	192	VAL	CB-CA-C	-5.11	105.29	111.88
17	X	139	GLU	N-CA-C	-5.10	102.23	110.14
15	V	87	GLU	N-CA-CB	5.10	117.61	110.12
3	C	241	PHE	CB-CA-C	5.09	118.04	109.69
14	T	89	LEU	N-CA-C	-5.09	105.73	111.28
21	q	69	ASN	CB-CA-C	-5.09	110.69	116.54
4	D	106	VAL	N-CA-CB	-5.09	105.26	111.21
3	C	108	LYS	N-CA-C	5.08	116.82	111.28
6	F	60	GLY	N-CA-C	-5.08	106.05	114.48
19	a	6	LEU	CA-C-N	-5.08	113.53	119.32
19	a	6	LEU	C-N-CA	-5.08	113.53	119.32
12	R	53	LYS	N-CA-C	5.07	116.67	108.41
3	C	181	PRO	CB-CA-C	-5.06	105.33	111.46
7	G	280	ASP	N-CA-CB	-5.06	102.68	110.12
8	H	202	GLU	N-CA-C	-5.06	105.22	111.90
7	G	150	ARG	N-CA-CB	-5.06	101.94	110.49
7	G	660	GLU	N-CA-C	5.05	118.05	109.76
3	C	139	ARG	N-CA-CB	-5.05	102.18	111.37
22	r	59	GLY	N-CA-C	-5.04	106.65	112.50
4	D	142	VAL	N-CA-CB	5.03	117.77	110.52
5	E	213	PRO	CB-CA-C	-5.03	106.30	112.89
10	P	52	SER	N-CA-C	-5.03	106.40	112.88
4	D	419	PRO	N-CA-C	5.02	118.51	111.33
6	F	366	ALA	N-CA-C	-5.02	105.50	110.97
2	B	98	ALA	N-CA-C	5.01	121.48	110.80
11	Q	165	SER	N-CA-C	-5.01	103.86	110.33
9	I	117	LYS	N-CA-C	-5.01	103.09	113.31
9	I	97	PHE	N-CA-C	5.00	121.46	110.80
14	T	149	ALA	N-CA-C	5.00	116.42	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	735	0	791	107	0
2	B	1241	0	1253	147	0
3	C	1643	0	1598	126	0
4	D	3083	0	3053	362	0
5	E	1635	0	1625	185	0
6	F	3288	0	3243	377	0
7	G	5287	0	5322	551	0
8	H	2493	0	2583	342	0
9	I	1380	0	1339	155	0
10	P	2720	0	2740	265	0
11	Q	940	0	930	86	0
12	R	660	0	639	71	0
13	S	667	0	685	72	0
14	T	604	0	596	73	0
15	V	915	0	954	81	0
16	W	970	0	991	90	0
17	X	1164	0	1150	105	0
18	Z	1145	0	1139	112	0
19	a	548	0	562	81	0
20	b	628	0	628	80	0
21	q	1025	0	980	77	0
22	r	686	0	710	73	0
23	s	193	0	187	35	0
24	A	90	0	131	28	0
24	H	51	0	82	11	0
25	B	8	0	0	10	0
25	F	8	0	0	11	0
25	G	16	0	0	8	0
25	I	16	0	0	8	0
26	B	78	0	107	25	0
27	E	4	0	0	3	0
27	G	4	0	0	4	0
28	F	31	0	19	3	0
29	H	35	0	43	10	0
30	P	48	0	26	6	0
31	R	1	0	0	0	0
32	W	35	0	0	0	0
33	q	57	0	58	16	0
All	All	34132	0	34164	3073	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 (3073) 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)
4:D:82:LEU:CD1	4:D:101:LEU:HD22	1.56	1.34
4:D:82:LEU:HD12	4:D:101:LEU:CD2	1.67	1.24
4:D:181:LEU:HD11	4:D:210:MET:SD	1.79	1.23
4:D:181:LEU:CD1	4:D:210:MET:SD	2.27	1.23
3:C:234:LEU:HD12	3:C:234:LEU:O	1.36	1.21
10:P:293:LEU:HB2	10:P:298:TYR:CE2	1.74	1.20
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
7:G:571:HIS:HD2	7:G:572:HIS:CD2	1.59	1.19
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.18
7:G:544:MET:HE3	7:G:546:PHE:CZ	1.78	1.18
3:C:223:VAL:CG2	3:C:225:LEU:CD1	2.22	1.18
3:C:87:ILE:HG13	3:C:144:THR:HG22	1.25	1.17
3:C:229:PHE:CE1	9:I:126:GLN:HG3	1.80	1.16
6:F:293:SER:HA	6:F:336:LEU:HD13	1.22	1.16
13:S:95:LEU:HD12	13:S:95:LEU:O	1.46	1.15
7:G:358:LEU:HD12	7:G:366:LEU:CD2	1.77	1.14
3:C:229:PHE:HE1	9:I:126:GLN:HG3	1.00	1.14
10:P:171:ASN:HB3	10:P:327:VAL:HB	1.26	1.13
1:A:18:ILE:CD1	8:H:76:THR:CG2	2.27	1.11
9:I:210:LEU:HD13	22:r:39:PRO:O	1.47	1.11
18:Z:120:LEU:HD23	18:Z:122:GLY:H	1.14	1.11
4:D:144:MET:SD	4:D:222:MET:HA	1.91	1.11
6:F:266:GLY:CA	6:F:271:SER:HA	1.78	1.10
1:A:18:ILE:HD12	8:H:76:THR:CG2	1.81	1.10
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.15	1.10
9:I:152:CYS:SG	25:I:301:SF4:FE1	1.41	1.10
2:B:100:CYS:SG	25:B:301:SF4:FE2	1.44	1.10
7:G:355:LYS:HA	7:G:366:LEU:CD1	1.82	1.10
10:P:350:ILE:HD11	10:P:366:ILE:HB	1.35	1.08
6:F:266:GLY:HA3	6:F:271:SER:CA	1.84	1.07
3:C:186:ILE:HG23	3:C:187:LEU:HG	1.35	1.06
4:D:86:PRO:CG	4:D:88:HIS:CE1	2.38	1.06
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.34	1.06
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.08	1.05
6:F:379:CYS:SG	25:F:502:SF4:FE4	1.46	1.05
8:H:90:PRO:HD3	8:H:162:LEU:HD13	1.36	1.05
19:a:3:PHE:CE1	33:q:201:CDL:H132	1.92	1.05
7:G:571:HIS:CD2	7:G:572:HIS:CD2	2.44	1.04
5:E:131:ILE:HD11	5:E:185:VAL:HB	1.36	1.04
4:D:299:GLN:NE2	9:I:36:TYR:CE2	2.26	1.04
7:G:355:LYS:HA	7:G:366:LEU:HD11	1.09	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:27:ARG:HB3	22:r:31:ILE:HG23	1.32	1.04
4:D:348:LEU:O	18:Z:11:PRO:HG3	1.56	1.03
4:D:267:ILE:HG22	8:H:278:PRO:HG2	1.33	1.03
7:G:358:LEU:HD12	7:G:366:LEU:HD21	1.06	1.03
21:q:71:LYS:HB3	21:q:73:THR:HG23	1.40	1.03
3:C:120:THR:HG21	15:V:116:ILE:HG21	1.36	1.02
4:D:256:ASP:HA	4:D:259:GLU:CB	1.89	1.02
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.42	1.02
8:H:184:MET:HG2	8:H:293:PHE:CD2	1.95	1.02
8:H:260:MET:HE3	19:a:13:GLY:O	1.58	1.02
3:C:223:VAL:HG22	3:C:225:LEU:CD1	1.90	1.02
6:F:300:ILE:HG23	6:F:305:GLY:O	1.58	1.02
6:F:382:CYS:SG	25:F:502:SF4:FE3	1.50	1.02
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
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.36	1.01
4:D:217:VAL:CG1	4:D:240:LEU:HD22	1.89	1.01
4:D:238:LEU:HB3	22:r:36:GLN:HG3	1.37	1.01
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	1.00
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.00
2:B:148:VAL:HG21	4:D:88:HIS:NE2	1.76	1.00
21:q:78:ASP:HB2	21:q:81:MET:HG3	1.42	0.99
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.28	0.99
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	0.98
4:D:241:LEU:HB3	18:Z:16:TYR:OH	1.63	0.98
19:a:58:ASN:HD22	19:a:60:TYR:HE1	1.10	0.98
8:H:184:MET:HG2	8:H:293:PHE:CE2	1.98	0.98
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.98
2:B:93:MET:CE	2:B:125:PRO:HD3	1.94	0.97
6:F:118:ASP:HA	6:F:159:ARG:HG3	1.45	0.97
4:D:376:GLU:HG3	7:G:121:LEU:HD12	1.46	0.97
1:A:18:ILE:HD12	8:H:76:THR:HG22	1.43	0.97
3:C:152:ILE:HD11	3:C:177:PHE:CE2	1.99	0.97
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.97
10:P:220:TYR:HD2	10:P:226:VAL:HG13	1.29	0.97
4:D:256:ASP:HA	4:D:259:GLU:HB3	1.45	0.96
7:G:75:CYS:SG	27:G:803:FES:FE1	1.57	0.96
7:G:114:GLU:OE2	22:r:53:TYR:HA	1.65	0.96
14:T:99:SER:HB2	14:T:102:SER:HB3	1.48	0.96
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
5:E:134:CYS:HG	27:E:301:FES:FE1	0.66	0.96
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	0.96
1:A:68:GLU:CG	1:A:98:LEU:HD13	1.93	0.96
4:D:86:PRO:HG2	4:D:88:HIS:CE1	2.00	0.95
7:G:611:THR:HG21	11:Q:105:GLU:CA	1.95	0.95
9:I:171:PRO:CB	21:q:93:MET:HE1	1.96	0.95
4:D:256:ASP:HB2	18:Z:25:LEU:HD12	1.46	0.95
6:F:300:ILE:HG22	6:F:306:GLY:HA2	1.46	0.95
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.95
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.95
4:D:238:LEU:HD23	22:r:36:GLN:HB2	1.47	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.95
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	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	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.94
8:H:117:LEU:CD2	8:H:136:VAL:HG11	1.97	0.94
7:G:674:LEU:HD11	13:S:46:LYS:HE2	1.49	0.94
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.94
7:G:338:VAL:CG1	7:G:546:PHE:HE1	1.81	0.94
8:H:199:ASP:HB3	8:H:279:ARG:HD3	1.48	0.94
10:P:306:GLY:HA2	10:P:312:PRO:HB3	1.48	0.93
7:G:544:MET:HE3	7:G:546:PHE:CE1	2.03	0.93
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.82	0.93
18:Z:97:ILE:HG23	18:Z:98:MET:HG3	1.51	0.93
8:H:196:ALA:HB1	8:H:198:PHE:CD1	2.02	0.93
4:D:267:ILE:HG21	8:H:278:PRO:O	1.67	0.93
6:F:293:SER:CA	6:F:336:LEU:HD13	1.97	0.93
6:F:382:CYS:HG	25:F:502:SF4:FE3	0.76	0.93
9:I:113:CYS:HG	25:I:302:SF4:FE3	0.62	0.93
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.93
1:A:68:GLU:HG2	1:A:98:LEU:HD13	1.49	0.92
7:G:611:THR:CG2	11:Q:105:GLU:HA	1.99	0.92
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.52	0.92
7:G:182:CYS:SG	25:G:802:SF4:FE2	1.61	0.92
19:a:3:PHE:CD1	33:q:201:CDL:H132	2.05	0.91
8:H:17:MET:HE1	29:H:401:UQ9:H17	1.50	0.91
7:G:662:THR:HG23	7:G:662:THR:O	1.71	0.91
9:I:152:CYS:HG	25:I:301:SF4:FE1	0.62	0.91
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.53	0.91
22:r:12:ARG:NH2	22:r:21:GLN:HE22	1.68	0.91
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.91
3:C:87:ILE:HG13	3:C:144:THR:CG2	2.00	0.90
4:D:376:GLU:HG3	7:G:121:LEU:CD1	2.00	0.90
7:G:541:PRO:HB2	7:G:561:PRO:HD3	1.52	0.90
7:G:661:GLU:O	7:G:661:GLU:HG2	1.68	0.90
2:B:141:MET:HE2	4:D:115:LEU:HB3	1.53	0.90
4:D:256:ASP:HB2	18:Z:25:LEU:CD1	2.02	0.90
7:G:176:CYS:HG	25:G:802:SF4:FE4	0.62	0.90
7:G:226:CYS:HG	25:G:802:SF4:FE1	0.70	0.90
9:I:123:CYS:HG	25:I:301:SF4:FE2	0.62	0.90
6:F:213:ILE:HG23	6:F:235:VAL:HG22	1.54	0.90
19:a:64:LYS:HE2	19:a:66:LEU:HB2	1.51	0.90
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.85	0.90
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.90
11:Q:57:GLU:OE1	11:Q:58:LYS:HG2	1.71	0.89
22:r:12:ARG:HH21	22:r:21:GLN:HE22	1.17	0.89
10:P:268:PRO:HG3	10:P:342:PRO:HB2	1.54	0.89
6:F:379:CYS:HG	25:F:502:SF4:FE4	0.58	0.89
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.89
2:B:93:MET:SD	2:B:125:PRO:HA	2.13	0.89
3:C:234:LEU:O	3:C:234:LEU:CD1	2.20	0.89
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.37	0.89
8:H:260:MET:HE1	19:a:16:LEU:HB2	1.53	0.89
17:X:20:VAL:HG23	17:X:25:LEU:CD1	2.03	0.88
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.38	0.88
4:D:259:GLU:HG3	18:Z:25:LEU:HD21	1.53	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
7:G:404:GLY:HA2	7:G:684:LEU:HD13	1.52	0.88
4:D:269:ARG:O	4:D:273:VAL:HG12	1.72	0.88
7:G:358:LEU:CD1	7:G:366:LEU:HD21	1.99	0.88
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.56	0.88
10:P:168:SER:O	10:P:202:ARG:HA	1.71	0.88
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.88
6:F:110:PRO:HB3	6:F:152:ARG:HE	1.39	0.87
10:P:293:LEU:HB2	10:P:298:TYR:CZ	2.08	0.87
19:a:58:ASN:HB3	19:a:60:TYR:CD1	2.08	0.87
4:D:120:THR:HG23	4:D:135:TYR:CD1	2.10	0.87
7:G:355:LYS:CA	7:G:366:LEU:HD11	2.02	0.87
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:CYS:SG	25:B:301:SF4:FE4	1.65	0.87
2:B:82:ILE:HD11	26:B:303:PC1:H362	1.55	0.86
3:C:229:PHE:HE1	9:I:126:GLN:CG	1.86	0.86
4:D:86:PRO:HG3	4:D:88:HIS:CE1	2.10	0.86
6:F:129:GLU:OE2	6:F:287:THR:HB	1.75	0.86
4:D:259:GLU:HG2	18:Z:23:ARG:HD2	1.57	0.86
3:C:87:ILE:CG1	3:C:144:THR:HG22	2.05	0.86
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.39	0.86
5:E:68:ASN:ND2	23:s:84:ASN:HD21	1.71	0.86
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.86
7:G:608:VAL:HG23	11:Q:103:THR:HB	1.57	0.86
1:A:18:ILE:CD1	8:H:76:THR:HG23	2.04	0.86
1:A:50:PRO:CG	4:D:80:MET:HG3	2.05	0.86
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.86
3:C:223:VAL:HG21	3:C:225:LEU:HD11	1.56	0.86
4:D:259:GLU:HB3	18:Z:25:LEU:HD11	1.57	0.86
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.74	0.86
11:Q:52:LEU:HD22	16:W:19:SER:HB3	1.58	0.86
22:r:27:ARG:HB3	22:r:31:ILE:CG2	2.05	0.86
4:D:137:ASP:OD2	4:D:223:HIS:HA	1.76	0.86
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.58	0.86
18:Z:120:LEU:HD23	18:Z:122:GLY:N	1.90	0.86
2:B:194:CYS:HG	25:B:301:SF4:FE4	0.55	0.85
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.85
6:F:45:LEU:HD11	6:F:129:GLU:CD	2.01	0.85
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.58	0.85
4:D:137:ASP:OD2	4:D:223:HIS:CA	2.24	0.85
6:F:293:SER:HA	6:F:336:LEU:CD1	2.05	0.85
10:P:293:LEU:CB	10:P:298:TYR:CE2	2.59	0.85
10:P:55:VAL:HG21	12:R:43:TYR:HB2	1.58	0.85
14:T:117:GLU:HA	14:T:120:MET:HE2	1.59	0.85
1:A:7:ILE:HD13	24:A:202:3PE:H371	1.56	0.85
1:A:18:ILE:HD11	8:H:76:THR:CG2	2.07	0.85
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.92	0.85
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.85
8:H:260:MET:HE3	19:a:13:GLY:C	2.00	0.85
17:X:7:LEU:HD12	18:Z:91:LEU:HD22	1.59	0.85
6:F:266:GLY:HA3	6:F:271:SER:HA	0.89	0.85
7:G:615:LEU:HG	10:P:41:ILE:HG23	1.57	0.85
10:P:293:LEU:HB2	10:P:298:TYR:HE2	1.34	0.85
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:662:THR:O	7:G:662:THR:CG2	2.25	0.84
10:P:220:TYR:CD2	10:P:226:VAL:HG13	2.12	0.84
4:D:451:ILE:HG23	4:D:456:ILE:HD11	1.57	0.84
7:G:388:ASN:H	7:G:514:ASN:CB	1.90	0.84
4:D:266:ARG:HH21	9:I:60:ILE:HA	1.42	0.84
7:G:544:MET:CE	7:G:546:PHE:CZ	2.61	0.84
5:E:68:ASN:HD21	23:s:84:ASN:ND2	1.76	0.84
4:D:236:LEU:HD22	4:D:240:LEU:HD23	1.59	0.84
3:C:223:VAL:CG2	3:C:225:LEU:HD12	2.08	0.84
6:F:254:ILE:HA	6:F:262:PHE:CE1	2.13	0.84
1:A:78:ALA:O	1:A:81:THR:HG22	1.78	0.83
8:H:87:VAL:HG12	8:H:96:ILE:HG12	1.56	0.83
7:G:126:LEU:O	7:G:126:LEU:CD1	2.24	0.83
13:S:95:LEU:O	13:S:95:LEU:CD1	2.26	0.83
6:F:425:CYS:HG	25:F:502:SF4:FE1	0.55	0.83
4:D:192:LEU:HD11	4:D:200:PHE:HB2	1.59	0.83
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.42	0.83
11:Q:131:LYS:HG2	11:Q:135:ILE:CD1	2.09	0.83
1:A:25:PRO:O	1:A:26:GLN:HB2	1.78	0.83
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.14	0.83
6:F:425:CYS:SG	25:F:502:SF4:FE1	1.70	0.83
7:G:617:ARG:HH12	16:W:128:GLY:C	1.86	0.82
24:A:202:3PE:H3D2	8:H:80:THR:HG21	1.61	0.82
4:D:256:ASP:CA	4:D:259:GLU:HB3	2.09	0.82
8:H:117:LEU:HD21	8:H:136:VAL:HG11	1.61	0.82
1:A:25:PRO:HG2	8:H:60:PRO:HD3	1.61	0.82
18:Z:58:ARG:HG2	20:b:45:ILE:HG12	1.59	0.82
4:D:390:GLN:OE1	7:G:145:MET:HE1	1.79	0.82
14:T:82:ARG:HD2	14:T:125:GLU:HG3	1.61	0.82
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.82
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.10	0.82
8:H:19:PHE:CE2	19:a:11:ILE:HG21	2.15	0.82
10:P:96:LEU:C	10:P:96:LEU:HD12	2.03	0.82
4:D:129:TYR:HE1	4:D:411:LEU:HD21	1.43	0.82
9:I:89:GLU:HG2	21:q:61:TRP:HB3	1.62	0.82
1:A:68:GLU:CD	1:A:98:LEU:HD13	2.04	0.82
4:D:82:LEU:HD12	4:D:101:LEU:HD22	0.85	0.82
4:D:144:MET:SD	4:D:222:MET:HG3	2.19	0.82
10:P:104:THR:HG21	12:R:46:VAL:HG12	1.60	0.82
12:R:47:ARG:HB2	21:q:125:VAL:HG11	1.61	0.82
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.82

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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	0.82
8:H:45:ILE:HD11	19:a:11:ILE:HD11	1.60	0.82
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.44	0.82
23:s:87:LEU:HA	23:s:90:PHE:HD2	1.44	0.82
5:E:68:ASN:HD21	23:s:84:ASN:HD21	1.26	0.81
8:H:260:MET:HE2	19:a:17:VAL:HG13	1.61	0.81
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.45	0.81
8:H:196:ALA:HB1	8:H:198:PHE:HD1	1.44	0.81
10:P:171:ASN:HB3	10:P:327:VAL:CB	2.11	0.81
18:Z:58:ARG:HG2	20:b:45:ILE:CG1	2.10	0.81
1:A:80:GLN:HA	20:b:46:ASN:HD21	1.43	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
8:H:19:PHE:HE2	19:a:11:ILE:HG21	1.44	0.81
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.63	0.81
7:G:403:VAL:HG23	7:G:432:ILE:HB	1.61	0.81
4:D:192:LEU:HD11	4:D:200:PHE:CB	2.10	0.81
8:H:187:ILE:HG23	8:H:198:PHE:CZ	2.15	0.81
8:H:229:THR:O	8:H:229:THR:HG22	1.81	0.81
7:G:75:CYS:HG	27:G:803:FES:FE1	0.98	0.80
7:G:89:VAL:HB	7:G:94:MET:HG3	1.62	0.80
7:G:355:LYS:CA	7:G:366:LEU:CD1	2.58	0.80
4:D:177:ILE:O	4:D:181:LEU:HD13	1.81	0.80
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.80
17:X:18:VAL:HG12	17:X:20:VAL:HG22	1.63	0.80
3:C:147:ASP:OD1	3:C:148:GLU:OE1	2.00	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
19:a:3:PHE:HE1	33:q:201:CDL:H132	1.44	0.80
26:B:303:PC1:H3C1	8:H:53:MET:HG3	1.63	0.80
7:G:544:MET:HE3	7:G:546:PHE:HZ	1.39	0.80
10:P:88:VAL:HG13	10:P:91:ILE:HD11	1.63	0.80
15:V:72:LEU:HD13	15:V:80:VAL:HG11	1.62	0.80
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.63	0.80
7:G:617:ARG:HH12	16:W:129:HIS:N	1.79	0.80
10:P:226:VAL:HG12	10:P:228:LEU:HG	1.63	0.80
24:A:201:3PE:H361	20:b:23:PHE:CZ	2.17	0.80
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
4:D:256:ASP:HA	4:D:259:GLU:HB2	1.63	0.79
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.22	0.79
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.79
4:D:82:LEU:HB2	4:D:101:LEU:HD13	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:241:LEU:CB	18:Z:16:TYR:OH	2.30	0.79
7:G:73:GLY:HA2	27:G:803:FES:S1	2.22	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
10:P:188:GLU:HG2	10:P:200:ILE:HD13	1.64	0.79
10:P:225:ALA:CB	10:P:289:ILE:HB	2.13	0.79
1:A:72:LEU:HD21	1:A:94:LEU:HD23	1.64	0.79
6:F:227:PRO:HB2	6:F:228:PRO:HD3	1.62	0.79
23:s:92:LEU:HB2	23:s:93:PRO:HD2	1.62	0.79
2:B:93:MET:HE1	2:B:125:PRO:HD3	1.62	0.79
6:F:224:ARG:HD3	11:Q:164:PHE:CE1	2.18	0.79
9:I:211:TYR:CZ	22:r:39:PRO:HG3	2.17	0.79
7:G:388:ASN:H	7:G:514:ASN:HB3	1.45	0.79
14:T:106:LYS:H	14:T:106:LYS:HD2	1.48	0.79
2:B:100:CYS:HG	25:B:301:SF4:FE2	0.99	0.78
4:D:259:GLU:HG3	18:Z:25:LEU:CD2	2.12	0.78
2:B:99:CYS:SG	25:B:301:SF4:S3	2.81	0.78
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.78
8:H:227:GLU:O	8:H:231:ILE:HG13	1.83	0.78
4:D:96:ARG:HG3	4:D:112:HIS:HB2	1.64	0.78
8:H:184:MET:CG	8:H:293:PHE:CD2	2.66	0.78
3:C:170:TRP:CG	3:C:183:LEU:HD21	2.18	0.78
6:F:424:ILE:HD11	7:G:73:GLY:O	1.84	0.78
3:C:160:ILE:HD12	4:D:285:ASN:HD22	1.49	0.78
7:G:338:VAL:HG13	7:G:546:PHE:HE1	1.47	0.78
2:B:93:MET:HE3	2:B:125:PRO:HD3	1.66	0.78
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.66	0.78
10:P:51:VAL:HG22	10:P:53:GLY:H	1.48	0.78
2:B:136:THR:HG21	4:D:118:ARG:HD3	1.66	0.78
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.98	0.78
1:A:73:LEU:O	1:A:76:PRO:HD2	1.84	0.78
1:A:50:PRO:HG3	4:D:80:MET:CG	2.14	0.77
10:P:363:SER:HA	16:W:54:GLN:HE22	1.46	0.77
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.77
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.13	0.77
1:A:72:LEU:CD2	1:A:94:LEU:HD23	2.13	0.77
3:C:103:THR:HG21	15:V:55:LYS:HE3	1.66	0.77
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.77
10:P:266:THR:HG21	10:P:329:PRO:HG3	1.67	0.77
17:X:20:VAL:HG23	17:X:25:LEU:HD11	1.66	0.77
1:A:3:LEU:HD23	24:A:202:3PE:H31	1.66	0.77
3:C:160:ILE:HD12	4:D:285:ASN:ND2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:210:LEU:HD12	22:r:39:PRO:HD2	1.66	0.77
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.65	0.77
8:H:190:LEU:O	8:H:196:ALA:HB2	1.83	0.77
1:A:68:GLU:HG2	1:A:98:LEU:CD1	2.13	0.77
4:D:137:ASP:CG	4:D:223:HIS:HA	2.09	0.77
5:E:196:THR:H	5:E:199:ASP:HB2	1.47	0.77
4:D:267:ILE:CG2	8:H:278:PRO:HG2	2.15	0.77
7:G:355:LYS:HG3	7:G:366:LEU:HD12	1.67	0.77
8:H:260:MET:CE	19:a:16:LEU:HB2	2.15	0.77
4:D:137:ASP:OD1	4:D:138:ARG:HG3	1.83	0.77
8:H:89:LEU:HD23	8:H:91:MET:HE2	1.64	0.77
6:F:36:LYS:HB3	6:F:38:GLU:HG2	1.66	0.76
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.76
7:G:652:ASN:HB3	7:G:655:ARG:NH2	2.00	0.76
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.76
8:H:117:LEU:HD23	8:H:136:VAL:HG11	1.67	0.76
3:C:70:LYS:HD3	15:V:101:GLU:HB2	1.67	0.76
7:G:126:LEU:HD13	12:R:89:PRO:HB3	1.67	0.76
10:P:217:PHE:HB2	10:P:280:ILE:HD13	1.66	0.76
14:T:123:GLU:HG2	14:T:130:ILE:HG12	1.65	0.76
3:C:89:PRO:O	3:C:92:VAL:HG23	1.85	0.76
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.21	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
7:G:127:ASP:HA	12:R:106:TYR:OH	1.86	0.76
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.21	0.76
1:A:50:PRO:HG3	4:D:80:MET:HG3	1.66	0.76
2:B:202:LEU:HD23	9:I:86:TYR:CG	2.20	0.76
4:D:299:GLN:NE2	9:I:36:TYR:CD2	2.53	0.76
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.66	0.76
2:B:148:VAL:CG2	4:D:88:HIS:NE2	2.48	0.75
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.75
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.05	0.75
21:q:25:ARG:HB3	21:q:29:ARG:HH12	1.52	0.75
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.75
11:Q:64:LEU:HG	16:W:84:LEU:HD12	1.68	0.75
13:S:22:HIS:C	13:S:58:CYS:SG	2.69	0.75
17:X:128:VAL:O	17:X:128:VAL:HG23	1.86	0.75
22:r:27:ARG:HD2	22:r:31:ILE:HG22	1.67	0.75
1:A:80:GLN:CA	20:b:46:ASN:HD21	1.97	0.75
8:H:90:PRO:HG2	8:H:240:ILE:HD13	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:277:VAL:HA	4:D:324:GLY:O	1.86	0.75
6:F:184:LYS:HB3	23:s:92:LEU:HD22	1.67	0.75
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.75
3:C:152:ILE:HD11	3:C:177:PHE:HE2	1.51	0.75
4:D:261:MET:HE1	9:I:73:THR:CG2	2.16	0.75
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.75
17:X:130:LYS:HD2	20:b:59:ASP:OD1	1.87	0.75
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
15:V:35:LEU:HD13	15:V:48:THR:HG23	1.68	0.75
9:I:90:LYS:HB2	21:q:90:LEU:CD2	2.17	0.75
9:I:180:HIS:CD2	10:P:100:LEU:HD21	2.21	0.75
18:Z:120:LEU:CD2	18:Z:122:GLY:H	1.94	0.75
2:B:126:ARG:HG3	8:H:216:ALA:HB2	1.66	0.74
3:C:118:VAL:HG12	3:C:120:THR:HG22	1.69	0.74
10:P:272:LEU:HG	10:P:375:VAL:HG21	1.68	0.74
10:P:301:ILE:HG22	10:P:305:PHE:HE2	1.52	0.74
11:Q:69:GLU:O	11:Q:72:ILE:HG22	1.86	0.74
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.01	0.74
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
7:G:335:GLY:HA3	7:G:362:ASP:HB3	1.68	0.74
10:P:359:TYR:O	10:P:360:ARG:HB3	1.86	0.74
17:X:49:GLU:HG3	17:X:50:GLU:HG3	1.70	0.74
4:D:86:PRO:HG2	4:D:88:HIS:ND1	2.02	0.74
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.22	0.74
12:R:31:ILE:HG12	12:R:37:VAL:HB	1.70	0.74
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.74
4:D:238:LEU:HB3	22:r:36:GLN:CG	2.17	0.74
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.22	0.74
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.74
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.74
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.74
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.74
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.74
10:P:225:ALA:HB1	10:P:289:ILE:HB	1.68	0.73
10:P:96:LEU:HD12	10:P:97:MET:N	2.01	0.73
4:D:368:ARG:NH2	9:I:165:ASP:OD1	2.21	0.73
6:F:67:GLU:HG3	6:F:71:LYS:HE3	1.70	0.73
8:H:260:MET:SD	19:a:13:GLY:HA2	2.28	0.73
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.23	0.73
10:P:134:TRP:HB3	10:P:312:PRO:HG3	1.71	0.73
14:T:104:PHE:HB3	14:T:110:LEU:HD22	1.71	0.73
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.71	0.73
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.73
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.24	0.73
10:P:55:VAL:HG21	12:R:43:TYR:CB	2.18	0.73
10:P:124:ASN:OD1	10:P:125:VAL:HG23	1.89	0.73
2:B:161:MET:HG2	2:B:196:PRO:HG2	1.71	0.73
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.73
8:H:304:HIS:O	8:H:308:PRO:HD3	1.87	0.73
10:P:226:VAL:CG1	10:P:228:LEU:HG	2.19	0.73
18:Z:129:THR:HG23	18:Z:132:GLU:H	1.52	0.73
2:B:93:MET:SD	2:B:125:PRO:CA	2.77	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.52	0.73
6:F:258:GLY:O	6:F:261:TRP:HB3	1.89	0.73
7:G:382:ARG:HG2	7:G:386:LEU:HD11	1.69	0.73
8:H:54:LYS:HE2	8:H:58:LYS:HD2	1.71	0.73
13:S:42:VAL:HG13	13:S:43:GLU:CD	2.13	0.73
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.69	0.73
24:H:402:3PE:H362	9:I:61:LEU:O	1.89	0.73
15:V:28:TYR:OH	15:V:55:LYS:HD3	1.89	0.73
6:F:228:PRO:HG2	11:Q:160:TYR:HD2	1.53	0.72
6:F:392:MET:CE	6:F:419:ILE:HD12	2.18	0.72
7:G:176:CYS:SG	25:G:802:SF4:FE4	1.78	0.72
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.72	0.72
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.70	0.72
10:P:64:PHE:HE1	10:P:209:ARG:O	1.72	0.72
4:D:144:MET:SD	4:D:222:MET:CA	2.73	0.72
5:E:176:LEU:HD12	5:E:184:MET:HE3	1.69	0.72
5:E:185:VAL:HG22	5:E:195:LEU:HD13	1.72	0.72
9:I:77:LEU:O	19:a:2:TRP:HB3	1.90	0.72
19:a:64:LYS:HE2	19:a:66:LEU:CB	2.19	0.72
7:G:544:MET:CE	7:G:546:PHE:HZ	2.01	0.72
19:a:58:ASN:ND2	19:a:60:TYR:HE1	1.84	0.72
1:A:65:PHE:O	1:A:68:GLU:HB2	1.90	0.72
3:C:120:THR:HG23	3:C:121:ARG:N	2.05	0.72
4:D:146:CYS:SG	4:D:178:THR:OG1	2.48	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.20	0.72
10:P:270:ARG:HH21	10:P:327:VAL:C	1.98	0.72
1:A:79:ILE:HA	1:A:87:MET:SD	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:302:PC1:H341	26:B:302:PC1:H222	1.70	0.72
4:D:215:GLU:OE2	9:I:94:SER:HB3	1.89	0.72
1:A:99:SER:HB3	24:A:201:3PE:H392	1.71	0.72
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.72
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.71
2:B:92:PRO:HD3	2:B:119:VAL:HG13	1.72	0.71
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.90	0.71
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.71	0.71
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.71
9:I:154:TYR:HA	9:I:169:GLU:OE2	1.90	0.71
13:S:25:GLN:HG3	13:S:57:GLU:CD	2.15	0.71
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.71
10:P:73:LEU:HA	10:P:76:MET:HE2	1.71	0.71
1:A:80:GLN:HA	20:b:46:ASN:ND2	2.05	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
8:H:45:ILE:CD1	19:a:11:ILE:HD11	2.19	0.71
11:Q:82:PRO:HD3	11:Q:98:LYS:HG3	1.70	0.71
10:P:274:PHE:HE1	10:P:290:PRO:HG3	1.54	0.71
21:q:10:GLY:HA3	33:q:201:CDL:HA32	1.72	0.71
4:D:203:MET:HE1	4:D:254:ARG:HB3	1.70	0.71
7:G:266:ARG:HH12	9:I:131:GLU:HG2	1.54	0.71
8:H:288:LEU:HD11	24:H:402:3PE:H2	1.71	0.71
10:P:276:LEU:HD23	10:P:280:ILE:HD12	1.72	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
8:H:157:ASN:ND2	8:H:165:LEU:HD11	2.06	0.71
21:q:25:ARG:O	21:q:29:ARG:HB3	1.91	0.71
1:A:22:PHE:HA	8:H:60:PRO:HG3	1.71	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
4:D:129:TYR:CE1	4:D:411:LEU:HD21	2.25	0.71
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
4:D:202:TRP:HH2	4:D:261:MET:CE	2.03	0.71
9:I:210:LEU:CD1	22:r:39:PRO:O	2.35	0.71
13:S:79:LEU:HA	13:S:82:LEU:HG	1.73	0.71
4:D:187:VAL:HG13	4:D:330:TYR:HE1	1.56	0.70
4:D:304:LYS:HG3	4:D:316:PHE:CZ	2.26	0.70
4:D:386:THR:CG2	9:I:118:LEU:HD13	2.21	0.70
21:q:26:VAL:HG12	21:q:32:ASP:O	1.91	0.70
4:D:436:ASP:OD1	4:D:437:LYS:N	2.25	0.70
10:P:64:PHE:CZ	10:P:242:VAL:HG21	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:ARG:HG2	8:H:214:GLU:O	1.90	0.70
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.21	0.70
8:H:200:LEU:HD11	8:H:285:LEU:HD23	1.74	0.70
4:D:217:VAL:HG11	4:D:240:LEU:HD22	1.72	0.70
5:E:131:ILE:HD13	5:E:187:ILE:HG12	1.72	0.70
4:D:202:TRP:HH2	4:D:261:MET:HE2	1.57	0.70
10:P:91:ILE:HG13	10:P:95:ARG:HH12	1.57	0.70
10:P:157:LYS:HB2	10:P:195:PHE:HD1	1.55	0.70
5:E:71:GLU:HG3	23:s:94:GLN:HE21	1.54	0.70
13:S:42:VAL:HG22	13:S:46:LYS:HE3	1.72	0.70
2:B:93:MET:HE1	2:B:125:PRO:CD	2.22	0.70
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.72	0.70
8:H:191:ALA:HB2	8:H:198:PHE:CD1	2.27	0.70
10:P:165:ILE:HD13	10:P:253:THR:HG22	1.73	0.70
21:q:26:VAL:CG1	21:q:32:ASP:O	2.40	0.70
7:G:617:ARG:NH1	16:W:128:GLY:C	2.50	0.70
10:P:174:MET:O	10:P:175:LYS:HG2	1.91	0.70
15:V:19:THR:HB	15:V:22:GLU:HG3	1.74	0.70
24:A:201:3PE:H361	20:b:23:PHE:CE1	2.27	0.69
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.69
8:H:90:PRO:HG2	8:H:240:ILE:HG21	1.74	0.69
19:a:7:PRO:O	19:a:11:ILE:HD12	1.92	0.69
4:D:348:LEU:O	18:Z:11:PRO:CG	2.37	0.69
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.69
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.69
8:H:97:ASN:ND2	19:a:38:VAL:HG13	2.07	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	1.92	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.69
8:H:90:PRO:CG	8:H:162:LEU:HB3	2.22	0.69
8:H:265:LEU:O	8:H:269:THR:N	2.24	0.69
9:I:123:CYS:SG	25:I:301:SF4:FE2	1.79	0.69
10:P:333:PRO:HA	10:P:337:ASP:OD2	1.92	0.69
14:T:82:ARG:HD2	14:T:125:GLU:CG	2.23	0.69
1:A:50:PRO:HG2	4:D:80:MET:HG3	1.74	0.69
4:D:259:GLU:CB	18:Z:25:LEU:HD11	2.23	0.69
13:S:62:GLN:HB2	13:S:80:ASN:HB2	1.75	0.69
19:a:18:ILE:N	19:a:19:PRO:CD	2.56	0.69
8:H:200:LEU:CD1	8:H:285:LEU:HD23	2.22	0.69
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:300:ILE:HG22	6:F:306:GLY:CA	2.22	0.69
20:b:78:LEU:HD22	20:b:80:TRP:HE1	1.56	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
6:F:410:ASP:OD1	6:F:411:SER:N	2.26	0.69
7:G:652:ASN:HB3	7:G:655:ARG:HH22	1.57	0.69
18:Z:130:LYS:HA	18:Z:133:MET:HE2	1.73	0.69
11:Q:99:MET:HE2	11:Q:126:LEU:HD12	1.73	0.69
1:A:80:GLN:C	20:b:46:ASN:HD21	2.01	0.69
5:E:185:VAL:HG22	5:E:195:LEU:CD1	2.23	0.69
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.69
7:G:338:VAL:CG1	7:G:546:PHE:CE1	2.72	0.68
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.75	0.68
1:A:50:PRO:CG	4:D:80:MET:CG	2.69	0.68
3:C:223:VAL:HG22	3:C:225:LEU:HD12	1.69	0.68
4:D:220:ALA:HB2	9:I:98:ARG:HH21	1.58	0.68
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.68
7:G:617:ARG:NH1	16:W:129:HIS:N	2.39	0.68
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.29	0.68
17:X:59:GLU:HA	17:X:62:LEU:HG	1.73	0.68
18:Z:92:GLU:O	18:Z:96:ILE:N	2.26	0.68
1:A:87:MET:HE1	8:H:309:ILE:HD11	1.73	0.68
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.68
8:H:90:PRO:HB3	8:H:162:LEU:HB3	1.75	0.68
17:X:130:LYS:HD3	20:b:63:MET:HG3	1.74	0.68
1:A:79:ILE:HD13	1:A:87:MET:SD	2.34	0.68
7:G:628:GLU:OE1	16:W:122:LEU:HB2	1.92	0.68
8:H:90:PRO:CG	8:H:240:ILE:HG21	2.24	0.68
16:W:87:ILE:HG22	16:W:91:MET:HE3	1.73	0.68
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.68
4:D:255:ILE:HG12	4:D:337:MET:HE2	1.74	0.68
5:E:178:ALA:HB3	5:E:184:MET:SD	2.34	0.68
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.74	0.68
8:H:287:HIS:CD2	8:H:291:LYS:HD2	2.28	0.68
3:C:63:TYR:CZ	3:C:67:ILE:HD11	2.28	0.68
8:H:155:LEU:O	8:H:315:PRO:HG2	1.94	0.68
20:b:31:ILE:HA	20:b:34:MET:HE2	1.76	0.68
2:B:94:THR:HG21	2:B:104:MET:HE2	1.76	0.67
8:H:314:VAL:HG23	18:Z:58:ARG:HH21	1.59	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.27	0.67
8:H:102:ILE:HG22	8:H:150:LEU:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:89:GLU:OE1	21:q:58:ARG:HG2	1.94	0.67
10:P:266:THR:HG21	10:P:329:PRO:HB3	1.76	0.67
14:T:111:ASP:H	14:T:114:ASP:HB2	1.58	0.67
21:q:137:TRP:CH2	21:q:140:PRO:HD3	2.29	0.67
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.67
17:X:134:ASP:OD1	17:X:135:ARG:N	2.27	0.67
18:Z:59:ARG:HG2	20:b:81:LEU:HG	1.77	0.67
18:Z:105:LYS:HD3	18:Z:108:GLU:OE1	1.95	0.67
19:a:58:ASN:HB3	19:a:60:TYR:HD1	1.59	0.67
10:P:266:THR:HG21	10:P:329:PRO:CG	2.25	0.67
15:V:106:GLU:HG3	15:V:107:PRO:HD2	1.75	0.67
1:A:113:TRP:HZ2	8:H:286:MET:HE2	1.59	0.67
2:B:113:ASP:OD1	8:H:34:ARG:HD3	1.94	0.67
7:G:356:ASP:O	7:G:360:LYS:HG3	1.93	0.67
19:a:2:TRP:CZ2	33:q:201:CDL:HB31	2.29	0.67
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.67
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.67
17:X:18:VAL:HG21	18:Z:74:LEU:HD11	1.77	0.67
1:A:68:GLU:OE2	1:A:98:LEU:HD22	1.95	0.67
2:B:93:MET:CE	2:B:125:PRO:CD	2.73	0.67
10:P:166:HIS:CD2	10:P:191:VAL:HG21	2.29	0.67
18:Z:69:ILE:HD12	20:b:54:PRO:HD3	1.75	0.67
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.67
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.67
21:q:39:VAL:HG21	21:q:89:TRP:CH2	2.30	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
7:G:382:ARG:NE	7:G:652:ASN:HD21	1.93	0.67
9:I:78:PHE:HA	19:a:2:TRP:CD1	2.28	0.67
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.48	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
13:S:40:ARG:HA	13:S:43:GLU:OE1	1.95	0.67
6:F:199:ARG:HD3	23:s:80:PHE:CE2	2.30	0.66
7:G:336:ASN:H	7:G:363:SER:HB2	1.60	0.66
17:X:46:CYS:HB2	17:X:135:ARG:CZ	2.25	0.66
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.66
19:a:32:GLY:HA3	19:a:60:TYR:CD2	2.30	0.66
22:r:8:ILE:O	22:r:11:LEU:HB2	1.95	0.66
2:B:107:MET:HE3	2:B:114:MET:HE2	1.77	0.66
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.66
4:D:326:CYS:SG	4:D:453:THR:HG21	2.35	0.66
6:F:300:ILE:CG2	6:F:307:VAL:N	2.59	0.66
7:G:126:LEU:CD1	12:R:89:PRO:HB3	2.26	0.66
7:G:651:PRO:HB2	13:S:57:GLU:O	1.96	0.66
6:F:117:ALA:HB1	6:F:131:MET:SD	2.35	0.66
6:F:300:ILE:HG21	6:F:307:VAL:N	2.11	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.66
6:F:300:ILE:HD11	6:F:356:VAL:HG21	1.78	0.66
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.95	0.66
10:P:209:ARG:HA	10:P:352:VAL:HG12	1.78	0.66
26:B:302:PC1:H112	21:q:75:TRP:CE3	2.31	0.66
3:C:120:THR:CG2	15:V:116:ILE:HG21	2.18	0.66
5:E:180:VAL:HG21	5:E:224:CYS:HA	1.78	0.66
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.66
8:H:196:ALA:CB	8:H:198:PHE:HD1	2.08	0.66
17:X:18:VAL:HA	17:X:68:LEU:HD21	1.76	0.66
10:P:187:GLY:HA2	10:P:190:GLU:HG2	1.78	0.66
17:X:24:VAL:HG12	17:X:86:TRP:CD1	2.31	0.66
18:Z:143:TYR:O	18:Z:144:THR:C	2.39	0.66
21:q:67:GLU:HG2	21:q:72:ASN:HA	1.78	0.66
1:A:25:PRO:CG	8:H:60:PRO:HD3	2.26	0.66
4:D:192:LEU:CD1	4:D:200:PHE:HB2	2.25	0.66
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.66
10:P:226:VAL:HG11	10:P:277:VAL:HG11	1.77	0.66
22:r:6:ARG:O	22:r:9:GLN:HG2	1.96	0.66
2:B:109:ALA:HB1	2:B:110:PRO:HD2	1.78	0.66
5:E:131:ILE:HG23	5:E:170:LEU:HA	1.77	0.66
5:E:192:TYR:HB3	5:E:195:LEU:HD21	1.78	0.66
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.66
1:A:17:LEU:HD13	8:H:225:MET:HE1	1.78	0.65
1:A:26:GLN:HG3	26:B:303:PC1:H232	1.77	0.65
4:D:266:ARG:HH21	9:I:60:ILE:CA	2.08	0.65
5:E:197:PRO:HA	5:E:200:ILE:HD12	1.77	0.65
6:F:109:ARG:HE	6:F:239:PRO:HD3	1.61	0.65
7:G:179:CYS:HG	25:G:802:SF4:FE3	1.11	0.65
2:B:202:LEU:CD2	9:I:86:TYR:CG	2.79	0.65
9:I:51:LYS:HA	18:Z:33:TYR:CE2	2.31	0.65
10:P:176:SER:H	10:P:182:ARG:HG2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:87:LEU:HD13	14:T:98:LEU:HD11	1.79	0.65
2:B:202:LEU:HD23	9:I:86:TYR:CD1	2.29	0.65
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.77	0.65
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.78	0.65
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.65
9:I:89:GLU:HG2	21:q:61:TRP:CB	2.26	0.65
19:a:55:SER:HB3	19:a:61:TYR:CD2	2.32	0.65
2:B:122:ARG:HH22	4:D:90:ALA:HB3	1.61	0.65
4:D:241:LEU:HB3	18:Z:16:TYR:HH	1.61	0.65
3:C:152:ILE:HD12	3:C:153:ASP:O	1.97	0.65
5:E:151:LEU:CD1	5:E:200:ILE:HG21	2.26	0.65
7:G:358:LEU:CD1	7:G:366:LEU:CD2	2.65	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
8:H:230:ASN:CB	8:H:233:LEU:HD12	2.25	0.65
10:P:171:ASN:CB	10:P:327:VAL:HB	2.16	0.65
22:r:68:ILE:HG13	22:r:68:ILE:O	1.97	0.65
2:B:95:PHE:CD1	2:B:97:LEU:CD1	2.80	0.65
13:S:44:LEU:HD11	13:S:95:LEU:HD21	1.78	0.65
4:D:97:LEU:HD21	4:D:435:LEU:HD21	1.78	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.77	0.65
4:D:266:ARG:HH22	9:I:63:TRP:HA	1.62	0.65
10:P:64:PHE:CZ	10:P:242:VAL:CG2	2.79	0.65
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.65
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.26	0.65
9:I:90:LYS:HD3	21:q:91:HIS:CE1	2.31	0.65
7:G:614:GLY:O	16:W:129:HIS:HE1	1.80	0.65
11:Q:75:ARG:HH22	11:Q:104:ARG:HG3	1.61	0.65
2:B:195:PRO:O	2:B:196:PRO:C	2.35	0.65
3:C:223:VAL:HG22	3:C:225:LEU:HD13	1.74	0.65
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.65
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.65
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.65
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.27	0.65
8:H:102:ILE:HD13	8:H:154:LEU:HD21	1.77	0.65
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.78	0.65
14:T:123:GLU:CD	14:T:130:ILE:H	2.03	0.65
17:X:54:ARG:HG2	18:Z:84:LEU:HD11	1.78	0.65
17:X:133:THR:HG22	17:X:135:ARG:H	1.62	0.64
4:D:259:GLU:CG	18:Z:25:LEU:HD11	2.27	0.64
7:G:652:ASN:CB	7:G:655:ARG:NH2	2.59	0.64
8:H:102:ILE:HD13	8:H:154:LEU:CD2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:184:MET:HA	8:H:293:PHE:HE2	1.62	0.64
14:T:105:MET:HE2	14:T:139:MET:HG2	1.79	0.64
3:C:87:ILE:CG1	3:C:144:THR:CG2	2.69	0.64
4:D:136:PHE:HA	4:D:139:LEU:HD12	1.80	0.64
9:I:171:PRO:HB3	21:q:93:MET:CE	2.04	0.64
14:T:93:ILE:HG13	14:T:110:LEU:HG	1.78	0.64
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.64
8:H:87:VAL:HB	8:H:88:PRO:HD3	1.79	0.64
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.78	0.64
5:E:176:LEU:HB2	5:E:184:MET:HE1	1.80	0.64
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.33	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.64
17:X:7:LEU:HD22	18:Z:87:LEU:CD1	2.27	0.64
6:F:196:PHE:HE1	23:s:91:ARG:HD3	1.62	0.64
7:G:401:LEU:HD21	7:G:432:ILE:CD1	2.28	0.64
12:R:36:GLN:NE2	21:q:127:TYR:HB3	2.13	0.64
4:D:315:GLU:HB3	4:D:346:GLN:HE22	1.62	0.64
6:F:224:ARG:NH1	11:Q:164:PHE:CD1	2.66	0.64
7:G:572:HIS:HB2	7:G:699:SER:OG	1.98	0.64
8:H:70:LEU:HA	8:H:73:ILE:HG22	1.79	0.64
13:S:44:LEU:HD11	13:S:95:LEU:CD2	2.28	0.64
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.78	0.64
5:E:226:PRO:HB2	5:E:229:GLY:O	1.98	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.33	0.64
1:A:23:TRP:CZ3	1:A:24:LEU:HD23	2.33	0.64
3:C:124:ARG:HD2	3:C:148:GLU:OE2	1.98	0.64
4:D:113:ILE:HG21	4:D:432:LEU:CD2	2.27	0.64
9:I:51:LYS:HA	18:Z:33:TYR:HE2	1.63	0.64
16:W:27:ASP:HB2	16:W:30:GLU:HG3	1.78	0.64
21:q:3:LEU:HD13	33:q:201:CDL:H521	1.80	0.64
8:H:45:ILE:HD11	19:a:11:ILE:CD1	2.28	0.64
8:H:307:LEU:HD23	8:H:310:PHE:CZ	2.33	0.64
1:A:24:LEU:CD1	26:B:303:PC1:H3B2	2.28	0.63
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.80	0.63
6:F:235:VAL:HG23	6:F:240:THR:HG21	1.80	0.63
2:B:138:THR:HG21	4:D:116:LEU:HA	1.79	0.63
4:D:137:ASP:OD2	4:D:223:HIS:HB3	1.98	0.63
6:F:388:GLY:HA3	6:F:419:ILE:HD11	1.80	0.63
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.80	0.63
8:H:102:ILE:CG2	8:H:150:LEU:HD11	2.28	0.63
22:r:6:ARG:HA	22:r:9:GLN:HG2	1.80	0.63
3:C:63:TYR:CE2	3:C:67:ILE:HD11	2.32	0.63
6:F:174:ARG:HG3	23:s:87:LEU:HD11	1.80	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.81	0.63
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.63	0.63
8:H:145:THR:O	8:H:149:ILE:HG12	1.97	0.63
17:X:31:HIS:HB2	17:X:70:PHE:HZ	1.63	0.63
2:B:137:LEU:HD22	2:B:145:LEU:CD2	2.29	0.63
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.62	0.63
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.39	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
2:B:108:ALA:HA	2:B:114:MET:HG2	1.80	0.63
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.81	0.63
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.63
7:G:388:ASN:HB3	7:G:511:LYS:HE2	1.81	0.63
8:H:87:VAL:HG13	8:H:95:LEU:HD23	1.80	0.63
10:P:169:HIS:H	10:P:184:LYS:HE3	1.64	0.63
18:Z:69:ILE:O	20:b:53:TYR:HE1	1.82	0.63
4:D:376:GLU:OE1	7:G:151:SER:HB2	1.99	0.63
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.80	0.63
14:T:106:LYS:HD2	14:T:106:LYS:N	2.13	0.63
15:V:8:THR:HG23	15:V:8:THR:O	1.97	0.63
22:r:5:THR:HG22	22:r:7:VAL:HG12	1.81	0.63
10:P:266:THR:HG21	10:P:329:PRO:CB	2.29	0.63
14:T:102:SER:O	14:T:141:PRO:HD3	1.98	0.63
4:D:87:GLN:HG3	4:D:93:GLY:HA2	1.80	0.63
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.63
5:E:68:ASN:HD21	23:s:84:ASN:CG	2.06	0.63
6:F:35:LEU:HD23	6:F:40:ARG:HG2	1.81	0.63
8:H:51:ASP:OD2	29:H:401:UQ9:H15	1.99	0.63
10:P:114:ASP:HA	10:P:117:ARG:HB2	1.80	0.63
10:P:207:PHE:CE2	10:P:241:TYR:HD1	2.17	0.63
12:R:98:GLU:CD	12:R:98:GLU:H	2.07	0.63
1:A:18:ILE:HD11	8:H:76:THR:HG23	1.72	0.62
2:B:106:HIS:CE1	4:D:211:PHE:HE2	2.16	0.62
7:G:173:MET:HE1	7:G:206:VAL:O	1.99	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.28	0.62
7:G:652:ASN:C	7:G:652:ASN:OD1	2.42	0.62
13:S:20:ARG:HG2	13:S:66:TRP:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:9:THR:HG21	15:V:78:GLU:HB2	1.81	0.62
20:b:65:ASP:O	20:b:66:VAL:C	2.41	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
8:H:51:ASP:OD1	29:H:401:UQ9:C15	2.46	0.62
8:H:189:THR:HB	8:H:234:MET:HB3	1.80	0.62
3:C:186:ILE:HG23	3:C:187:LEU:N	2.14	0.62
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.99	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.82	0.62
7:G:473:MET:CE	7:G:514:ASN:HD21	2.12	0.62
2:B:207:GLN:HG3	2:B:210:ARG:HH21	1.65	0.62
4:D:82:LEU:CD1	4:D:101:LEU:CD2	2.49	0.62
5:E:183:PRO:HB2	5:E:195:LEU:N	2.14	0.62
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.80	0.62
8:H:5:ASN:ND2	8:H:95:LEU:HD13	2.14	0.62
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.29	0.62
3:C:103:THR:HG21	15:V:55:LYS:CE	2.28	0.62
3:C:189:ASP:OD1	3:C:190:TYR:N	2.32	0.62
4:D:320:ILE:HD11	9:I:38:TYR:CE1	2.35	0.62
4:D:386:THR:HG23	9:I:118:LEU:HD13	1.81	0.62
8:H:90:PRO:CG	8:H:240:ILE:HD13	2.30	0.62
10:P:276:LEU:HD23	10:P:280:ILE:CD1	2.30	0.62
10:P:363:SER:HB3	16:W:51:HIS:CE1	2.35	0.62
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.80	0.62
1:A:106:TRP:CH2	20:b:19:LEU:HD21	2.34	0.62
4:D:217:VAL:HG11	4:D:240:LEU:CD2	2.29	0.62
8:H:260:MET:CE	19:a:17:VAL:HG13	2.29	0.62
15:V:27:LEU:O	15:V:31:THR:HG23	1.99	0.62
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.82	0.62
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
8:H:85:LEU:O	8:H:88:PRO:HD2	1.99	0.62
8:H:91:MET:O	8:H:92:PRO:C	2.42	0.62
17:X:86:TRP:CZ2	19:a:64:LYS:HA	2.35	0.62
2:B:90:LEU:O	2:B:119:VAL:HA	2.00	0.62
3:C:63:TYR:CE2	3:C:67:ILE:CD1	2.83	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
8:H:119:SER:HB2	8:H:215:TYR:CE1	2.34	0.62
8:H:195:ARG:CZ	8:H:274:ARG:HB2	2.29	0.62
16:W:104:THR:O	16:W:108:ARG:HG3	1.99	0.62
4:D:202:TRP:CD2	9:I:76:TYR:HE2	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.35	0.62
4:D:187:VAL:HG13	4:D:330:TYR:CE1	2.35	0.62
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.62
13:S:22:HIS:O	13:S:58:CYS:SG	2.58	0.62
16:W:58:THR:HG23	16:W:61:GLN:H	1.65	0.62
2:B:184:ILE:HG22	2:B:185:VAL:HG13	1.82	0.61
4:D:250:ASN:HA	22:r:23:LYS:HD3	1.82	0.61
5:E:71:GLU:OE1	23:s:96:SER:HB3	2.00	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.61
8:H:195:ARG:HH22	8:H:271:LEU:HA	1.65	0.61
10:P:209:ARG:O	10:P:210:GLU:HG2	2.00	0.61
10:P:320:GLU:O	10:P:324:ILE:HG22	2.00	0.61
11:Q:62:THR:HB	11:Q:72:ILE:HD11	1.82	0.61
1:A:13:LEU:HD21	8:H:14:LEU:HD11	1.82	0.61
3:C:126:GLU:OE2	3:C:143:LYS:HD3	1.99	0.61
7:G:136:GLU:HG2	11:Q:85:ASN:HD21	1.64	0.61
8:H:1:MET:HE2	19:a:26:ILE:HG23	1.82	0.61
8:H:288:LEU:HG	8:H:293:PHE:CE1	2.35	0.61
10:P:235:THR:HG21	10:P:323:HIS:O	2.00	0.61
6:F:45:LEU:HD11	6:F:129:GLU:OE1	1.99	0.61
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.30	0.61
3:C:195:HIS:HE1	16:W:88:LYS:NZ	1.98	0.61
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.82	0.61
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.61
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.29	0.61
8:H:303:TRP:HE3	20:b:29:ALA:HB2	1.65	0.61
10:P:252:ALA:HB2	10:P:338:LEU:HD21	1.81	0.61
21:q:68:MET:HG3	21:q:71:LYS:HB2	1.83	0.61
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.61
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.61
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.81	0.61
8:H:195:ARG:NH1	8:H:274:ARG:HB2	2.14	0.61
10:P:97:MET:O	10:P:103:LEU:HD11	2.00	0.61
10:P:293:LEU:CB	10:P:298:TYR:HE2	2.05	0.61
24:A:201:3PE:H391	20:b:23:PHE:HE1	1.65	0.61
4:D:149:GLN:HE21	4:D:171:ARG:HB3	1.65	0.61
5:E:136:THR:HB	27:E:301:FES:S2	2.41	0.61
18:Z:101:VAL:HB	18:Z:102:PRO:HD2	1.81	0.61
24:A:201:3PE:H361	20:b:23:PHE:HZ	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:TYR:OH	4:D:117:HIS:HE1	1.83	0.61
5:E:68:ASN:ND2	23:s:84:ASN:ND2	2.41	0.61
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
19:a:58:ASN:CB	19:a:60:TYR:CE1	2.84	0.61
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.30	0.61
4:D:348:LEU:HB3	18:Z:16:TYR:CE2	2.36	0.61
7:G:182:CYS:HG	25:G:802:SF4:FE2	0.44	0.61
13:S:18:GLU:HB2	13:S:52:PRO:HB2	1.81	0.61
13:S:42:VAL:CG1	13:S:43:GLU:OE2	2.49	0.61
24:A:201:3PE:H2A1	20:b:20:VAL:HG13	1.83	0.61
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.61
8:H:195:ARG:NH2	8:H:271:LEU:HD23	2.15	0.61
10:P:228:LEU:HD21	10:P:277:VAL:HG21	1.81	0.61
17:X:7:LEU:CD2	18:Z:87:LEU:CD1	2.78	0.61
22:r:9:GLN:HA	22:r:12:ARG:HG2	1.80	0.61
2:B:97:LEU:HD23	2:B:136:THR:O	2.01	0.61
4:D:124:ILE:HG13	4:D:135:TYR:CD2	2.36	0.61
6:F:299:LEU:CD1	6:F:300:ILE:HG13	2.30	0.61
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.61
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.61
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.61
14:T:92:LYS:HE3	16:W:67:ARG:NH1	2.16	0.61
3:C:73:GLN:HG2	15:V:103:LEU:HD21	1.83	0.60
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.82	0.60
8:H:85:LEU:HD21	8:H:108:THR:HB	1.82	0.60
9:I:68:ARG:NH2	18:Z:26:PRO:O	2.34	0.60
4:D:220:ALA:CB	9:I:98:ARG:HH21	2.14	0.60
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.82	0.60
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.60
10:P:236:VAL:HG21	10:P:270:ARG:HG2	1.84	0.60
10:P:300:TRP:HE3	10:P:301:ILE:HD13	1.67	0.60
1:A:1:MET:O	1:A:4:TYR:N	2.34	0.60
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.60
4:D:267:ILE:HG22	8:H:278:PRO:CG	2.22	0.60
7:G:571:HIS:CD2	7:G:572:HIS:HD2	2.11	0.60
8:H:260:MET:HE1	19:a:16:LEU:CB	2.28	0.60
10:P:321:ARG:O	10:P:325:SER:HB3	2.01	0.60
2:B:115:ASP:HA	2:B:119:VAL:O	2.01	0.60
3:C:120:THR:HG21	15:V:116:ILE:CG2	2.22	0.60
4:D:325:ASP:OD1	4:D:328:ASP:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.37	0.60
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.60
17:X:130:LYS:HD2	20:b:59:ASP:CG	2.25	0.60
2:B:153:PRO:HG3	8:H:58:LYS:HE3	1.83	0.60
5:E:142:ARG:HG2	5:E:183:PRO:HD3	1.83	0.60
7:G:614:GLY:O	16:W:129:HIS:CE1	2.54	0.60
8:H:190:LEU:HD13	8:H:270:PHE:CD1	2.36	0.60
9:I:87:PRO:HG2	9:I:88:PHE:CD2	2.37	0.60
11:Q:69:GLU:HA	11:Q:72:ILE:HG22	1.82	0.60
2:B:167:GLY:H	2:B:180:GLY:HA2	1.67	0.60
5:E:147:ILE:HD11	5:E:195:LEU:HB2	1.84	0.60
6:F:225:LEU:HD22	7:G:93:ALA:HB3	1.84	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
20:b:63:MET:HB2	20:b:66:VAL:HG12	1.83	0.60
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.83	0.60
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.60
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	0.60
7:G:541:PRO:HB2	7:G:561:PRO:CD	2.28	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.60
8:H:90:PRO:HB3	8:H:162:LEU:CB	2.31	0.60
17:X:60:GLY:C	18:Z:81:ARG:HH22	2.09	0.60
3:C:84:GLU:HG2	3:C:141:ARG:HD2	1.83	0.60
6:F:45:LEU:CD1	6:F:129:GLU:OE1	2.50	0.60
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.60
9:I:80:GLU:N	19:a:1:MET:HE1	2.16	0.60
9:I:135:ARG:O	9:I:135:ARG:HG2	2.00	0.60
14:T:80:LYS:HG3	14:T:145:VAL:HG21	1.84	0.60
15:V:14:LEU:CD2	15:V:79:GLU:HG2	2.32	0.60
16:W:26:ARG:HB2	16:W:26:ARG:NH1	2.16	0.60
20:b:69:HIS:CD2	20:b:70:PRO:HD2	2.36	0.60
2:B:99:CYS:HB2	4:D:222:MET:HE2	1.83	0.60
26:B:303:PC1:H3B1	8:H:57:MET:CE	2.32	0.60
4:D:217:VAL:CG1	4:D:240:LEU:CD2	2.74	0.60
4:D:353:PRO:HA	18:Z:10:MET:HE1	1.82	0.60
6:F:224:ARG:HD3	11:Q:164:PHE:CZ	2.37	0.60
8:H:66:THR:OG1	8:H:124:ASN:HB2	2.02	0.60
8:H:307:LEU:HA	8:H:310:PHE:CE2	2.36	0.60
9:I:93:LEU:HD11	9:I:173:PHE:CE2	2.37	0.60
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.10	0.59
5:E:195:LEU:HD23	5:E:218:ARG:HG3	1.83	0.59
7:G:136:GLU:HG2	11:Q:85:ASN:ND2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:145:MET:O	22:r:61:ARG:NH2	2.35	0.59
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.82	0.59
9:I:68:ARG:HH12	18:Z:28:ARG:HG2	1.67	0.59
9:I:105:ARG:NH2	9:I:191:LEU:HD22	2.17	0.59
10:P:297:VAL:O	10:P:301:ILE:HG12	2.01	0.59
12:R:33:HIS:CD2	12:R:34:THR:HG23	2.37	0.59
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.59
8:H:51:ASP:CG	29:H:401:UQ9:H15	2.27	0.59
8:H:102:ILE:CD1	8:H:154:LEU:CD2	2.80	0.59
15:V:38:PHE:CE1	15:V:95:LEU:HB2	2.37	0.59
4:D:137:ASP:OD2	4:D:223:HIS:CB	2.50	0.59
5:E:143:ASP:O	5:E:146:SER:HB3	2.02	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.17	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.59
9:I:106:TYR:OH	12:R:88:HIS:HB3	2.01	0.59
10:P:192:ARG:HH12	10:P:260:GLY:HA2	1.67	0.59
7:G:401:LEU:HD21	7:G:432:ILE:HD12	1.83	0.59
2:B:106:HIS:CE1	4:D:211:PHE:CE2	2.90	0.59
3:C:208:GLU:CG	3:C:221:GLU:HG3	2.31	0.59
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.27	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.67	0.59
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.59
8:H:190:LEU:HD23	8:H:198:PHE:HE1	1.67	0.59
10:P:228:LEU:HD13	10:P:232:GLY:HA3	1.84	0.59
17:X:44:MET:HE2	18:Z:73:PRO:HA	1.84	0.59
4:D:232:VAL:HG22	4:D:356:ILE:HB	1.85	0.59
12:R:84:GLY:O	12:R:85:ALA:HB3	2.02	0.59
24:A:202:3PE:H391	8:H:81:LEU:HD23	1.85	0.59
4:D:87:GLN:O	4:D:93:GLY:HA3	2.02	0.59
6:F:261:TRP:HE3	6:F:262:PHE:CD1	2.21	0.59
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.65	0.59
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.67	0.59
7:G:130:ILE:HA	9:I:140:ARG:HH11	1.68	0.59
9:I:38:TYR:CD2	9:I:41:LYS:HD3	2.38	0.59
15:V:75:GLY:HA3	15:V:79:GLU:OE1	2.01	0.59
5:E:233:LEU:HD21	6:F:45:LEU:HB3	1.84	0.59
8:H:51:ASP:OD1	29:H:401:UQ9:H15	2.03	0.59
9:I:113:CYS:SG	25:I:302:SF4:FE3	1.80	0.59
10:P:282:GLY:O	10:P:285:HIS:CE1	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:237:PRO:HG2	11:Q:88:GLN:OE1	2.02	0.59
5:E:184:MET:HG3	5:E:192:TYR:O	2.03	0.59
6:F:64:LYS:H	6:F:256:ARG:HE	1.49	0.59
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.85	0.59
8:H:119:SER:HB2	8:H:215:TYR:HE1	1.66	0.59
9:I:189:LYS:HG3	9:I:189:LYS:O	2.02	0.59
10:P:170:LEU:O	10:P:171:ASN:OD1	2.21	0.59
11:Q:161:GLY:HA2	11:Q:164:PHE:CD2	2.38	0.59
17:X:125:LEU:HB2	18:Z:66:GLU:HB3	1.84	0.59
3:C:223:VAL:HG23	3:C:225:LEU:CD1	2.26	0.59
7:G:32:ILE:HG12	7:G:45:PRO:HG3	1.85	0.59
8:H:90:PRO:CB	8:H:162:LEU:HB3	2.31	0.59
12:R:47:ARG:HG3	12:R:48:PHE:CD2	2.38	0.59
4:D:259:GLU:CG	18:Z:25:LEU:CD1	2.81	0.58
6:F:119:GLU:HB3	6:F:124:THR:CG2	2.32	0.58
6:F:329:LYS:HA	6:F:332:CYS:SG	2.43	0.58
7:G:372:PHE:H	7:G:532:PRO:HB2	1.68	0.58
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.68	0.58
10:P:227:PRO:HB2	10:P:298:TYR:CE1	2.38	0.58
10:P:238:GLN:HG2	10:P:270:ARG:HG3	1.83	0.58
12:R:47:ARG:HB2	21:q:125:VAL:CG1	2.31	0.58
23:s:79:THR:O	23:s:83:LEU:HG	2.03	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
4:D:222:MET:O	4:D:223:HIS:HB2	2.02	0.58
5:E:134:CYS:SG	5:E:175:CYS:HA	2.43	0.58
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.83	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.17	0.58
9:I:90:LYS:H	21:q:90:LEU:HD21	1.68	0.58
1:A:23:TRP:CZ3	1:A:24:LEU:CD2	2.86	0.58
1:A:51:PHE:CD2	1:A:53:MET:HB2	2.38	0.58
4:D:376:GLU:HG3	7:G:121:LEU:HD13	1.85	0.58
5:E:188:ASN:O	5:E:189:ASP:HB3	2.03	0.58
6:F:174:ARG:HB2	23:s:87:LEU:HD11	1.85	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
1:A:55:PHE:HE1	8:H:134:ARG:HA	1.68	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.85	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.86	0.58
8:H:198:PHE:CE2	24:H:402:3PE:H242	2.39	0.58
11:Q:64:LEU:HD12	16:W:85:LEU:HD21	1.86	0.58
2:B:91:TRP:HA	2:B:120:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:144:MET:SD	4:D:223:HIS:N	2.74	0.58
4:D:238:LEU:CB	22:r:36:GLN:HG3	2.23	0.58
6:F:231:ALA:O	6:F:239:PRO:HA	2.04	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.58
10:P:96:LEU:C	10:P:96:LEU:CD1	2.72	0.58
10:P:302:GLY:HA2	10:P:305:PHE:HD2	1.68	0.58
17:X:9:THR:HB	17:X:12:GLU:HG3	1.86	0.58
19:a:50:ARG:O	19:a:54:ILE:HG13	2.03	0.58
26:B:302:PC1:H112	21:q:75:TRP:HE3	1.68	0.58
6:F:133:HIS:O	6:F:134:ASP:C	2.46	0.58
6:F:184:LYS:HB3	23:s:92:LEU:CD2	2.33	0.58
6:F:379:CYS:SG	25:F:502:SF4:S1	3.02	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.86	0.58
2:B:194:CYS:O	25:B:301:SF4:S3	2.61	0.58
4:D:267:ILE:CG2	8:H:278:PRO:O	2.48	0.58
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.68	0.58
7:G:388:ASN:H	7:G:514:ASN:HB2	1.65	0.58
13:S:42:VAL:CG1	13:S:43:GLU:CD	2.76	0.58
21:q:88:ARG:HG2	21:q:94:THR:OG1	2.03	0.58
5:E:243:GLY:O	6:F:257:ARG:HG3	2.03	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
8:H:81:LEU:O	8:H:82:ALA:C	2.45	0.58
9:I:163:PRO:O	12:R:89:PRO:HD3	2.04	0.58
10:P:91:ILE:HD12	10:P:105:PHE:CD2	2.39	0.58
15:V:114:TRP:CD2	15:V:114:TRP:O	2.57	0.58
19:a:18:ILE:N	19:a:19:PRO:HD3	2.19	0.58
1:A:18:ILE:HD11	8:H:76:THR:HG22	1.69	0.58
1:A:51:PHE:HD2	1:A:53:MET:HB2	1.69	0.58
24:A:201:3PE:H3C1	20:b:23:PHE:CD1	2.39	0.58
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.63	0.58
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.58
17:X:15:VAL:HG21	17:X:61:LYS:HG2	1.84	0.58
17:X:132:LYS:HB3	20:b:59:ASP:HB3	1.84	0.58
4:D:235:ASP:HA	4:D:356:ILE:HG21	1.85	0.58
4:D:253:LEU:HD22	22:r:23:LYS:HB2	1.85	0.58
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.04	0.58
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.58
7:G:136:GLU:OE2	7:G:272:ARG:NH1	2.36	0.58
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.58
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:103:LEU:HD21	8:H:160:TYR:CE1	2.39	0.58
10:P:236:VAL:HG22	10:P:270:ARG:HG2	1.85	0.58
3:C:45:THR:OG1	22:r:57:ARG:HD2	2.04	0.57
3:C:229:PHE:CE1	9:I:126:GLN:CG	2.71	0.57
5:E:189:ASP:OD1	6:F:163:TYR:HB3	2.04	0.57
8:H:150:LEU:C	8:H:150:LEU:HD13	2.29	0.57
8:H:157:ASN:C	8:H:157:ASN:OD1	2.46	0.57
13:S:14:LEU:HB3	13:S:70:ALA:HB2	1.85	0.57
1:A:64:LEU:O	1:A:68:GLU:HG3	2.03	0.57
5:E:221:ARG:O	5:E:225:GLU:HB3	2.03	0.57
7:G:330:LEU:HD13	7:G:546:PHE:CZ	2.39	0.57
8:H:318:MET:SD	19:a:41:VAL:HG11	2.43	0.57
17:X:15:VAL:CG2	17:X:61:LYS:HG2	2.35	0.57
17:X:24:VAL:HG12	17:X:86:TRP:CG	2.39	0.57
18:Z:7:LYS:HD2	22:r:40:LYS:O	2.04	0.57
2:B:193:GLY:HA2	9:I:154:TYR:CE2	2.39	0.57
8:H:138:GLN:NE2	8:H:191:ALA:O	2.31	0.57
8:H:305:ILE:O	8:H:308:PRO:HD2	2.04	0.57
13:S:42:VAL:O	13:S:46:LYS:HG3	2.04	0.57
14:T:90:TYR:CE2	14:T:93:ILE:HG12	2.38	0.57
15:V:45:ARG:O	15:V:49:GLU:HB2	2.04	0.57
2:B:199:GLU:HB2	9:I:173:PHE:CE1	2.40	0.57
4:D:192:LEU:HD11	4:D:200:PHE:HB3	1.85	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
7:G:355:LYS:CB	7:G:366:LEU:CD1	2.82	0.57
8:H:62:ARG:HD3	8:H:68:MET:SD	2.44	0.57
13:S:42:VAL:HG13	13:S:43:GLU:OE2	2.03	0.57
15:V:50:GLN:HE22	22:r:93:LYS:HA	1.69	0.57
2:B:157:TYR:HB3	2:B:188:ASP:OD2	2.03	0.57
7:G:330:LEU:HA	7:G:544:MET:HE1	1.86	0.57
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.40	0.57
10:P:169:HIS:ND1	30:P:401:NDP:H5N	2.20	0.57
2:B:99:CYS:HB3	4:D:141:TYR:CB	2.34	0.57
5:E:183:PRO:HB2	5:E:195:LEU:H	1.68	0.57
5:E:233:LEU:CD2	6:F:45:LEU:HB3	2.34	0.57
8:H:287:HIS:HD2	8:H:291:LYS:HD2	1.67	0.57
10:P:88:VAL:HA	10:P:91:ILE:HG12	1.86	0.57
10:P:128:ASN:ND2	10:P:149:PRO:HB3	2.20	0.57
12:R:38:TYR:HE1	12:R:44:ARG:HE	1.53	0.57
3:C:184:ARG:NH2	4:D:110:ASP:OD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.87	0.57
7:G:386:LEU:O	7:G:387:LEU:C	2.46	0.57
10:P:209:ARG:CA	10:P:352:VAL:HG12	2.34	0.57
5:E:131:ILE:HD11	5:E:185:VAL:CB	2.24	0.57
8:H:96:ILE:HG13	8:H:96:ILE:O	2.04	0.57
8:H:158:GLY:HA3	8:H:315:PRO:HB2	1.86	0.57
8:H:200:LEU:HD11	8:H:285:LEU:CD2	2.34	0.57
10:P:271:TYR:HA	10:P:375:VAL:HG22	1.86	0.57
15:V:81:ILE:O	15:V:82:LEU:C	2.47	0.57
21:q:68:MET:O	21:q:71:LYS:HB2	2.05	0.57
22:r:13:ASN:OD1	22:r:20:LEU:HB2	2.05	0.57
1:A:55:PHE:O	1:A:56:PHE:C	2.46	0.57
4:D:137:ASP:OD1	4:D:137:ASP:C	2.48	0.57
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.70	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.87	0.57
15:V:6:LYS:CG	15:V:16:VAL:HG23	2.34	0.57
17:X:20:VAL:HG23	17:X:25:LEU:HD12	1.83	0.57
21:q:6:VAL:HG21	33:q:201:CDL:HB61	1.86	0.57
2:B:224:ARG:HD3	10:P:85:ARG:HH12	1.70	0.56
4:D:202:TRP:CH2	4:D:261:MET:CE	2.86	0.56
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.87	0.56
14:T:104:PHE:HE2	14:T:144:ILE:HD11	1.69	0.56
4:D:361:ALA:O	4:D:384:LEU:HD11	2.05	0.56
6:F:226:LYS:O	6:F:227:PRO:C	2.47	0.56
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.40	0.56
10:P:192:ARG:HE	10:P:200:ILE:HD12	1.70	0.56
13:S:55:ILE:O	13:S:55:ILE:HG13	2.05	0.56
19:a:58:ASN:HB3	19:a:60:TYR:CE1	2.39	0.56
2:B:95:PHE:CD1	2:B:97:LEU:HD11	2.40	0.56
3:C:67:ILE:HA	15:V:43:ALA:HB3	1.86	0.56
3:C:210:ARG:NH2	10:P:75:ARG:HD3	2.21	0.56
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.56
5:E:165:ASP:C	5:E:167:LEU:H	2.13	0.56
6:F:213:ILE:HG23	6:F:235:VAL:CG2	2.32	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
9:I:36:TYR:HD2	22:r:104:TRP:HB2	1.70	0.56
10:P:54:VAL:O	10:P:54:VAL:HG23	2.05	0.56
10:P:217:PHE:CB	10:P:280:ILE:HD13	2.33	0.56
11:Q:126:LEU:HD13	11:Q:137:PHE:CE2	2.40	0.56
11:Q:163:ASN:C	11:Q:163:ASN:OD1	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:33:HIS:HD2	12:R:34:THR:HG23	1.70	0.56
15:V:111:GLN:HG3	15:V:111:GLN:O	2.04	0.56
18:Z:125:TYR:HA	18:Z:128:ARG:HD3	1.87	0.56
23:s:76:ASN:O	23:s:79:THR:HG22	2.05	0.56
23:s:92:LEU:HD12	23:s:93:PRO:O	2.05	0.56
2:B:93:MET:HE1	2:B:125:PRO:CG	2.36	0.56
6:F:129:GLU:OE2	6:F:287:THR:CB	2.53	0.56
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.56
7:G:400:VAL:HG22	7:G:473:MET:HG2	1.87	0.56
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.56
10:P:258:ALA:O	10:P:261:LYS:HB2	2.05	0.56
13:S:44:LEU:HD12	13:S:48:HIS:CD2	2.40	0.56
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.40	0.56
17:X:20:VAL:CG2	17:X:25:LEU:HD11	2.33	0.56
18:Z:97:ILE:HG13	18:Z:98:MET:H	1.71	0.56
4:D:82:LEU:HB2	4:D:101:LEU:CD1	2.35	0.56
4:D:301:ASP:O	4:D:302:LEU:HB2	2.05	0.56
7:G:275:PRO:HB3	7:G:286:ILE:HG23	1.86	0.56
9:I:90:LYS:HE2	21:q:79:GLY:O	2.06	0.56
11:Q:163:ASN:OD1	11:Q:164:PHE:CD1	2.58	0.56
20:b:69:HIS:CG	20:b:70:PRO:HD2	2.41	0.56
4:D:158:LEU:HD12	4:D:411:LEU:HD23	1.87	0.56
8:H:253:GLU:HG3	19:a:21:VAL:CG2	2.35	0.56
9:I:180:HIS:CD2	10:P:100:LEU:CD2	2.87	0.56
10:P:223:PHE:CZ	10:P:227:PRO:HG3	2.39	0.56
10:P:223:PHE:CE2	10:P:227:PRO:HG3	2.40	0.56
12:R:35:GLY:O	12:R:36:GLN:HB3	2.06	0.56
13:S:25:GLN:HG3	13:S:57:GLU:OE1	2.05	0.56
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.56
3:C:184:ARG:HH22	4:D:112:HIS:CD2	2.24	0.56
4:D:166:ARG:NH1	18:Z:9:ASP:O	2.26	0.56
5:E:240:PRO:HB3	6:F:60:GLY:HA3	1.88	0.56
8:H:68:MET:O	8:H:69:SER:C	2.49	0.56
12:R:69:VAL:CG1	12:R:112:LYS:HB2	2.35	0.56
20:b:69:HIS:HB3	20:b:72:ASP:OD1	2.06	0.56
1:A:75:LEU:HD13	8:H:305:ILE:HD11	1.86	0.56
2:B:77:LYS:HE3	26:B:302:PC1:H271	1.88	0.56
4:D:92:HIS:CD2	4:D:95:LEU:HD21	2.41	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.56
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:91:ILE:HD12	10:P:105:PHE:HD2	1.70	0.56
20:b:11:ASN:OD1	20:b:12:ALA:N	2.39	0.56
8:H:90:PRO:HD2	8:H:240:ILE:HD13	1.88	0.56
9:I:180:HIS:NE2	10:P:100:LEU:HD21	2.21	0.56
19:a:37:ARG:HH11	19:a:59:ARG:HD2	1.70	0.56
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.41	0.56
3:C:120:THR:CG2	3:C:121:ARG:N	2.68	0.56
4:D:97:LEU:HB3	4:D:99:LEU:HD21	1.86	0.56
12:R:69:VAL:HG12	12:R:112:LYS:N	2.21	0.56
22:r:64:VAL:HB	22:r:65:PRO:HD2	1.87	0.56
1:A:1:MET:O	1:A:2:ASN:C	2.48	0.55
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.55
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.17	0.55
8:H:30:TYR:CE1	19:a:1:MET:O	2.58	0.55
8:H:68:MET:O	8:H:72:ILE:HG12	2.07	0.55
9:I:79:ARG:HH21	22:r:20:LEU:HD13	1.70	0.55
10:P:232:GLY:HA2	10:P:273:LEU:HD23	1.89	0.55
10:P:249:ILE:O	10:P:253:THR:HG23	2.05	0.55
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.34	0.55
3:C:223:VAL:HG23	3:C:225:LEU:HD12	1.88	0.55
4:D:171:ARG:HG2	4:D:227:ILE:HD12	1.88	0.55
6:F:42:PHE:HD2	6:F:275:LEU:HD11	1.70	0.55
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.86	0.55
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.55
7:G:652:ASN:OD1	7:G:652:ASN:O	2.23	0.55
8:H:48:PRO:HA	8:H:51:ASP:OD2	2.06	0.55
17:X:133:THR:HG21	17:X:135:ARG:CZ	2.35	0.55
2:B:99:CYS:C	2:B:101:ALA:N	2.61	0.55
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.87	0.55
5:E:130:HIS:NE2	5:E:132:GLN:HG2	2.21	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.55
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.55
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.55
17:X:7:LEU:HD22	18:Z:87:LEU:HD12	1.86	0.55
18:Z:89:GLU:O	18:Z:93:GLU:HG2	2.06	0.55
19:a:6:LEU:O	19:a:7:PRO:C	2.44	0.55
3:C:186:ILE:CG2	3:C:187:LEU:HG	2.23	0.55
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.67	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.18	0.55
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.55
8:H:96:ILE:O	8:H:98:LEU:HG	2.06	0.55
8:H:157:ASN:OD1	8:H:158:GLY:N	2.40	0.55
10:P:304:LEU:H	10:P:304:LEU:HD12	1.71	0.55
24:A:201:3PE:H3C1	20:b:23:PHE:HD1	1.72	0.55
2:B:168:GLY:HA3	2:B:172:HIS:HB2	1.87	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
8:H:181:MET:HE3	8:H:300:LEU:HD13	1.89	0.55
9:I:211:TYR:CE1	22:r:39:PRO:HG3	2.41	0.55
1:A:106:TRP:CZ3	20:b:19:LEU:HD21	2.41	0.55
2:B:117:PHE:HZ	9:I:86:TYR:HB3	1.72	0.55
4:D:133:LEU:HB3	4:D:134:PRO:HD3	1.88	0.55
4:D:140:ASP:H	4:D:147:ASN:ND2	2.05	0.55
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.42	0.55
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.84	0.55
7:G:388:ASN:N	7:G:514:ASN:HB2	2.22	0.55
8:H:150:LEU:O	8:H:154:LEU:HG	2.07	0.55
1:A:5:THR:O	1:A:9:ILE:HG12	2.07	0.55
1:A:113:TRP:CZ2	8:H:286:MET:HG3	2.42	0.55
3:C:104:ASN:O	22:r:97:PRO:HD3	2.06	0.55
4:D:163:PRO:HG2	4:D:168:GLN:HE21	1.71	0.55
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.55
7:G:375:GLU:O	7:G:675:VAL:HG21	2.06	0.55
7:G:382:ARG:CZ	7:G:652:ASN:HD21	2.19	0.55
7:G:545:LEU:HD21	7:G:547:LEU:HD21	1.88	0.55
22:r:12:ARG:NH2	22:r:21:GLN:NE2	2.46	0.55
1:A:96:THR:OG1	20:b:26:TRP:NE1	2.39	0.55
2:B:81:LEU:HA	26:B:302:PC1:H242	1.88	0.55
4:D:380:HIS:O	4:D:384:LEU:HG	2.07	0.55
5:E:91:TRP:CE3	5:E:125:PRO:HB3	2.41	0.55
11:Q:81:VAL:O	11:Q:81:VAL:HG13	2.06	0.55
17:X:9:THR:HG22	17:X:11:GLU:H	1.72	0.55
2:B:84:TRP:CZ3	26:B:302:PC1:H371	2.42	0.55
3:C:79:CYS:SG	22:r:64:VAL:HG23	2.46	0.55
3:C:219:VAL:HG11	16:W:113:THR:CG2	2.37	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.55
8:H:161:SER:HB2	8:H:164:THR:HG23	1.87	0.55
8:H:200:LEU:HD13	8:H:282:TYR:HD1	1.71	0.55
9:I:68:ARG:NH1	18:Z:28:ARG:HG2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:272:LEU:HG	10:P:375:VAL:HG11	1.89	0.55
12:R:44:ARG:HB3	12:R:47:ARG:NH1	2.22	0.55
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.21	0.55
15:V:22:GLU:O	15:V:23:ARG:C	2.50	0.55
19:a:40:ARG:HG2	19:a:41:VAL:HG13	1.87	0.55
1:A:3:LEU:CD2	24:A:202:3PE:H31	2.35	0.55
4:D:123:LEU:HB3	4:D:135:TYR:OH	2.07	0.55
6:F:254:ILE:HG23	6:F:259:GLY:HA2	1.89	0.55
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.40	0.55
15:V:35:LEU:CD1	15:V:48:THR:HG23	2.37	0.55
4:D:202:TRP:CH2	4:D:261:MET:HE3	2.42	0.54
6:F:119:GLU:HG3	6:F:127:ASP:OD2	2.07	0.54
7:G:360:LYS:HD3	7:G:632:ILE:HB	1.89	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
9:I:153:ILE:O	9:I:154:TYR:C	2.48	0.54
10:P:206:ILE:HG13	30:P:401:NDP:H42N	1.89	0.54
10:P:335:LEU:O	10:P:339:GLY:N	2.38	0.54
20:b:45:ILE:HA	20:b:80:TRP:HH2	1.72	0.54
1:A:92:PHE:CE1	8:H:302:MET:HG3	2.43	0.54
4:D:181:LEU:CD1	4:D:210:MET:CE	2.84	0.54
6:F:35:LEU:HB2	6:F:291:GLU:HB2	1.89	0.54
12:R:40:GLU:HA	12:R:45:ARG:HH11	1.72	0.54
13:S:16:LEU:HD21	13:S:19:ILE:HD11	1.89	0.54
21:q:69:ASN:CG	21:q:70:GLY:H	2.15	0.54
2:B:107:MET:CE	2:B:114:MET:HE2	2.37	0.54
26:B:303:PC1:C3C	8:H:53:MET:HG3	2.37	0.54
4:D:82:LEU:HD12	4:D:101:LEU:CG	2.34	0.54
4:D:411:LEU:HD11	4:D:419:PRO:HB3	1.90	0.54
7:G:629:ILE:CD1	16:W:122:LEU:HD21	2.37	0.54
8:H:84:SER:O	8:H:87:VAL:HG23	2.07	0.54
11:Q:161:GLY:HA2	11:Q:164:PHE:HD2	1.72	0.54
16:W:42:TRP:CE2	16:W:93:LEU:HG	2.41	0.54
17:X:64:ASN:OD1	17:X:64:ASN:O	2.25	0.54
2:B:175:TYR:OH	4:D:117:HIS:CE1	2.61	0.54
4:D:95:LEU:HB3	4:D:458:PHE:CZ	2.42	0.54
4:D:95:LEU:HD23	4:D:458:PHE:CZ	2.41	0.54
4:D:255:ILE:HG22	4:D:338:ARG:NH2	2.22	0.54
4:D:311:TYR:HA	4:D:314:VAL:HG22	1.90	0.54
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.89	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.54
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.54
7:G:380:ASP:O	13:S:55:ILE:HG12	2.07	0.54
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.54
9:I:143:THR:HA	12:R:34:THR:HG21	1.89	0.54
10:P:296:PHE:CE1	10:P:297:VAL:HG23	2.42	0.54
17:X:60:GLY:C	18:Z:81:ARG:NH2	2.65	0.54
4:D:198:THR:N	4:D:199:PRO:HD2	2.22	0.54
5:E:221:ARG:NH1	6:F:285:PRO:HG2	2.23	0.54
6:F:388:GLY:CA	6:F:419:ILE:HD11	2.38	0.54
7:G:330:LEU:HD13	7:G:546:PHE:HZ	1.71	0.54
8:H:102:ILE:HG13	8:H:160:TYR:O	2.08	0.54
13:S:26:ARG:HA	13:S:34:ARG:NH1	2.23	0.54
2:B:194:CYS:HB3	2:B:195:PRO:CD	2.33	0.54
3:C:70:LYS:HE3	3:C:71:TYR:CZ	2.43	0.54
4:D:84:PHE:CZ	8:H:205:SER:HB3	2.43	0.54
4:D:386:THR:CG2	9:I:118:LEU:CD1	2.85	0.54
4:D:444:LEU:HD21	8:H:205:SER:HB2	1.89	0.54
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.90	0.54
5:E:151:LEU:CD1	5:E:200:ILE:HD13	2.37	0.54
5:E:165:ASP:C	5:E:167:LEU:N	2.64	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.07	0.54
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.22	0.54
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.54
8:H:129:LEU:O	8:H:133:LEU:HG	2.08	0.54
11:Q:53:ILE:HG12	16:W:26:ARG:O	2.08	0.54
4:D:159:LEU:HD21	4:D:391:VAL:HG12	1.90	0.54
4:D:256:ASP:O	4:D:260:GLU:N	2.33	0.54
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
8:H:196:ALA:HB1	8:H:198:PHE:H	1.73	0.54
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.54
16:W:93:LEU:HD22	16:W:97:ILE:HG13	1.89	0.54
4:D:451:ILE:CG2	4:D:456:ILE:HD11	2.33	0.54
6:F:228:PRO:CG	11:Q:160:TYR:HD2	2.19	0.54
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.54
7:G:304:GLU:HG3	7:G:305:PRO:HD2	1.89	0.54
8:H:197:PRO:HB3	8:H:277:TYR:HB2	1.90	0.54
8:H:288:LEU:HD21	24:H:402:3PE:H222	1.90	0.54
9:I:65:GLU:HG3	9:I:65:GLU:O	2.08	0.54
17:X:41:LYS:CB	17:X:131:VAL:HG11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.37	0.54
4:D:451:ILE:HG23	4:D:456:ILE:CD1	2.35	0.54
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.54
6:F:167:SER:CB	23:s:75:TYR:CE2	2.91	0.54
7:G:130:ILE:HA	9:I:140:ARG:NH1	2.23	0.54
7:G:557:ARG:HD3	21:q:144:TYR:CD2	2.43	0.54
8:H:102:ILE:HD12	8:H:160:TYR:HA	1.89	0.54
10:P:91:ILE:HG13	10:P:95:ARG:NH1	2.23	0.54
10:P:130:ILE:HD13	10:P:148:ILE:HG21	1.90	0.54
10:P:227:PRO:O	10:P:298:TYR:CZ	2.61	0.54
6:F:167:SER:HB3	23:s:75:TYR:CE2	2.43	0.54
6:F:362:ASP:O	6:F:363:ILE:C	2.51	0.54
8:H:130:PHE:HA	8:H:133:LEU:HD12	1.90	0.54
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.54
13:S:51:LEU:O	13:S:53:ILE:HG13	2.07	0.54
14:T:90:TYR:HD2	14:T:93:ILE:HB	1.73	0.54
2:B:219:LYS:HD2	2:B:223:ARG:CZ	2.38	0.53
6:F:45:LEU:CD1	6:F:129:GLU:CD	2.77	0.53
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.53
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.53
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.53
8:H:86:TRP:HE1	8:H:229:THR:HG22	1.73	0.53
8:H:130:PHE:CE2	8:H:134:ARG:HD2	2.43	0.53
8:H:157:ASN:ND2	8:H:165:LEU:CD1	2.71	0.53
8:H:317:TYR:O	8:H:318:MET:HB2	2.08	0.53
17:X:133:THR:HG21	17:X:135:ARG:NH1	2.23	0.53
19:a:3:PHE:CD1	33:q:201:CDL:C13	2.84	0.53
24:A:201:3PE:H221	20:b:16:GLU:HG3	1.90	0.53
4:D:154:ALA:HB2	4:D:398:THR:HG21	1.90	0.53
4:D:232:VAL:CG2	4:D:356:ILE:HB	2.37	0.53
4:D:333:ARG:HH12	4:D:453:THR:HA	1.73	0.53
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.53
6:F:382:CYS:SG	25:F:502:SF4:S4	3.06	0.53
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.53
8:H:198:PHE:O	8:H:200:LEU:HG	2.08	0.53
1:A:113:TRP:CZ2	8:H:286:MET:HE2	2.40	0.53
4:D:136:PHE:HZ	4:D:422:CYS:SG	2.31	0.53
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.53
7:G:557:ARG:CG	7:G:579:MET:HE3	2.38	0.53
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.53
8:H:261:MET:O	8:H:265:LEU:HD23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:44:ARG:O	12:R:47:ARG:HG2	2.09	0.53
13:S:44:LEU:HD12	13:S:48:HIS:HD2	1.72	0.53
14:T:79:ILE:HD13	14:T:148:ILE:HG22	1.90	0.53
18:Z:128:ARG:HE	18:Z:132:GLU:CD	2.16	0.53
1:A:18:ILE:HD12	8:H:76:THR:HG21	1.86	0.53
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.90	0.53
6:F:166:ALA:HB1	23:s:80:PHE:CE1	2.44	0.53
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.09	0.53
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.53
13:S:22:HIS:HB3	13:S:58:CYS:SG	2.48	0.53
14:T:133:ILE:HG13	14:T:137:LYS:HZ2	1.73	0.53
15:V:44:TYR:CE2	15:V:94:MET:HG3	2.44	0.53
17:X:137:LEU:HG	17:X:138:PRO:HD2	1.90	0.53
2:B:92:PRO:CD	2:B:119:VAL:HG13	2.38	0.53
2:B:175:TYR:OH	3:C:197:PHE:CE1	2.60	0.53
6:F:228:PRO:HG2	11:Q:160:TYR:CD2	2.41	0.53
7:G:173:MET:SD	7:G:206:VAL:O	2.66	0.53
7:G:289:LYS:NZ	7:G:697:THR:OG1	2.36	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.09	0.53
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.90	0.53
10:P:366:ILE:O	10:P:369:THR:HG22	2.08	0.53
13:S:44:LEU:HD22	13:S:91:MET:HG2	1.89	0.53
14:T:110:LEU:HD21	14:T:118:ILE:HD12	1.91	0.53
17:X:17:GLU:HA	17:X:64:ASN:HD21	1.74	0.53
17:X:122:LEU:HD11	18:Z:59:ARG:O	2.08	0.53
18:Z:134:SER:O	18:Z:137:ASN:N	2.41	0.53
3:C:125:PHE:HZ	3:C:198:ARG:HE	1.56	0.53
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.53
10:P:48:ARG:NH2	10:P:98:GLY:O	2.42	0.53
10:P:143:ASP:O	10:P:148:ILE:HG12	2.09	0.53
10:P:227:PRO:HB2	10:P:298:TYR:OH	2.08	0.53
10:P:302:GLY:O	10:P:303:LYS:C	2.50	0.53
15:V:97:TRP:O	15:V:98:LYS:C	2.52	0.53
16:W:130:ASP:O	16:W:130:ASP:OD1	2.26	0.53
20:b:19:LEU:HB3	20:b:23:PHE:CE2	2.44	0.53
2:B:84:TRP:CH2	8:H:50:ALA:HB2	2.44	0.53
2:B:137:LEU:CD2	2:B:145:LEU:CD2	2.86	0.53
2:B:148:VAL:HG21	4:D:88:HIS:CD2	2.43	0.53
5:E:244:VAL:HG11	6:F:64:LYS:NZ	2.23	0.53
6:F:196:PHE:CE1	23:s:91:ARG:HD3	2.44	0.53
7:G:36:VAL:O	7:G:39:GLN:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:338:VAL:HG13	7:G:546:PHE:CE1	2.37	0.53
7:G:402:LEU:O	7:G:431:LEU:HA	2.09	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
14:T:80:LYS:O	14:T:84:LEU:HG	2.08	0.53
16:W:120:ASP:HB3	16:W:123:SER:OG	2.08	0.53
3:C:160:ILE:CD1	4:D:285:ASN:HD22	2.18	0.53
5:E:87:ARG:HD2	23:s:77:THR:HB	1.89	0.53
8:H:29:GLY:O	8:H:32:GLN:N	2.41	0.53
8:H:181:MET:HE3	8:H:300:LEU:CD1	2.39	0.53
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
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.53
17:X:18:VAL:HA	17:X:68:LEU:CD2	2.39	0.53
17:X:41:LYS:HB2	17:X:131:VAL:HG11	1.91	0.53
5:E:162:THR:CG2	5:E:166:LYS:HA	2.39	0.53
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.24	0.53
6:F:80:MET:HE2	6:F:95:THR:HG21	1.89	0.53
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.53
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.53
7:G:243:TRP:NE1	9:I:121:ALA:HB2	2.23	0.53
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.53
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.53
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.53
8:H:245:PRO:HG2	8:H:255:TYR:CE2	2.44	0.53
14:T:102:SER:HB2	14:T:107:ASP:HB2	1.91	0.53
20:b:74:LEU:H	20:b:74:LEU:HD12	1.73	0.53
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.43	0.53
5:E:162:THR:HG22	5:E:166:LYS:HA	1.91	0.53
8:H:102:ILE:CD1	8:H:154:LEU:HD21	2.38	0.53
22:r:6:ARG:HA	22:r:9:GLN:CG	2.39	0.53
3:C:209:LEU:HD21	16:W:108:ARG:NH1	2.25	0.52
5:E:143:ASP:HB3	5:E:146:SER:HB2	1.91	0.52
5:E:179:CYS:HA	27:E:301:FES:S1	2.49	0.52
7:G:67:GLU:HB3	11:Q:156:LYS:HD2	1.91	0.52
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.52
7:G:617:ARG:NH1	16:W:129:HIS:HA	2.24	0.52
9:I:210:LEU:HD12	22:r:39:PRO:CD	2.39	0.52
14:T:86:VAL:HG11	14:T:122:MET:SD	2.48	0.52
17:X:13:LEU:O	17:X:15:VAL:HG23	2.08	0.52
18:Z:50:MET:SD	18:Z:54:ASN:ND2	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:6:ARG:C	22:r:9:GLN:HG2	2.34	0.52
2:B:100:CYS:SG	25:B:301:SF4:S4	3.07	0.52
2:B:124:SER:HB3	2:B:125:PRO:HD2	1.91	0.52
4:D:390:GLN:HG3	4:D:415:GLY:O	2.09	0.52
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.75	0.52
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.52
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.69	0.52
7:G:524:ALA:HB2	7:G:597:VAL:HG22	1.91	0.52
8:H:132:ALA:O	8:H:133:LEU:C	2.50	0.52
8:H:197:PRO:HD3	8:H:273:ILE:CG2	2.39	0.52
9:I:64:THR:HG21	18:Z:35:MET:HE1	1.92	0.52
10:P:122:HIS:CD2	12:R:45:ARG:HB2	2.43	0.52
11:Q:61:ILE:O	11:Q:65:THR:HG23	2.09	0.52
15:V:42:ALA:O	15:V:43:ALA:C	2.53	0.52
18:Z:24:ASN:O	18:Z:25:LEU:C	2.52	0.52
22:r:6:ARG:HA	22:r:9:GLN:CD	2.34	0.52
2:B:168:GLY:HA3	2:B:172:HIS:CB	2.39	0.52
5:E:198:LYS:O	5:E:201:GLU:HB3	2.10	0.52
6:F:110:PRO:CB	6:F:152:ARG:HE	2.18	0.52
6:F:225:LEU:CD2	7:G:93:ALA:HB3	2.40	0.52
7:G:35:PHE:HB2	7:G:101:ASN:HA	1.90	0.52
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.92	0.52
8:H:27:ILE:HD12	8:H:271:LEU:HD12	1.91	0.52
8:H:264:LEU:O	8:H:268:SER:N	2.37	0.52
11:Q:111:LEU:HD12	12:R:47:ARG:HH21	1.75	0.52
2:B:194:CYS:O	2:B:196:PRO:HD3	2.09	0.52
3:C:223:VAL:HG21	3:C:225:LEU:CD1	2.17	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.91	0.52
1:A:24:LEU:HD11	26:B:303:PC1:H3B2	1.91	0.52
2:B:79:ASP:HA	2:B:82:ILE:HB	1.92	0.52
4:D:266:ARG:NH1	9:I:66:LEU:HG	2.24	0.52
6:F:126:LYS:HG3	6:F:275:LEU:CB	2.39	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
8:H:95:LEU:HG	8:H:96:ILE:HG23	1.90	0.52
10:P:59:PHE:CD1	10:P:83:PRO:HG2	2.45	0.52
10:P:203:PRO:HG2	30:P:401:NDP:C5N	2.39	0.52
10:P:293:LEU:HB2	10:P:298:TYR:OH	2.09	0.52
15:V:33:ASP:O	15:V:36:LYS:N	2.34	0.52
15:V:67:LYS:O	15:V:68:LEU:C	2.52	0.52
17:X:48:TRP:CE2	20:b:55:VAL:HG22	2.45	0.52
21:q:21:ARG:O	21:q:25:ARG:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:ARG:NH1	9:I:128:ILE:O	2.43	0.52
4:D:216:ARG:O	4:D:237:PRO:HG3	2.09	0.52
10:P:137:ARG:HG3	10:P:138:ASN:OD1	2.10	0.52
10:P:236:VAL:HG23	10:P:271:TYR:C	2.35	0.52
1:A:106:TRP:NE1	24:A:201:3PE:H32	2.24	0.52
4:D:254:ARG:HE	22:r:25:GLN:HB3	1.74	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.52
8:H:260:MET:CE	19:a:13:GLY:C	2.79	0.52
9:I:90:LYS:HD3	21:q:91:HIS:HE1	1.72	0.52
23:s:89:LYS:HG3	23:s:90:PHE:N	2.24	0.52
4:D:222:MET:HG2	4:D:223:HIS:CD2	2.44	0.52
4:D:444:LEU:HD21	8:H:205:SER:C	2.35	0.52
6:F:119:GLU:CD	28:F:501:FMN:HN3	2.18	0.52
6:F:294:VAL:HG12	6:F:337:MET:HB2	1.92	0.52
7:G:391:ILE:HG22	7:G:417:ARG:HE	1.75	0.52
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.52
10:P:316:LYS:O	10:P:320:GLU:HG3	2.10	0.52
16:W:31:ALA:O	16:W:34:ARG:N	2.40	0.52
18:Z:87:LEU:O	18:Z:91:LEU:HB2	2.10	0.52
3:C:132:LEU:HD11	4:D:300:TRP:CZ2	2.44	0.52
4:D:113:ILE:CG2	4:D:432:LEU:CD2	2.87	0.52
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.52
6:F:234:GLY:HA3	6:F:238:CYS:O	2.10	0.52
8:H:318:MET:HG2	19:a:40:ARG:HD2	1.92	0.52
18:Z:97:ILE:HG13	18:Z:98:MET:N	2.25	0.52
3:C:149:LEU:O	16:W:23:ILE:HD11	2.10	0.52
3:C:170:TRP:CD1	3:C:183:LEU:HD21	2.44	0.52
3:C:186:ILE:CG2	3:C:187:LEU:N	2.73	0.52
4:D:105:MET:HA	4:D:443:MET:HA	1.92	0.52
7:G:35:PHE:CE1	7:G:40:SER:HB2	2.45	0.52
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.52
10:P:229:VAL:HG22	10:P:298:TYR:CD2	2.44	0.52
11:Q:112:MET:SD	21:q:126:PRO:HB3	2.50	0.52
3:C:63:TYR:OH	3:C:102:HIS:HE1	1.93	0.51
4:D:271:ARG:NH1	8:H:279:ARG:O	2.43	0.51
4:D:320:ILE:HD11	9:I:38:TYR:HE1	1.73	0.51
4:D:375:MET:HE1	7:G:126:LEU:HA	1.90	0.51
4:D:385:TYR:HB2	9:I:118:LEU:HD11	1.92	0.51
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.51
7:G:670:GLU:HB2	13:S:42:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:253:GLU:O	8:H:254:LEU:C	2.52	0.51
24:H:402:3PE:H322	9:I:63:TRP:CZ3	2.45	0.51
13:S:90:ALA:O	13:S:94:VAL:HG23	2.09	0.51
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.75	0.51
16:W:110:PHE:O	16:W:111:HIS:C	2.53	0.51
5:E:143:ASP:HB3	5:E:146:SER:CB	2.40	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.53	0.51
3:C:190:TYR:HB3	16:W:101:LYS:HG2	1.92	0.51
4:D:386:THR:HG23	9:I:118:LEU:CD1	2.40	0.51
5:E:59:TYR:O	5:E:62:ILE:HB	2.10	0.51
5:E:178:ALA:HB2	5:E:191:TYR:CE2	2.45	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.46	0.51
8:H:91:MET:C	8:H:93:HIS:N	2.67	0.51
10:P:154:GLN:O	10:P:158:GLU:HG3	2.10	0.51
11:Q:135:ILE:HD11	11:Q:147:VAL:HG21	1.91	0.51
2:B:189:ILE:HD12	2:B:207:GLN:HB3	1.93	0.51
26:B:303:PC1:H3B1	8:H:57:MET:HE2	1.92	0.51
3:C:136:PHE:CE1	22:r:96:THR:HB	2.44	0.51
5:E:39:VAL:HG11	7:G:163:LYS:HE3	1.93	0.51
6:F:300:ILE:CG2	6:F:305:GLY:O	2.44	0.51
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.51
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.51
7:G:611:THR:HG21	11:Q:105:GLU:N	2.25	0.51
12:R:69:VAL:HG11	12:R:112:LYS:HB2	1.93	0.51
22:r:7:VAL:O	22:r:11:LEU:HG	2.10	0.51
4:D:179:ARG:NH2	4:D:401:GLU:O	2.43	0.51
5:E:176:LEU:HB2	5:E:184:MET:CE	2.41	0.51
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.74	0.51
8:H:51:ASP:OD1	8:H:52:ALA:N	2.44	0.51
9:I:79:ARG:C	19:a:1:MET:HE1	2.35	0.51
10:P:279:TYR:CD1	10:P:372:ALA:HB2	2.45	0.51
13:S:18:GLU:CB	13:S:52:PRO:HB2	2.40	0.51
17:X:52:ASP:OD1	17:X:53:PRO:HD2	2.11	0.51
2:B:91:TRP:CD1	2:B:120:VAL:HG13	2.46	0.51
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.25	0.51
3:C:186:ILE:HG13	4:D:113:ILE:HD11	1.92	0.51
5:E:229:GLY:O	5:E:231:THR:HG23	2.10	0.51
7:G:304:GLU:HG3	7:G:615:LEU:HD12	1.93	0.51
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.51
9:I:79:ARG:NH2	22:r:20:LEU:HD13	2.24	0.51
13:S:19:ILE:O	13:S:53:ILE:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:32:TYR:HE1	17:X:67:ALA:HA	1.76	0.51
17:X:108:ASP:O	17:X:112:LEU:N	2.41	0.51
4:D:259:GLU:HG2	18:Z:25:LEU:HD13	1.92	0.51
4:D:270:ASN:HB3	8:H:284:GLN:NE2	2.25	0.51
4:D:356:ILE:HD11	4:D:357:LYS:HE3	1.93	0.51
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.45	0.51
6:F:382:CYS:HA	7:G:74:ASN:O	2.11	0.51
10:P:215:ASN:O	10:P:216:HIS:C	2.54	0.51
13:S:24:CYS:HB2	13:S:30:SER:HB3	1.93	0.51
4:D:174:PHE:CZ	4:D:240:LEU:HD21	2.42	0.51
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.51
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.51
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
8:H:39:ILE:HG12	21:q:31:ASN:OD1	2.11	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
10:P:157:LYS:HD3	10:P:195:PHE:CE1	2.46	0.51
10:P:294:PRO:O	10:P:298:TYR:HD2	1.94	0.51
15:V:31:THR:HG22	15:V:88:LEU:HB2	1.92	0.51
4:D:399:ALA:HB1	4:D:406:GLU:HG3	1.93	0.51
6:F:335:VAL:HG12	6:F:336:LEU:O	2.11	0.51
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.92	0.51
8:H:86:TRP:HH2	8:H:232:ILE:HG22	1.76	0.51
9:I:111:GLU:OE2	9:I:187:LYS:HE3	2.11	0.51
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.51
1:A:54:LYS:O	1:A:58:VAL:HG23	2.11	0.51
5:E:178:ALA:HB2	5:E:191:TYR:HE2	1.76	0.51
8:H:318:MET:HG2	19:a:40:ARG:CD	2.41	0.51
9:I:203:ALA:HB2	21:q:88:ARG:HH11	1.76	0.51
16:W:95:GLU:HB3	16:W:101:LYS:HG3	1.93	0.51
18:Z:10:MET:HG3	18:Z:11:PRO:HD2	1.93	0.51
3:C:70:LYS:O	15:V:103:LEU:HD12	2.11	0.50
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.50
6:F:226:LYS:HD2	6:F:229:PHE:CD2	2.46	0.50
6:F:299:LEU:HD11	6:F:300:ILE:HG13	1.93	0.50
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.08	0.50
7:G:406:ASN:O	7:G:407:PRO:C	2.53	0.50
7:G:661:GLU:O	7:G:661:GLU:CG	2.46	0.50
11:Q:85:ASN:O	11:Q:86:ASN:C	2.52	0.50
14:T:104:PHE:CG	14:T:110:LEU:HD22	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:86:ILE:HG21	18:Z:124:MET:O	2.11	0.50
20:b:27:GLY:O	20:b:28:LEU:C	2.51	0.50
2:B:200:ALA:O	2:B:201:LEU:C	2.53	0.50
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.92	0.50
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.77	0.50
7:G:253:VAL:HG12	7:G:253:VAL:O	2.10	0.50
8:H:14:LEU:HB3	29:H:401:UQ9:H23	1.92	0.50
10:P:335:LEU:HB3	10:P:340:VAL:HB	1.92	0.50
16:W:69:MET:C	16:W:71:MET:N	2.63	0.50
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.25	0.50
5:E:140:MET:HE1	6:F:366:ALA:HA	1.92	0.50
5:E:225:GLU:O	5:E:226:PRO:C	2.48	0.50
6:F:42:PHE:HE1	6:F:137:LYS:HG2	1.76	0.50
6:F:109:ARG:NE	6:F:239:PRO:HD3	2.25	0.50
6:F:299:LEU:HD12	6:F:300:ILE:HG13	1.92	0.50
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.12	0.50
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.50
9:I:72:MET:O	9:I:75:SER:OG	2.23	0.50
10:P:165:ILE:HG21	10:P:249:ILE:HG23	1.93	0.50
11:Q:131:LYS:HG2	11:Q:135:ILE:HD11	1.89	0.50
14:T:130:ILE:HG23	14:T:134:ASP:OD2	2.12	0.50
15:V:8:THR:O	15:V:8:THR:CG2	2.59	0.50
17:X:45:LEU:HG	17:X:131:VAL:HG23	1.93	0.50
18:Z:92:GLU:O	18:Z:95:ALA:N	2.45	0.50
2:B:109:ALA:HB1	2:B:110:PRO:CD	2.41	0.50
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.50
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.50
8:H:253:GLU:HG3	19:a:21:VAL:HG22	1.93	0.50
10:P:45:LYS:O	10:P:50:SER:HB3	2.11	0.50
14:T:144:ILE:O	14:T:148:ILE:HG12	2.12	0.50
1:A:84:THR:HG22	20:b:43:SER:HB2	1.93	0.50
4:D:259:GLU:HG2	18:Z:25:LEU:CD1	2.40	0.50
5:E:203:ILE:HD11	5:E:218:ARG:HD3	1.93	0.50
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.50
6:F:391:TRP:HH2	7:G:118:GLU:OE2	1.92	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
8:H:224:PHE:CE2	29:H:401:UQ9:H11	2.46	0.50
10:P:153:ALA:HB2	10:P:164:PHE:CE2	2.46	0.50
14:T:104:PHE:CB	14:T:110:LEU:HD22	2.39	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
21:q:43:LYS:O	21:q:44:TYR:HB2	2.10	0.50
2:B:170:TYR:HE1	4:D:127:LYS:HD3	1.77	0.50
2:B:182:ASP:HA	2:B:187:VAL:HG23	1.93	0.50
4:D:95:LEU:O	4:D:95:LEU:HD12	2.12	0.50
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.50
10:P:163:ARG:HH22	10:P:256:PRO:HA	1.76	0.50
10:P:206:ILE:H	30:P:401:NDP:H71N	1.58	0.50
10:P:223:PHE:CG	10:P:223:PHE:O	2.65	0.50
11:Q:53:ILE:HG23	16:W:20:VAL:HG23	1.94	0.50
15:V:9:THR:HG21	15:V:78:GLU:CB	2.42	0.50
18:Z:69:ILE:HD12	20:b:54:PRO:CD	2.41	0.50
19:a:43:TYR:CZ	19:a:47:LEU:HD11	2.46	0.50
24:A:201:3PE:H3A2	20:b:22:SER:OG	2.12	0.50
4:D:137:ASP:CB	4:D:223:HIS:HA	2.41	0.50
5:E:131:ILE:CD1	5:E:185:VAL:HB	2.25	0.50
6:F:109:ARG:NH2	6:F:232:ASP:O	2.41	0.50
6:F:185:ASN:HA	6:F:189:SER:O	2.12	0.50
12:R:48:PHE:HD1	12:R:52:GLN:O	1.95	0.50
14:T:92:LYS:NZ	14:T:92:LYS:HB3	2.27	0.50
14:T:134:ASP:HA	14:T:137:LYS:HZ3	1.76	0.50
21:q:66:THR:HG23	21:q:74:PHE:CD1	2.47	0.50
4:D:92:HIS:HD2	4:D:95:LEU:HD21	1.76	0.50
4:D:140:ASP:H	4:D:147:ASN:HD21	1.60	0.50
4:D:181:LEU:HD11	4:D:210:MET:CG	2.41	0.50
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.50
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.25	0.50
8:H:181:MET:CE	8:H:300:LEU:CD1	2.90	0.50
9:I:105:ARG:NH2	12:R:56:ASN:HD21	2.10	0.50
10:P:68:TYR:CD2	10:P:242:VAL:HG11	2.46	0.50
16:W:67:ARG:O	16:W:71:MET:HB2	2.11	0.50
17:X:130:LYS:HG2	20:b:59:ASP:HB2	1.92	0.50
1:A:3:LEU:HD13	8:H:96:ILE:CD1	2.42	0.50
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.93	0.50
3:C:96:LEU:HD22	3:C:155:ILE:HG21	1.94	0.50
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.50
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
7:G:372:PHE:CZ	7:G:385:TYR:HB3	2.47	0.50
8:H:200:LEU:CD1	8:H:285:LEU:CD2	2.89	0.50
9:I:78:PHE:CD1	22:r:8:ILE:HG23	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:95:LEU:O	15:V:95:LEU:HD23	2.12	0.50
16:W:107:MET:HE3	16:W:112:GLU:OE2	2.11	0.50
17:X:49:GLU:CG	17:X:50:GLU:HG3	2.40	0.50
24:A:202:3PE:H122	18:Z:143:TYR:HB3	1.94	0.49
4:D:95:LEU:HD13	4:D:97:LEU:HD13	1.94	0.49
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.49
7:G:648:GLU:O	13:S:22:HIS:HE1	1.95	0.49
8:H:181:MET:CE	8:H:300:LEU:HD12	2.42	0.49
9:I:200:GLU:HG2	21:q:88:ARG:HB2	1.93	0.49
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.49
13:S:23:LEU:HD12	13:S:23:LEU:O	2.12	0.49
14:T:79:ILE:HG23	14:T:126:PHE:CE1	2.47	0.49
20:b:67:PRO:HB3	20:b:74:LEU:HB2	1.93	0.49
24:A:202:3PE:H111	8:H:98:LEU:HA	1.94	0.49
3:C:234:LEU:O	3:C:234:LEU:CG	2.60	0.49
4:D:123:LEU:CB	4:D:135:TYR:OH	2.60	0.49
4:D:462:ASP:O	4:D:463:ARG:C	2.54	0.49
5:E:214:LYS:HG3	5:E:214:LYS:O	2.11	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
16:W:102:GLN:H	16:W:105:HIS:CD2	2.30	0.49
17:X:7:LEU:CD2	18:Z:87:LEU:HD12	2.42	0.49
20:b:41:TYR:CD1	20:b:84:LEU:HD11	2.46	0.49
21:q:19:GLY:O	21:q:23:LEU:N	2.41	0.49
1:A:57:LEU:O	1:A:58:VAL:C	2.53	0.49
3:C:92:VAL:O	3:C:96:LEU:HD13	2.11	0.49
4:D:83:ASN:HA	4:D:97:LEU:O	2.11	0.49
4:D:326:CYS:O	4:D:327:TYR:C	2.56	0.49
5:E:200:ILE:HG22	5:E:204:ILE:HG13	1.92	0.49
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.49
7:G:403:VAL:HG23	7:G:432:ILE:CB	2.38	0.49
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.49
10:P:157:LYS:HD3	10:P:195:PHE:CD1	2.47	0.49
10:P:209:ARG:CG	10:P:352:VAL:HG12	2.43	0.49
14:T:90:TYR:HE2	14:T:93:ILE:HG12	1.77	0.49
20:b:60:ASP:HB2	20:b:62:ASN:OD1	2.12	0.49
21:q:60:ARG:HH12	21:q:95:ASP:CA	2.16	0.49
2:B:93:MET:HE1	2:B:125:PRO:CB	2.43	0.49
3:C:80:LEU:O	3:C:81:ASP:HB2	2.12	0.49
4:D:371:MET:CE	9:I:163:PRO:HB3	2.41	0.49
8:H:204:GLU:O	8:H:205:SER:C	2.54	0.49
8:H:216:ALA:O	8:H:217:ALA:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:270:ARG:HB3	10:P:375:VAL:O	2.11	0.49
14:T:115:GLN:O	14:T:119:ILE:HG12	2.12	0.49
1:A:108:GLN:O	1:A:109:LYS:HB2	2.13	0.49
6:F:40:ARG:HB3	6:F:289:GLU:CD	2.37	0.49
6:F:45:LEU:O	6:F:46:TYR:HB2	2.13	0.49
6:F:235:VAL:HG12	6:F:236:PHE:CD2	2.47	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
8:H:152:SER:O	8:H:153:VAL:C	2.55	0.49
9:I:106:TYR:O	9:I:107:PRO:C	2.55	0.49
14:T:84:LEU:HD22	14:T:98:LEU:CD2	2.42	0.49
17:X:76:SER:OG	17:X:77:HIS:N	2.45	0.49
22:r:6:ARG:CA	22:r:9:GLN:HG2	2.42	0.49
3:C:45:THR:HG22	4:D:358:VAL:CG2	2.42	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.49
8:H:136:VAL:O	8:H:137:ALA:C	2.54	0.49
10:P:113:LYS:C	10:P:115:SER:H	2.21	0.49
13:S:16:LEU:HD13	13:S:94:VAL:HG12	1.95	0.49
14:T:120:MET:HE1	16:W:43:TYR:CG	2.47	0.49
17:X:24:VAL:HG23	17:X:25:LEU:HD12	1.95	0.49
19:a:3:PHE:CE1	33:q:201:CDL:C13	2.82	0.49
22:r:6:ARG:O	22:r:9:GLN:CG	2.60	0.49
4:D:112:HIS:HE1	16:W:100:TRP:CD1	2.30	0.49
4:D:299:GLN:NE2	9:I:36:TYR:CZ	2.80	0.49
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.49
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
7:G:181:ARG:HA	7:G:184:ARG:HH21	1.77	0.49
7:G:617:ARG:HH22	16:W:128:GLY:N	2.11	0.49
8:H:17:MET:HG2	8:H:228:TYR:HB2	1.94	0.49
8:H:179:TRP:NE1	18:Z:43:LEU:HD12	2.28	0.49
8:H:184:MET:CG	8:H:293:PHE:HD2	2.23	0.49
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.95	0.49
10:P:209:ARG:HG2	10:P:352:VAL:HG12	1.93	0.49
10:P:227:PRO:HB3	10:P:291:TYR:CE1	2.47	0.49
14:T:95:PRO:HG2	14:T:97:LYS:HB3	1.95	0.49
16:W:130:ASP:O	16:W:131:PRO:C	2.52	0.49
23:s:87:LEU:O	23:s:91:ARG:HG3	2.12	0.49
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.27	0.49
8:H:151:LEU:O	8:H:152:SER:C	2.54	0.49
8:H:231:ILE:O	8:H:235:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:93:LEU:HD11	9:I:173:PHE:HE2	1.77	0.49
10:P:80:VAL:HB	10:P:103:LEU:HD22	1.94	0.49
10:P:335:LEU:HD12	10:P:342:PRO:HG3	1.94	0.49
16:W:93:LEU:O	16:W:94:GLN:C	2.55	0.49
1:A:50:PRO:HG2	4:D:80:MET:CG	2.37	0.49
4:D:89:PRO:O	4:D:90:ALA:C	2.56	0.49
6:F:167:SER:OG	23:s:75:TYR:CE2	2.63	0.49
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.49
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.49
7:G:403:VAL:HG13	7:G:403:VAL:O	2.12	0.49
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.76	0.49
9:I:41:LYS:HG2	9:I:41:LYS:O	2.13	0.49
9:I:76:TYR:CE1	9:I:79:ARG:CZ	2.96	0.49
10:P:150:ARG:HE	10:P:190:GLU:HB3	1.78	0.49
16:W:46:VAL:HB	16:W:47:PRO:HD3	1.95	0.49
17:X:10:LEU:H	17:X:10:LEU:HD12	1.77	0.49
4:D:163:PRO:HG2	4:D:168:GLN:HG2	1.94	0.49
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.49
4:D:211:PHE:O	4:D:212:GLU:C	2.56	0.49
4:D:256:ASP:CG	22:r:18:GLN:HE22	2.20	0.49
6:F:67:GLU:O	6:F:71:LYS:HG2	2.13	0.49
6:F:126:LYS:HG3	6:F:275:LEU:HB3	1.94	0.49
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.49
7:G:475:VAL:HG11	7:G:516:LEU:HD23	1.95	0.49
8:H:90:PRO:CD	8:H:240:ILE:HD13	2.43	0.49
10:P:236:VAL:HG23	10:P:271:TYR:O	2.13	0.49
12:R:51:ARG:O	12:R:52:GLN:HG3	2.13	0.49
21:q:26:VAL:HG11	21:q:32:ASP:O	2.10	0.49
21:q:65:THR:HG22	21:q:81:MET:HE1	1.95	0.49
23:s:92:LEU:HB2	23:s:93:PRO:CD	2.40	0.49
1:A:2:ASN:HB3	8:H:2:PHE:CZ	2.48	0.48
3:C:221:GLU:O	3:C:222:PRO:C	2.56	0.48
4:D:260:GLU:OE1	9:I:72:MET:SD	2.71	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
7:G:665:PHE:O	7:G:668:ALA:N	2.45	0.48
8:H:68:MET:HG2	8:H:72:ILE:HD13	1.95	0.48
9:I:144:ARG:NE	9:I:146:ASP:OD2	2.46	0.48
10:P:223:PHE:CZ	10:P:227:PRO:CG	2.96	0.48
17:X:74:ILE:O	17:X:77:HIS:O	2.31	0.48
17:X:141:PRO:O	17:X:142:TYR:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:THR:HG1	20:b:26:TRP:NE1	2.11	0.48
2:B:137:LEU:CD2	2:B:145:LEU:HD22	2.42	0.48
2:B:222:TYR:HA	10:P:137:ARG:HH12	1.77	0.48
4:D:95:LEU:HD23	4:D:458:PHE:HZ	1.78	0.48
4:D:253:LEU:O	4:D:256:ASP:OD1	2.31	0.48
5:E:129:TYR:HA	5:E:188:ASN:ND2	2.28	0.48
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.42	0.48
10:P:165:ILE:CD1	10:P:253:THR:HG22	2.42	0.48
10:P:227:PRO:HB2	10:P:298:TYR:HE1	1.79	0.48
10:P:307:LEU:O	10:P:308:SER:C	2.55	0.48
13:S:63:PRO:HB2	13:S:79:LEU:HD12	1.93	0.48
16:W:49:THR:O	16:W:50:VAL:C	2.56	0.48
17:X:7:LEU:HD22	18:Z:87:LEU:HD11	1.93	0.48
17:X:53:PRO:O	18:Z:84:LEU:HD22	2.13	0.48
20:b:35:ILE:HG12	20:b:35:ILE:O	2.13	0.48
1:A:72:LEU:HD23	1:A:94:LEU:HD23	1.94	0.48
2:B:99:CYS:C	2:B:101:ALA:H	2.21	0.48
26:B:303:PC1:H241	10:P:310:PHE:HE1	1.79	0.48
3:C:130:ASN:HD21	3:C:141:ARG:HE	1.62	0.48
4:D:444:LEU:HD11	8:H:205:SER:HB2	1.95	0.48
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.74	0.48
6:F:383:THR:O	6:F:384:PRO:C	2.56	0.48
7:G:70:SER:O	7:G:184:ARG:NH1	2.46	0.48
8:H:154:LEU:O	8:H:155:LEU:C	2.55	0.48
8:H:313:GLY:O	8:H:314:VAL:C	2.56	0.48
11:Q:62:THR:HB	11:Q:72:ILE:CD1	2.43	0.48
15:V:31:THR:O	15:V:35:LEU:HG	2.13	0.48
17:X:49:GLU:CG	17:X:50:GLU:N	2.77	0.48
1:A:7:ILE:CD1	24:A:202:3PE:H371	2.36	0.48
4:D:79:ASN:OD1	4:D:107:ARG:NH1	2.46	0.48
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.95	0.48
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.48
6:F:134:ASP:CG	6:F:137:LYS:HB2	2.39	0.48
6:F:234:GLY:O	6:F:237:GLY:N	2.45	0.48
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.48
10:P:132:ARG:HD2	10:P:134:TRP:CZ2	2.47	0.48
10:P:140:ASP:C	10:P:142:GLU:N	2.68	0.48
10:P:157:LYS:CB	10:P:195:PHE:HD1	2.24	0.48
14:T:119:ILE:HD12	14:T:138:LEU:CD1	2.40	0.48
5:E:228:GLY:H	6:F:284:HIS:CG	2.32	0.48
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.48
7:G:170:LYS:O	7:G:231:LEU:HA	2.13	0.48
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.94	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
8:H:147:ALA:O	8:H:151:LEU:N	2.42	0.48
10:P:94:LEU:O	10:P:97:MET:HG2	2.14	0.48
17:X:119:ARG:NH1	18:Z:63:GLU:OE2	2.45	0.48
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.66	0.48
26:B:303:PC1:H3B1	8:H:57:MET:HE3	1.94	0.48
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.48
7:G:183:ILE:HD11	7:G:197:THR:HG23	1.95	0.48
13:S:30:SER:O	13:S:31:GLN:C	2.56	0.48
2:B:176:SER:O	2:B:177:VAL:HG23	2.14	0.48
6:F:47:GLY:O	6:F:48:ARG:HB2	2.13	0.48
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.96	0.48
8:H:183:MET:SD	24:H:402:3PE:H331	2.53	0.48
9:I:62:MET:O	9:I:63:TRP:C	2.56	0.48
10:P:59:PHE:CD2	10:P:152:ILE:HD13	2.49	0.48
10:P:59:PHE:HA	10:P:83:PRO:HD2	1.96	0.48
10:P:292:PRO:O	10:P:293:LEU:HG	2.14	0.48
10:P:365:GLU:N	10:P:365:GLU:OE1	2.46	0.48
14:T:110:LEU:CD2	14:T:118:ILE:HD12	2.43	0.48
1:A:111:LEU:HB2	8:H:291:LYS:HE2	1.96	0.48
2:B:194:CYS:CB	2:B:195:PRO:HD3	2.36	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48
5:E:147:ILE:CD1	5:E:195:LEU:HB2	2.43	0.48
7:G:545:LEU:CD2	7:G:547:LEU:HD21	2.44	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:277:TYR:CE2	24:H:402:3PE:H272	2.48	0.48
9:I:76:TYR:HE1	9:I:79:ARG:NH2	2.12	0.48
16:W:65:LYS:O	16:W:69:MET:HG2	2.14	0.48
16:W:84:LEU:HD11	16:W:88:LYS:HE3	1.96	0.48
17:X:20:VAL:HB	17:X:24:VAL:HG21	1.96	0.48
3:C:208:GLU:HG2	3:C:221:GLU:HG3	1.95	0.48
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.78	0.48
5:E:206:GLU:HB3	5:E:213:PRO:HB3	1.96	0.48
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.53	0.48
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
9:I:152:CYS:SG	25:I:301:SF4:S4	3.12	0.48
13:S:46:LYS:O	13:S:49:PRO:HD3	2.13	0.48
15:V:6:LYS:HG2	15:V:16:VAL:HG23	1.96	0.48
17:X:49:GLU:CD	20:b:58:ARG:HH21	2.22	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
4:D:203:MET:HE3	4:D:258:VAL:HG23	1.95	0.48
4:D:240:LEU:HG	4:D:244:ILE:CD1	2.44	0.48
5:E:71:GLU:CG	23:s:94:GLN:HE21	2.26	0.48
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.79	0.48
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.78	0.48
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.14	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
10:P:146:VAL:HG13	10:P:190:GLU:HG3	1.95	0.48
17:X:124:GLN:HB3	20:b:70:PRO:O	2.14	0.48
19:a:2:TRP:HE1	22:r:8:ILE:HG21	1.79	0.48
1:A:24:LEU:O	1:A:25:PRO:C	2.56	0.47
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.47
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.47
7:G:665:PHE:O	7:G:666:GLN:C	2.57	0.47
8:H:229:THR:O	8:H:229:THR:CG2	2.52	0.47
9:I:180:HIS:HD2	10:P:100:LEU:CD2	2.26	0.47
11:Q:78:ARG:O	11:Q:80:PHE:HD1	1.96	0.47
1:A:7:ILE:HD12	24:A:202:3PE:H292	1.96	0.47
1:A:65:PHE:HA	1:A:68:GLU:CD	2.39	0.47
2:B:182:ASP:HA	2:B:185:VAL:O	2.14	0.47
26:B:303:PC1:H382	8:H:57:MET:HE2	1.95	0.47
4:D:304:LYS:HD3	4:D:318:VAL:HG23	1.95	0.47
4:D:384:LEU:HD21	7:G:144:MET:HE1	1.95	0.47
6:F:337:MET:HE2	6:F:337:MET:HA	1.96	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:517:HIS:H	7:G:599:THR:CG2	2.27	0.47
8:H:249:ILE:HG12	17:X:99:HIS:CE1	2.50	0.47
9:I:50:MET:HG2	18:Z:33:TYR:OH	2.13	0.47
10:P:54:VAL:O	10:P:78:SER:HB3	2.14	0.47
10:P:263:PHE:CE1	10:P:333:PRO:HB2	2.48	0.47
14:T:120:MET:HE1	16:W:43:TYR:CD2	2.49	0.47
20:b:78:LEU:HD22	20:b:80:TRP:NE1	2.27	0.47
21:q:41:GLU:HG3	21:q:47:LYS:HD3	1.95	0.47
22:r:27:ARG:HD2	22:r:31:ILE:CG2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:VAL:HG11	16:W:113:THR:HG21	1.96	0.47
5:E:47:ASN:HB2	5:E:48:PRO:HD2	1.97	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.47
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.92	0.47
8:H:260:MET:SD	19:a:16:LEU:HB2	2.54	0.47
15:V:77:VAL:C	15:V:79:GLU:N	2.66	0.47
17:X:49:GLU:O	17:X:51:LYS:HD2	2.13	0.47
19:a:12:MET:O	19:a:12:MET:HG2	2.14	0.47
24:A:201:3PE:C39	20:b:23:PHE:HE1	2.27	0.47
3:C:67:ILE:HD13	3:C:98:PHE:CZ	2.49	0.47
4:D:80:MET:O	4:D:100:GLU:HA	2.14	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	0.47
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.47
7:G:380:ASP:CB	13:S:41:TYR:OH	2.62	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
8:H:47:GLN:O	8:H:50:ALA:HB3	2.15	0.47
8:H:90:PRO:HG3	8:H:240:ILE:HG21	1.93	0.47
14:T:80:LYS:HB2	14:T:145:VAL:HG11	1.96	0.47
22:r:110:GLN:HG2	22:r:113:LEU:HD22	1.95	0.47
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.50	0.47
5:E:230:LEU:C	5:E:232:SER:H	2.22	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
10:P:285:HIS:HB3	10:P:361:TRP:CE3	2.47	0.47
12:R:67:GLN:HG3	12:R:68:PRO:HD2	1.96	0.47
17:X:7:LEU:HD12	18:Z:91:LEU:CD2	2.37	0.47
4:D:97:LEU:HB3	4:D:99:LEU:CD2	2.45	0.47
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.47
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.44	0.47
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.47
6:F:327:ILE:HG13	6:F:331:VAL:HB	1.95	0.47
6:F:357:MET:HE1	6:F:363:ILE:HD12	1.95	0.47
8:H:122:ALA:O	8:H:123:SER:C	2.57	0.47
8:H:215:TYR:HD2	8:H:219:PRO:CB	2.28	0.47
10:P:74:GLY:HA2	10:P:102:GLN:OE1	2.14	0.47
10:P:76:MET:SD	10:P:254:LYS:HE3	2.54	0.47
17:X:123:GLY:HA2	18:Z:66:GLU:OE2	2.15	0.47
24:A:202:3PE:H111	8:H:98:LEU:HD23	1.96	0.47
4:D:87:GLN:HG3	4:D:93:GLY:CA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:361:ALA:O	4:D:362:LYS:C	2.58	0.47
4:D:392:PRO:HD3	22:r:60:ARG:HG3	1.96	0.47
5:E:45:GLU:H	5:E:45:GLU:CD	2.21	0.47
5:E:92:LEU:HG	5:E:92:LEU:O	2.15	0.47
5:E:129:TYR:HA	5:E:188:ASN:HD21	1.80	0.47
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.47
7:G:648:GLU:O	13:S:22:HIS:CE1	2.68	0.47
8:H:193:THR:O	8:H:194:ASN:HB2	2.15	0.47
9:I:64:THR:CG2	18:Z:35:MET:HE1	2.44	0.47
10:P:134:TRP:HB3	10:P:312:PRO:CG	2.41	0.47
10:P:169:HIS:HB2	10:P:184:LYS:HE2	1.96	0.47
10:P:235:THR:CG2	10:P:323:HIS:O	2.63	0.47
10:P:376:ASN:O	10:P:377:TYR:C	2.57	0.47
14:T:116:VAL:O	14:T:120:MET:HG3	2.15	0.47
14:T:140:CYS:O	14:T:143:GLU:HB2	2.15	0.47
17:X:48:TRP:O	17:X:51:LYS:HE3	2.15	0.47
18:Z:10:MET:HE2	18:Z:10:MET:HB2	1.59	0.47
18:Z:72:MET:HG3	20:b:53:TYR:CD1	2.49	0.47
18:Z:120:LEU:HD23	18:Z:121:ILE:N	2.29	0.47
20:b:63:MET:HB2	20:b:66:VAL:CG1	2.45	0.47
2:B:136:THR:HG22	2:B:164:CYS:HB2	1.97	0.47
3:C:168:GLU:HB2	3:C:186:ILE:HG21	1.97	0.47
4:D:159:LEU:CG	4:D:391:VAL:HG12	2.45	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
5:E:107:PRO:O	5:E:110:ARG:HB3	2.15	0.47
6:F:212:LEU:HD12	6:F:212:LEU:O	2.15	0.47
7:G:385:TYR:CE2	7:G:526:LEU:HB2	2.49	0.47
8:H:65:THR:HG21	8:H:71:PHE:HB2	1.96	0.47
8:H:230:ASN:HB3	8:H:233:LEU:HD12	1.97	0.47
10:P:40:VAL:O	10:P:42:PRO:HD3	2.15	0.47
10:P:131:GLY:HA3	30:P:401:NDP:O3D	2.15	0.47
13:S:87:VAL:O	13:S:88:THR:C	2.55	0.47
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.45	0.47
3:C:45:THR:OG1	22:r:57:ARG:CD	2.63	0.47
3:C:232:PHE:HE1	7:G:244:GLU:HG3	1.80	0.47
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.47
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.49	0.47
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.47
6:F:364:VAL:HA	6:F:438:LEU:HD11	1.97	0.47
7:G:691:ILE:HG12	7:G:695:TYR:CE2	2.50	0.47
10:P:73:LEU:HD23	10:P:250:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:88:HIS:ND1	12:R:89:PRO:O	2.47	0.47
13:S:24:CYS:SG	13:S:61:VAL:O	2.72	0.47
16:W:38:LEU:HG	16:W:70:PHE:HZ	1.80	0.47
17:X:15:VAL:O	17:X:17:GLU:HG3	2.15	0.47
18:Z:88:ARG:O	18:Z:92:GLU:HG3	2.14	0.47
2:B:146:ARG:NH1	2:B:149:TYR:CD2	2.83	0.47
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
8:H:42:PRO:HB3	21:q:27:PHE:CZ	2.49	0.47
8:H:96:ILE:O	8:H:97:ASN:C	2.57	0.47
8:H:199:ASP:HB3	8:H:279:ARG:CD	2.33	0.47
13:S:24:CYS:N	13:S:58:CYS:HB2	2.29	0.47
2:B:99:CYS:HB3	4:D:141:TYR:HB3	1.95	0.46
3:C:69:PRO:HD2	15:V:99:PRO:O	2.15	0.46
5:E:243:GLY:O	5:E:244:VAL:C	2.58	0.46
7:G:400:VAL:HG22	7:G:473:MET:CG	2.45	0.46
10:P:73:LEU:CD2	10:P:250:VAL:HG22	2.45	0.46
10:P:223:PHE:HZ	10:P:227:PRO:CG	2.28	0.46
13:S:35:ASP:O	13:S:38:VAL:HG22	2.15	0.46
14:T:107:ASP:O	14:T:108:LEU:HB2	2.15	0.46
33:q:201:CDL:HB4	22:r:5:THR:OG1	2.16	0.46
2:B:207:GLN:HA	2:B:210:ARG:NH2	2.30	0.46
3:C:123:ASN:HB2	15:V:111:GLN:OE1	2.14	0.46
5:E:196:THR:O	5:E:197:PRO:C	2.56	0.46
5:E:232:SER:O	5:E:233:LEU:HB2	2.15	0.46
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.97	0.46
6:F:128:ARG:HA	6:F:131:MET:HE2	1.96	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
6:F:299:LEU:CD1	6:F:300:ILE:N	2.68	0.46
6:F:313:ASN:OD1	6:F:359:ARG:NH1	2.48	0.46
6:F:382:CYS:SG	25:F:502:SF4:S1	3.13	0.46
7:G:35:PHE:O	7:G:101:ASN:HA	2.16	0.46
9:I:85:ASN:HB3	9:I:89:GLU:HG3	1.98	0.46
9:I:116:CYS:HB2	9:I:118:LEU:H	1.80	0.46
10:P:81:ILE:HD11	12:R:46:VAL:HG21	1.97	0.46
15:V:31:THR:C	15:V:33:ASP:N	2.73	0.46
15:V:44:TYR:O	15:V:48:THR:HG22	2.15	0.46
18:Z:69:ILE:HG23	20:b:54:PRO:HD2	1.96	0.46
2:B:169:GLY:C	2:B:171:TYR:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:300:ILE:HD13	6:F:307:VAL:HG22	1.96	0.46
7:G:544:MET:HA	7:G:565:PHE:O	2.14	0.46
8:H:264:LEU:HD23	19:a:12:MET:HE2	1.97	0.46
10:P:229:VAL:C	10:P:231:LEU:N	2.73	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
16:W:61:GLN:O	16:W:64:ASP:HB2	2.15	0.46
21:q:60:ARG:HD2	21:q:92:CYS:SG	2.56	0.46
4:D:409:VAL:HG13	4:D:422:CYS:SG	2.55	0.46
5:E:43:THR:O	5:E:47:ASN:HB3	2.15	0.46
5:E:61:ARG:O	5:E:62:ILE:C	2.57	0.46
5:E:142:ARG:CB	5:E:182:ALA:HB3	2.45	0.46
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.45	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.15	0.46
7:G:137:CYS:N	11:Q:88:GLN:HE21	2.13	0.46
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.84	0.46
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.46
7:G:462:PHE:CD1	7:G:465:VAL:HB	2.50	0.46
10:P:141:PHE:HD1	10:P:145:PHE:HE2	1.64	0.46
10:P:169:HIS:H	10:P:184:LYS:CE	2.28	0.46
15:V:33:ASP:O	15:V:34:ILE:C	2.59	0.46
15:V:51:ILE:O	15:V:52:THR:C	2.58	0.46
16:W:28:LEU:O	16:W:32:LYS:HG3	2.15	0.46
16:W:124:LYS:O	16:W:125:PHE:C	2.58	0.46
17:X:49:GLU:OE1	20:b:58:ARG:NH2	2.49	0.46
19:a:43:TYR:CE1	19:a:47:LEU:HD11	2.50	0.46
20:b:28:LEU:O	20:b:31:ILE:HG12	2.15	0.46
21:q:10:GLY:HA3	33:q:201:CDL:CA3	2.43	0.46
22:r:8:ILE:HA	22:r:11:LEU:HD12	1.98	0.46
2:B:95:PHE:CD1	2:B:97:LEU:HD12	2.51	0.46
2:B:97:LEU:HD21	2:B:141:MET:HG2	1.98	0.46
2:B:112:TYR:O	2:B:113:ASP:C	2.56	0.46
1:A:91:ALA:O	1:A:92:PHE:C	2.58	0.46
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.16	0.46
7:G:30:ASN:O	7:G:45:PRO:HD3	2.15	0.46
7:G:330:LEU:HD12	7:G:544:MET:HE1	1.98	0.46
8:H:149:ILE:HG21	8:H:185:TRP:HB2	1.98	0.46
8:H:200:LEU:HD12	8:H:285:LEU:HD23	1.96	0.46
10:P:230:SER:HB3	10:P:234:LYS:HE3	1.98	0.46
19:a:22:SER:O	19:a:23:THR:C	2.58	0.46
1:A:13:LEU:HD21	8:H:14:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:TYR:CE2	4:D:117:HIS:HE1	2.34	0.46
4:D:98:VAL:HG21	4:D:112:HIS:CE1	2.51	0.46
4:D:100:GLU:HB2	4:D:107:ARG:HB3	1.96	0.46
4:D:412:VAL:HG12	15:V:114:TRP:CZ2	2.50	0.46
5:E:71:GLU:HG3	23:s:94:GLN:NE2	2.27	0.46
6:F:157:TYR:CG	6:F:212:LEU:HD11	2.51	0.46
6:F:410:ASP:OD1	6:F:410:ASP:C	2.58	0.46
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.46
7:G:114:GLU:OE1	22:r:53:TYR:HB3	2.15	0.46
7:G:158:ARG:NH2	7:G:202:ASN:OD1	2.49	0.46
7:G:651:PRO:HD2	13:S:56:ARG:HB3	1.96	0.46
8:H:123:SER:O	8:H:124:ASN:HB3	2.15	0.46
10:P:276:LEU:CD2	10:P:280:ILE:HD11	2.46	0.46
14:T:133:ILE:HG13	14:T:137:LYS:NZ	2.30	0.46
16:W:69:MET:C	16:W:71:MET:H	2.24	0.46
6:F:253:THR:O	6:F:257:ARG:HB3	2.16	0.46
7:G:330:LEU:CA	7:G:544:MET:HE1	2.46	0.46
7:G:355:LYS:HG3	7:G:366:LEU:CD1	2.43	0.46
10:P:220:TYR:CD1	10:P:223:PHE:HE1	2.34	0.46
10:P:228:LEU:HD22	10:P:273:LEU:HD21	1.97	0.46
10:P:301:ILE:HG22	10:P:305:PHE:CE2	2.42	0.46
10:P:318:LYS:HA	10:P:321:ARG:HG2	1.97	0.46
11:Q:63:THR:O	16:W:85:LEU:HD21	2.16	0.46
16:W:36:ARG:O	16:W:40:ARG:HG3	2.16	0.46
33:q:201:CDL:H711	33:q:201:CDL:H321	1.98	0.46
1:A:24:LEU:HD22	26:B:303:PC1:H352	1.98	0.46
2:B:153:PRO:O	2:B:156:ARG:HB3	2.16	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
7:G:49:VAL:HB	7:G:91:ALA:HA	1.98	0.46
7:G:405:THR:O	7:G:407:PRO:HD3	2.16	0.46
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.97	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
12:R:88:HIS:O	12:R:89:PRO:C	2.56	0.46
13:S:24:CYS:CA	13:S:58:CYS:HB2	2.46	0.46
17:X:7:LEU:CD2	18:Z:87:LEU:HD11	2.46	0.46
21:q:17:HIS:CD2	21:q:35:ILE:HD13	2.50	0.46
21:q:42:ASP:CG	21:q:46:ASN:HB2	2.41	0.46
25:B:301:SF4:S2	4:D:138:ARG:HD3	2.55	0.46
4:D:238:LEU:O	4:D:238:LEU:HG	2.16	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:83:GLU:O	7:G:84:LYS:C	2.59	0.46
7:G:97:MET:SD	7:G:100:TRP:CZ2	3.10	0.46
7:G:114:GLU:OE2	22:r:53:TYR:CA	2.51	0.46
8:H:142:TYR:CD1	8:H:289:LEU:HD13	2.51	0.46
10:P:106:LEU:HB2	12:R:50:ASP:OD2	2.16	0.46
16:W:22:PRO:HG3	16:W:26:ARG:NH2	2.30	0.46
17:X:130:LYS:HE2	17:X:130:LYS:HB3	1.79	0.46
19:a:3:PHE:HD1	33:q:201:CDL:C13	2.28	0.46
21:q:6:VAL:HG21	33:q:201:CDL:CB6	2.46	0.46
21:q:24:LEU:O	21:q:28:PHE:HB2	2.16	0.46
4:D:123:LEU:HD13	4:D:135:TYR:OH	2.14	0.45
6:F:262:PHE:HA	6:F:265:PHE:HD2	1.81	0.45
7:G:35:PHE:CD1	7:G:40:SER:HB2	2.51	0.45
8:H:230:ASN:HA	8:H:233:LEU:HD12	1.97	0.45
9:I:78:PHE:HA	19:a:2:TRP:HD1	1.80	0.45
12:R:46:VAL:O	12:R:47:ARG:C	2.58	0.45
14:T:102:SER:HB2	14:T:107:ASP:CB	2.46	0.45
16:W:77:THR:O	16:W:79:PRO:HD3	2.17	0.45
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.98	0.45
1:A:65:PHE:HA	1:A:68:GLU:CG	2.46	0.45
5:E:195:LEU:HD23	5:E:218:ARG:CG	2.45	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.31	0.45
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.16	0.45
7:G:173:MET:CE	7:G:206:VAL:O	2.64	0.45
8:H:25:ARG:NH2	29:H:401:UQ9:C10	2.79	0.45
8:H:148:ILE:HG21	8:H:297:THR:HG22	1.99	0.45
8:H:201:THR:C	8:H:203:GLY:N	2.71	0.45
9:I:135:ARG:O	9:I:136:ALA:HB3	2.16	0.45
11:Q:163:ASN:OD1	11:Q:164:PHE:CG	2.69	0.45
13:S:20:ARG:CG	13:S:66:TRP:HB2	2.46	0.45
17:X:128:VAL:HG12	20:b:54:PRO:HB2	1.97	0.45
18:Z:108:GLU:O	18:Z:109:SER:C	2.57	0.45
5:E:73:HIS:CE1	11:Q:166:TRP:CD2	3.05	0.45
5:E:131:ILE:N	5:E:169:THR:O	2.49	0.45
6:F:196:PHE:HD1	23:s:91:ARG:HE	1.65	0.45
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.45
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.98	0.45
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.45
8:H:233:LEU:O	8:H:236:ALA:N	2.49	0.45
10:P:244:ASP:HB3	10:P:335:LEU:HD13	1.98	0.45
10:P:315:THR:O	10:P:319:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:65:LYS:HE3	16:W:69:MET:SD	2.56	0.45
2:B:93:MET:HE1	2:B:125:PRO:HB3	1.98	0.45
2:B:174:SER:HB3	4:D:123:LEU:HD11	1.99	0.45
4:D:163:PRO:HG2	4:D:168:GLN:NE2	2.32	0.45
4:D:232:VAL:HG23	4:D:356:ILE:HD13	1.98	0.45
4:D:234:GLN:HE21	9:I:212:ARG:HB3	1.79	0.45
4:D:261:MET:CE	9:I:73:THR:CG2	2.90	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:300:ILE:CG2	6:F:306:GLY:C	2.90	0.45
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.46	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.45
8:H:65:THR:HG22	8:H:67:SER:H	1.80	0.45
8:H:151:LEU:HD23	8:H:151:LEU:C	2.41	0.45
8:H:157:ASN:HD22	8:H:165:LEU:HD11	1.78	0.45
9:I:56:ASN:O	9:I:60:ILE:HG13	2.16	0.45
10:P:203:PRO:HG2	30:P:401:NDP:C6N	2.47	0.45
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.45
14:T:98:LEU:O	14:T:99:SER:C	2.57	0.45
18:Z:133:MET:O	18:Z:134:SER:C	2.60	0.45
21:q:17:HIS:ND1	21:q:26:VAL:HG21	2.30	0.45
23:s:94:GLN:OE1	23:s:94:GLN:N	2.49	0.45
3:C:118:VAL:HB	3:C:121:ARG:HD2	1.98	0.45
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.45
5:E:241:GLY:HA2	6:F:63:TYR:CE2	2.51	0.45
6:F:50:ASP:C	6:F:52:ARG:N	2.73	0.45
6:F:136:HIS:O	6:F:137:LYS:C	2.59	0.45
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.91	0.45
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.98	0.45
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.45
8:H:112:SER:O	8:H:113:VAL:C	2.59	0.45
10:P:128:ASN:HD22	10:P:166:HIS:CD2	2.35	0.45
10:P:303:LYS:O	10:P:307:LEU:HG	2.15	0.45
10:P:354:ARG:HD2	10:P:362:LEU:O	2.16	0.45
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.98	0.45
22:r:57:ARG:HG3	22:r:57:ARG:O	2.16	0.45
1:A:24:LEU:HD13	26:B:303:PC1:H3B2	1.99	0.45
1:A:52:SER:O	1:A:53:MET:HB3	2.15	0.45
1:A:73:LEU:HD23	8:H:151:LEU:HD12	1.97	0.45
4:D:174:PHE:O	4:D:178:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:226:TYR:CZ	4:D:232:VAL:HB	2.52	0.45
8:H:138:GLN:HG3	8:H:285:LEU:HD21	1.98	0.45
8:H:142:TYR:CE1	8:H:285:LEU:HD11	2.51	0.45
10:P:88:VAL:O	10:P:91:ILE:HG12	2.17	0.45
10:P:192:ARG:NE	10:P:200:ILE:HD12	2.30	0.45
11:Q:69:GLU:HA	11:Q:72:ILE:CG2	2.45	0.45
13:S:95:LEU:HD12	13:S:95:LEU:C	2.33	0.45
14:T:123:GLU:HA	14:T:128:PHE:O	2.16	0.45
2:B:95:PHE:HD1	2:B:97:LEU:HD12	1.81	0.45
4:D:87:GLN:CG	4:D:93:GLY:HA2	2.46	0.45
6:F:174:ARG:CG	23:s:87:LEU:HD11	2.47	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:182:CYS:SG	25:G:802:SF4:S1	3.14	0.45
8:H:102:ILE:HG21	8:H:154:LEU:HD21	1.99	0.45
8:H:157:ASN:HD22	8:H:165:LEU:CD1	2.29	0.45
8:H:198:PHE:HE2	24:H:402:3PE:H242	1.82	0.45
10:P:188:GLU:HG3	10:P:202:ARG:HH21	1.82	0.45
15:V:43:ALA:O	15:V:44:TYR:C	2.60	0.45
2:B:99:CYS:SG	25:B:301:SF4:S4	3.14	0.45
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.52	0.45
3:C:223:VAL:CG2	3:C:225:LEU:HD13	2.33	0.45
4:D:304:LYS:HD3	4:D:318:VAL:CG2	2.47	0.45
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.96	0.45
6:F:261:TRP:HZ3	6:F:262:PHE:CE2	2.35	0.45
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.45
7:G:35:PHE:CE1	7:G:40:SER:CB	2.99	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.99	0.45
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.45
7:G:283:GLU:O	7:G:283:GLU:CG	2.50	0.45
7:G:382:ARG:HG2	7:G:386:LEU:CD1	2.41	0.45
7:G:382:ARG:CZ	7:G:652:ASN:ND2	2.80	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
7:G:671:LEU:CD2	13:S:45:LYS:HG2	2.44	0.45
9:I:114:ILE:HD13	12:R:106:TYR:CD1	2.51	0.45
10:P:81:ILE:HG12	12:R:46:VAL:HG11	1.99	0.45
10:P:99:ASP:CG	10:P:100:LEU:H	2.24	0.45
10:P:370:LYS:HD3	10:P:371:PRO:O	2.16	0.45
11:Q:53:ILE:HG22	16:W:20:VAL:O	2.17	0.45
17:X:27:ALA:HB1	17:X:85:TYR:CD2	2.52	0.45
19:a:4:GLU:O	19:a:7:PRO:HD2	2.16	0.45
2:B:154:GLU:O	2:B:155:PRO:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:ASP:OD1	4:D:138:ARG:N	2.50	0.45
4:D:265:ASN:O	4:D:266:ARG:C	2.56	0.45
4:D:266:ARG:HH11	9:I:66:LEU:HG	1.81	0.45
5:E:163:THR:HG23	5:E:168:PHE:O	2.17	0.45
5:E:180:VAL:HG13	5:E:181:ASN:N	2.31	0.45
6:F:227:PRO:HB2	6:F:228:PRO:CD	2.40	0.45
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.46	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.45
7:G:473:MET:HE3	7:G:514:ASN:ND2	2.22	0.45
9:I:98:ARG:NH1	9:I:155:CYS:O	2.50	0.45
10:P:168:SER:O	10:P:203:PRO:HD2	2.16	0.45
11:Q:112:MET:HG2	11:Q:114:TRP:CE2	2.52	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
16:W:104:THR:HG22	16:W:108:ARG:HE	1.82	0.45
3:C:118:VAL:CG1	3:C:120:THR:HG22	2.45	0.45
3:C:120:THR:HG23	3:C:121:ARG:H	1.81	0.45
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.45
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.45
7:G:176:CYS:SG	25:G:802:SF4:S1	3.14	0.45
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.45
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
8:H:243:LEU:HB3	8:H:262:GLU:OE1	2.15	0.45
22:r:27:ARG:CB	22:r:31:ILE:CG2	2.87	0.45
4:D:152:SER:OG	4:D:227:ILE:O	2.35	0.44
4:D:460:GLU:O	4:D:463:ARG:HG2	2.16	0.44
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.44
7:G:341:ILE:HD12	7:G:555:ILE:CG1	2.47	0.44
7:G:399:VAL:HG21	7:G:462:PHE:CZ	2.51	0.44
8:H:51:ASP:OD1	29:H:401:UQ9:C13	2.64	0.44
10:P:171:ASN:OD1	10:P:171:ASN:O	2.34	0.44
15:V:50:GLN:NE2	22:r:94:ALA:H	2.15	0.44
2:B:127:GLN:NE2	8:H:213:VAL:O	2.50	0.44
2:B:140:LYS:HD2	4:D:115:LEU:HD23	1.99	0.44
4:D:168:GLN:HB3	4:D:310:VAL:HG13	1.99	0.44
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.44
6:F:335:VAL:HG13	6:F:341:ALA:HB1	1.99	0.44
7:G:308:ARG:NH1	7:G:578:PRO:O	2.50	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:227:GLU:C	8:H:228:TYR:HD1	2.25	0.44
8:H:260:MET:HE1	19:a:16:LEU:CA	2.47	0.44
9:I:48:VAL:HG23	20:b:10:LYS:HZ2	1.82	0.44
10:P:276:LEU:CD2	10:P:280:ILE:CD1	2.95	0.44
14:T:99:SER:HB2	14:T:102:SER:CB	2.33	0.44
15:V:48:THR:HA	15:V:51:ILE:HD12	1.98	0.44
15:V:79:GLU:O	15:V:80:VAL:C	2.58	0.44
19:a:66:LEU:HD13	19:a:66:LEU:O	2.17	0.44
21:q:48:TYR:OH	21:q:83:PRO:HD2	2.18	0.44
2:B:192:PRO:HD3	9:I:176:SER:HA	1.98	0.44
4:D:319:PRO:HG3	4:D:336:GLU:HG3	2.00	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
5:E:81:VAL:O	5:E:82:LEU:C	2.59	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
6:F:226:LYS:N	6:F:227:PRO:CD	2.80	0.44
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.44
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.16	0.44
15:V:35:LEU:HD22	15:V:48:THR:HG21	1.98	0.44
4:D:88:HIS:N	4:D:89:PRO:HD2	2.32	0.44
4:D:142:VAL:HG11	4:D:185:MET:CB	2.48	0.44
4:D:150:ALA:O	4:D:151:TYR:C	2.57	0.44
4:D:326:CYS:O	4:D:329:ARG:N	2.51	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
6:F:398:ARG:HH21	7:G:155:GLU:HG3	1.83	0.44
7:G:629:ILE:HD11	16:W:122:LEU:HD21	1.98	0.44
8:H:74:ALA:N	8:H:75:PRO:HD2	2.32	0.44
8:H:184:MET:CG	8:H:293:PHE:CE2	2.88	0.44
8:H:218:GLY:O	8:H:219:PRO:C	2.57	0.44
9:I:54:THR:HA	20:b:13:TRP:HE1	1.82	0.44
12:R:44:ARG:HB3	12:R:47:ARG:HH12	1.82	0.44
15:V:39:PRO:O	15:V:40:LYS:C	2.60	0.44
15:V:56:LEU:O	15:V:60:LYS:HG2	2.17	0.44
21:q:68:MET:HE2	21:q:71:LYS:HD3	1.99	0.44
2:B:197:THR:O	2:B:200:ALA:HB3	2.17	0.44
3:C:117:ASP:OD1	3:C:124:ARG:HB2	2.18	0.44
3:C:149:LEU:O	3:C:151:PRO:HD3	2.17	0.44
3:C:183:LEU:HD22	16:W:91:MET:HE1	1.99	0.44
4:D:126:TYR:HA	4:D:418:ARG:HH11	1.83	0.44
5:E:47:ASN:HB2	5:E:48:PRO:CD	2.47	0.44
6:F:36:LYS:CB	6:F:38:GLU:HG2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:174:ARG:CB	23:s:87:LEU:HD11	2.48	0.44
6:F:227:PRO:CB	6:F:228:PRO:HD3	2.40	0.44
6:F:410:ASP:O	6:F:413:TRP:HB3	2.17	0.44
7:G:75:CYS:SG	27:G:803:FES:S2	3.16	0.44
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.44
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.44
7:G:629:ILE:HD11	16:W:122:LEU:HD11	2.00	0.44
8:H:45:ILE:CD1	19:a:11:ILE:CD1	2.90	0.44
8:H:187:ILE:HD11	9:I:63:TRP:CH2	2.53	0.44
8:H:196:ALA:C	8:H:198:PHE:N	2.69	0.44
16:W:31:ALA:O	16:W:32:LYS:C	2.58	0.44
21:q:37:THR:O	21:q:49:TYR:HA	2.17	0.44
1:A:111:LEU:CB	8:H:291:LYS:HE2	2.48	0.44
2:B:170:TYR:CZ	4:D:135:TYR:CE2	3.06	0.44
3:C:126:GLU:O	3:C:128:VAL:HG23	2.17	0.44
4:D:144:MET:SD	4:D:222:MET:CG	2.98	0.44
4:D:256:ASP:HB2	18:Z:25:LEU:HD11	1.93	0.44
4:D:256:ASP:C	4:D:259:GLU:HB3	2.43	0.44
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.44
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.44
8:H:190:LEU:HD23	8:H:198:PHE:CE1	2.51	0.44
10:P:266:THR:CG2	10:P:329:PRO:HB3	2.47	0.44
15:V:65:VAL:O	15:V:66:LYS:C	2.60	0.44
15:V:82:LEU:HG	15:V:86:LYS:HE2	2.00	0.44
16:W:98:LYS:HD3	16:W:100:TRP:CZ2	2.53	0.44
18:Z:58:ARG:HG2	20:b:45:ILE:CD1	2.48	0.44
1:A:109:LYS:HB2	1:A:109:LYS:HE2	1.88	0.44
24:A:202:3PE:H2A1	24:A:202:3PE:H2D2	1.80	0.44
2:B:104:MET:HE3	2:B:104:MET:HB3	1.84	0.44
26:B:302:PC1:H341	26:B:302:PC1:C22	2.45	0.44
3:C:153:ASP:OD1	3:C:153:ASP:N	2.50	0.44
4:D:113:ILE:CG2	4:D:432:LEU:HD21	2.48	0.44
4:D:133:LEU:HD11	4:D:148:GLU:HB3	1.98	0.44
4:D:256:ASP:OD1	4:D:257:GLU:N	2.50	0.44
6:F:157:TYR:CG	6:F:212:LEU:CD1	3.01	0.44
7:G:447:ASP:O	7:G:447:ASP:CG	2.60	0.44
10:P:221:ARG:HD2	10:P:286:ARG:CD	2.43	0.44
13:S:85:ASP:OD1	13:S:86:GLU:N	2.51	0.44
15:V:31:THR:O	15:V:33:ASP:N	2.50	0.44
2:B:137:LEU:HD13	2:B:145:LEU:HD22	1.99	0.44
4:D:83:ASN:C	4:D:85:GLY:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:119:GLU:HB3	6:F:124:THR:HG22	2.00	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.58	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:304:GLU:CG	7:G:305:PRO:HD2	2.47	0.44
7:G:309:ASN:OD1	7:G:310:GLU:N	2.51	0.44
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
7:G:359:ASN:C	7:G:361:VAL:O	2.61	0.44
8:H:19:PHE:CD2	19:a:11:ILE:HG21	2.53	0.44
10:P:92:MET:C	10:P:94:LEU:N	2.74	0.44
10:P:224:LEU:HB3	10:P:225:ALA:H	1.53	0.44
10:P:293:LEU:HB3	10:P:294:PRO:HD2	2.00	0.44
10:P:299:SER:HB3	10:P:316:LYS:NZ	2.33	0.44
10:P:304:LEU:HA	10:P:307:LEU:HG	1.99	0.44
14:T:105:MET:HE1	14:T:115:GLN:HG3	1.99	0.44
17:X:84:GLU:C	17:X:87:THR:HG22	2.42	0.44
21:q:42:ASP:OD1	21:q:46:ASN:N	2.45	0.44
1:A:96:THR:HG1	20:b:26:TRP:HZ2	1.63	0.44
2:B:79:ASP:OD1	2:B:80:ASP:N	2.51	0.44
3:C:148:GLU:OE2	11:Q:140:LYS:NZ	2.30	0.44
4:D:87:GLN:OE1	4:D:87:GLN:HA	2.18	0.44
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.83	0.44
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.98	0.44
7:G:383:SER:O	7:G:384:ASN:C	2.58	0.44
8:H:102:ILE:CG2	8:H:150:LEU:HD21	2.48	0.44
8:H:228:TYR:N	8:H:228:TYR:CD1	2.85	0.44
10:P:111:ARG:NH1	10:P:138:ASN:HB3	2.33	0.44
14:T:103:HIS:O	14:T:107:ASP:N	2.51	0.44
17:X:54:ARG:HG2	18:Z:84:LEU:CD1	2.45	0.44
17:X:129:THR:HA	20:b:67:PRO:O	2.18	0.44
21:q:26:VAL:HG13	21:q:30:ALA:HB3	2.00	0.44
4:D:137:ASP:HB2	4:D:223:HIS:HA	1.99	0.43
5:E:79:LEU:HB2	5:E:80:PRO:HD3	2.00	0.43
7:G:61:PRO:HB3	7:G:146:PHE:CD2	2.53	0.43
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.58	0.43
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.43
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.43
7:G:617:ARG:HH22	16:W:128:GLY:H	1.64	0.43
8:H:249:ILE:HD13	8:H:249:ILE:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:114:ASP:O	10:P:118:LYS:HG2	2.18	0.43
10:P:275:HIS:CE1	10:P:373:LYS:HE2	2.53	0.43
14:T:99:SER:C	14:T:101:ASN:N	2.75	0.43
15:V:56:LEU:HG	15:V:60:LYS:HE3	2.00	0.43
15:V:62:GLU:HA	15:V:63:PRO:HD3	1.82	0.43
17:X:49:GLU:CG	17:X:50:GLU:H	2.30	0.43
18:Z:128:ARG:HB3	18:Z:132:GLU:OE1	2.18	0.43
20:b:37:PRO:O	20:b:40:LYS:NZ	2.51	0.43
22:r:5:THR:CG2	22:r:7:VAL:HG12	2.46	0.43
4:D:188:THR:O	4:D:192:LEU:HD13	2.18	0.43
4:D:327:TYR:CE2	4:D:331:LEU:HD11	2.53	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.34	0.43
6:F:412:LEU:CD2	6:F:435:VAL:HG13	2.48	0.43
7:G:450:LYS:CD	7:G:453:GLN:HG3	2.32	0.43
8:H:27:ILE:HD12	8:H:271:LEU:CD1	2.48	0.43
9:I:57:ALA:O	9:I:61:LEU:HB2	2.18	0.43
10:P:283:MET:HG2	10:P:353:LEU:HD12	1.99	0.43
17:X:73:GLN:O	17:X:77:HIS:N	2.51	0.43
17:X:140:ASN:N	17:X:141:PRO:CD	2.81	0.43
23:s:83:LEU:O	23:s:87:LEU:HD13	2.18	0.43
2:B:224:ARG:HG3	10:P:136:THR:HG21	2.00	0.43
4:D:142:VAL:HG12	4:D:182:ASN:HA	2.01	0.43
4:D:159:LEU:CD2	4:D:391:VAL:HG12	2.48	0.43
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.42	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
6:F:311:TRP:CH2	6:F:333:GLU:HB3	2.53	0.43
7:G:165:ILE:CG2	7:G:169:VAL:HB	2.48	0.43
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.43
7:G:291:ARG:HD2	7:G:292:PHE:CE2	2.54	0.43
7:G:355:LYS:CG	7:G:366:LEU:HD12	2.43	0.43
7:G:611:THR:CG2	11:Q:104:ARG:C	2.91	0.43
7:G:664:TYR:OH	13:S:23:LEU:HD11	2.18	0.43
8:H:62:ARG:HD2	8:H:68:MET:HB2	2.00	0.43
16:W:69:MET:O	16:W:70:PHE:C	2.60	0.43
4:D:95:LEU:HD12	4:D:95:LEU:C	2.43	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.43
15:V:90:LEU:O	15:V:94:MET:N	2.44	0.43
16:W:98:LYS:HD3	16:W:100:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:O	8:H:151:LEU:HD11	2.18	0.43
3:C:127:ILE:H	3:C:127:ILE:HD12	1.83	0.43
4:D:129:TYR:CE2	4:D:391:VAL:HG22	2.54	0.43
4:D:133:LEU:O	4:D:134:PRO:C	2.59	0.43
4:D:172:VAL:HG21	4:D:310:VAL:CG2	2.49	0.43
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.43
4:D:385:TYR:HD2	9:I:122:ILE:CD1	2.31	0.43
5:E:145:ASP:O	5:E:146:SER:C	2.62	0.43
7:G:117:MET:SD	7:G:143:SER:HB2	2.58	0.43
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.28	0.43
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.18	0.43
7:G:662:THR:HB	13:S:25:GLN:NE2	2.33	0.43
8:H:288:LEU:HG	8:H:293:PHE:HE1	1.84	0.43
10:P:110:ALA:HB1	10:P:148:ILE:CD1	2.48	0.43
10:P:231:LEU:HB2	10:P:233:PHE:HD1	1.82	0.43
15:V:62:GLU:OE2	15:V:64:ASP:HB3	2.19	0.43
19:a:57:VAL:HG22	19:a:57:VAL:O	2.18	0.43
21:q:9:ARG:O	21:q:13:GLN:HG3	2.18	0.43
4:D:211:PHE:HD1	4:D:221:ARG:O	2.02	0.43
6:F:261:TRP:CE3	6:F:262:PHE:CD1	3.05	0.43
6:F:311:TRP:HZ2	6:F:333:GLU:HB3	1.80	0.43
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.50	0.43
7:G:571:HIS:HD2	7:G:572:HIS:NE2	2.09	0.43
12:R:43:TYR:C	12:R:45:ARG:H	2.26	0.43
13:S:35:ASP:O	13:S:36:PHE:C	2.60	0.43
16:W:87:ILE:O	16:W:88:LYS:C	2.61	0.43
18:Z:30:LEU:HD12	18:Z:30:LEU:H	1.84	0.43
1:A:96:THR:O	1:A:97:ILE:C	2.60	0.43
2:B:74:VAL:O	2:B:78:LEU:HG	2.19	0.43
2:B:100:CYS:SG	25:B:301:SF4:S3	3.17	0.43
5:E:133:VAL:HG22	5:E:185:VAL:HG12	2.00	0.43
5:E:138:PRO:HG3	6:F:355:ILE:HD13	1.99	0.43
5:E:233:LEU:HD23	6:F:43:THR:O	2.18	0.43
5:E:238:LYS:HB3	5:E:242:PHE:CG	2.53	0.43
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.43
8:H:52:ALA:HB2	29:H:401:UQ9:H18	2.00	0.43
8:H:61:MET:O	8:H:63:PRO:HD3	2.18	0.43
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.54	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
10:P:146:VAL:O	10:P:147:ASN:C	2.60	0.43
10:P:293:LEU:HD12	10:P:298:TYR:OH	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:84:GLY:O	12:R:85:ALA:CB	2.65	0.43
13:S:44:LEU:CD2	13:S:91:MET:HG2	2.48	0.43
14:T:147:TYR:O	14:T:148:ILE:C	2.61	0.43
17:X:18:VAL:CG1	17:X:20:VAL:HG22	2.44	0.43
18:Z:87:LEU:HA	18:Z:90:ASN:HB2	2.01	0.43
21:q:42:ASP:OD1	21:q:46:ASN:HB2	2.18	0.43
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.82	0.43
2:B:202:LEU:HD21	9:I:86:TYR:CB	2.48	0.43
3:C:226:ALA:O	11:Q:116:SER:OG	2.31	0.43
4:D:82:LEU:CD2	8:H:126:LYS:HD2	2.49	0.43
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.43
5:E:144:SER:O	5:E:147:ILE:HB	2.19	0.43
5:E:167:LEU:HD12	5:E:167:LEU:HA	1.79	0.43
6:F:363:ILE:HG23	6:F:364:VAL:N	2.33	0.43
8:H:2:PHE:CE1	8:H:95:LEU:HD11	2.54	0.43
8:H:142:TYR:CD2	8:H:289:LEU:HD12	2.54	0.43
8:H:231:ILE:HG23	8:H:270:PHE:CD2	2.54	0.43
9:I:71:GLY:O	22:r:15:ALA:HB1	2.19	0.43
10:P:144:VAL:HG23	10:P:145:PHE:CD2	2.54	0.43
10:P:232:GLY:O	10:P:273:LEU:HB3	2.18	0.43
15:V:31:THR:O	15:V:32:LEU:C	2.61	0.43
1:A:51:PHE:HE2	1:A:53:MET:SD	2.42	0.43
2:B:153:PRO:CG	8:H:58:LYS:HE3	2.47	0.43
4:D:138:ARG:HG2	4:D:223:HIS:CE1	2.53	0.43
4:D:212:GLU:OE1	22:r:27:ARG:NH2	2.50	0.43
4:D:259:GLU:OE2	18:Z:23:ARG:NH2	2.51	0.43
5:E:196:THR:O	5:E:199:ASP:N	2.51	0.43
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.43
7:G:422:TRP:HZ2	7:G:441:ARG:HB3	1.82	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
8:H:28:LEU:HG	8:H:275:ALA:HB2	2.01	0.43
9:I:135:ARG:HD2	12:R:61:ILE:CG1	2.49	0.43
10:P:140:ASP:O	10:P:141:PHE:C	2.62	0.43
10:P:231:LEU:CD2	10:P:292:PRO:HB3	2.48	0.43
10:P:293:LEU:C	10:P:298:TYR:HE2	2.27	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
14:T:90:TYR:HD2	14:T:93:ILE:CB	2.32	0.43
16:W:87:ILE:CG2	16:W:91:MET:HE3	2.45	0.43
18:Z:120:LEU:O	18:Z:121:ILE:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:31:ILE:O	20:b:35:ILE:HG22	2.18	0.43
24:A:201:3PE:H272	20:b:23:PHE:HD2	1.84	0.43
26:B:303:PC1:H241	10:P:310:PHE:CE1	2.53	0.43
3:C:53:THR:O	3:C:54:HIS:C	2.60	0.43
3:C:152:ILE:HD11	3:C:177:PHE:CD2	2.50	0.43
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.43
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.34	0.43
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.43
6:F:234:GLY:O	6:F:235:VAL:C	2.62	0.43
6:F:392:MET:HE2	6:F:416:SER:HA	1.93	0.43
7:G:496:MET:O	7:G:500:ILE:HG13	2.19	0.43
7:G:517:HIS:H	7:G:599:THR:HG21	1.84	0.43
10:P:92:MET:C	10:P:94:LEU:H	2.26	0.43
10:P:134:TRP:CZ2	10:P:311:GLU:HG2	2.54	0.43
10:P:187:GLY:O	10:P:188:GLU:C	2.62	0.43
11:Q:57:GLU:HG3	11:Q:58:LYS:O	2.19	0.43
11:Q:98:LYS:NZ	11:Q:127:THR:OG1	2.52	0.43
17:X:129:THR:HG21	20:b:70:PRO:HD3	2.00	0.43
19:a:58:ASN:O	19:a:59:ARG:C	2.61	0.43
20:b:45:ILE:N	20:b:80:TRP:HH2	2.17	0.43
2:B:108:ALA:N	2:B:114:MET:HE3	2.33	0.42
3:C:229:PHE:CD1	9:I:126:GLN:HG3	2.43	0.42
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.84	0.42
4:D:266:ARG:NH2	9:I:59:ARG:O	2.52	0.42
10:P:321:ARG:HA	10:P:325:SER:HB2	2.00	0.42
16:W:45:GLU:O	16:W:46:VAL:C	2.59	0.42
17:X:131:VAL:HG23	17:X:131:VAL:O	2.19	0.42
19:a:58:ASN:CB	19:a:60:TYR:CD1	2.89	0.42
21:q:14:VAL:HG13	21:q:23:LEU:HG	2.01	0.42
2:B:108:ALA:HB2	2:B:114:MET:HE3	2.01	0.42
2:B:154:GLU:O	10:P:89:TYR:OH	2.27	0.42
3:C:208:GLU:HG3	3:C:221:GLU:HG3	2.00	0.42
3:C:227:GLN:NE2	9:I:129:THR:HG21	2.34	0.42
4:D:159:LEU:HG	4:D:391:VAL:HG12	2.01	0.42
4:D:326:CYS:O	4:D:330:TYR:N	2.33	0.42
5:E:65:ILE:O	5:E:66:VAL:C	2.62	0.42
5:E:73:HIS:HE1	11:Q:166:TRP:CG	2.38	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42
7:G:304:GLU:HB3	7:G:316:TYR:HD1	1.83	0.42
7:G:376:GLY:C	7:G:378:GLY:N	2.77	0.42
7:G:380:ASP:HB2	13:S:41:TYR:OH	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.42
8:H:123:SER:O	8:H:124:ASN:CB	2.66	0.42
8:H:195:ARG:HH21	8:H:271:LEU:HD23	1.84	0.42
9:I:152:CYS:SG	25:I:301:SF4:S2	3.16	0.42
10:P:336:GLU:H	10:P:336:GLU:CD	2.25	0.42
12:R:32:THR:C	12:R:34:THR:N	2.76	0.42
2:B:87:ARG:HH12	26:B:302:PC1:P	2.42	0.42
3:C:72:VAL:HG22	3:C:87:ILE:HG22	2.01	0.42
3:C:155:ILE:O	3:C:156:VAL:C	2.58	0.42
4:D:264:ASN:HB2	9:I:65:GLU:OE2	2.18	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
6:F:41:ILE:HD13	6:F:250:VAL:HG12	2.01	0.42
6:F:119:GLU:H	6:F:159:ARG:HD2	1.83	0.42
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.42
11:Q:52:LEU:HD23	11:Q:52:LEU:HA	1.73	0.42
16:W:53:MET:O	16:W:54:GLN:C	2.62	0.42
16:W:59:VAL:HG12	16:W:63:ARG:HD2	2.01	0.42
16:W:104:THR:HG22	16:W:108:ARG:NE	2.34	0.42
17:X:7:LEU:HD21	18:Z:87:LEU:CD1	2.48	0.42
17:X:59:GLU:OE2	17:X:135:ARG:HD3	2.19	0.42
17:X:128:VAL:O	17:X:128:VAL:CG2	2.58	0.42
1:A:13:LEU:O	1:A:17:LEU:HG	2.19	0.42
1:A:75:LEU:O	1:A:76:PRO:C	2.60	0.42
2:B:92:PRO:HG3	2:B:119:VAL:HG13	2.01	0.42
3:C:120:THR:CG2	3:C:121:ARG:H	2.32	0.42
3:C:202:PRO:O	3:C:203:LEU:C	2.62	0.42
4:D:184:ILE:HG23	4:D:203:MET:HB3	2.00	0.42
4:D:234:GLN:NE2	9:I:212:ARG:HB3	2.35	0.42
5:E:78:VAL:HG21	6:F:218:GLY:O	2.20	0.42
5:E:190:ASN:HB3	5:E:192:TYR:CE1	2.55	0.42
5:E:230:LEU:C	5:E:232:SER:N	2.78	0.42
6:F:226:LYS:N	6:F:227:PRO:HD2	2.35	0.42
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.42
7:G:114:GLU:CD	22:r:53:TYR:HD1	2.26	0.42
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.42
7:G:480:ALA:O	7:G:481:LEU:C	2.63	0.42
10:P:97:MET:HE2	10:P:97:MET:HB3	1.84	0.42
11:Q:69:GLU:O	11:Q:72:ILE:CG2	2.61	0.42
11:Q:75:ARG:NH1	11:Q:102:ASP:OD1	2.51	0.42
14:T:85:TYR:CZ	14:T:89:LEU:HD11	2.55	0.42
15:V:13:GLY:O	15:V:14:LEU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:14:VAL:HA	19:a:17:VAL:HG22	2.00	0.42
19:a:37:ARG:NH1	19:a:59:ARG:HD2	2.34	0.42
2:B:224:ARG:HH21	10:P:85:ARG:NH1	2.17	0.42
26:B:303:PC1:H3I3	8:H:53:MET:HE2	2.01	0.42
6:F:126:LYS:HE2	6:F:274:LYS:HZ3	1.85	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
7:G:65:TYR:HB2	7:G:92:CYS:SG	2.60	0.42
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.42
7:G:651:PRO:O	7:G:654:VAL:HG12	2.19	0.42
8:H:91:MET:O	8:H:93:HIS:N	2.52	0.42
8:H:135:ALA:HB2	8:H:201:THR:HB	2.01	0.42
8:H:204:GLU:HG2	8:H:279:ARG:HH22	1.84	0.42
8:H:231:ILE:O	8:H:231:ILE:HG22	2.19	0.42
10:P:220:TYR:HA	10:P:223:PHE:CE1	2.55	0.42
11:Q:130:ALA:O	11:Q:131:LYS:C	2.62	0.42
15:V:20:PRO:HG3	15:V:65:VAL:HG22	2.02	0.42
16:W:69:MET:O	16:W:71:MET:N	2.53	0.42
17:X:41:LYS:HB3	17:X:131:VAL:HG11	2.02	0.42
1:A:108:GLN:HG3	1:A:110:GLY:H	1.85	0.42
2:B:169:GLY:C	2:B:171:TYR:H	2.27	0.42
4:D:86:PRO:CD	4:D:88:HIS:CE1	3.02	0.42
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42
6:F:336:LEU:C	6:F:336:LEU:HD12	2.44	0.42
7:G:114:GLU:OE2	22:r:54:TYR:N	2.51	0.42
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.42
9:I:144:ARG:NH2	11:Q:112:MET:O	2.53	0.42
10:P:299:SER:HB3	10:P:316:LYS:HZ2	1.85	0.42
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.42
13:S:32:GLY:HA2	13:S:35:ASP:CG	2.45	0.42
13:S:41:TYR:O	13:S:42:VAL:C	2.63	0.42
2:B:110:PRO:HA	8:H:34:ARG:HB3	2.02	0.42
4:D:218:SER:OG	4:D:219:GLY:N	2.51	0.42
4:D:259:GLU:CD	4:D:263:THR:HG1	2.28	0.42
4:D:359:ASP:OD1	4:D:360:ASP:N	2.52	0.42
6:F:291:GLU:OE2	6:F:292:MET:N	2.53	0.42
7:G:184:ARG:O	7:G:185:PHE:C	2.60	0.42
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.37	0.42
8:H:231:ILE:HG23	8:H:270:PHE:HD2	1.83	0.42
24:H:402:3PE:H352	24:H:402:3PE:H381	1.80	0.42
9:I:79:ARG:HH21	22:r:20:LEU:CD1	2.33	0.42
10:P:309:PRO:HG2	10:P:310:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:99:MET:HB2	11:Q:128:PHE:HE2	1.84	0.42
12:R:79:CYS:O	12:R:88:HIS:CE1	2.73	0.42
13:S:18:GLU:OE2	13:S:68:ARG:NE	2.50	0.42
15:V:114:TRP:O	15:V:116:ILE:N	2.52	0.42
18:Z:111:PHE:CD1	18:Z:117:VAL:HG21	2.55	0.42
18:Z:125:TYR:O	18:Z:128:ARG:HB2	2.20	0.42
19:a:18:ILE:O	19:a:22:SER:HB3	2.18	0.42
19:a:18:ILE:H	19:a:19:PRO:HD3	1.85	0.42
2:B:79:ASP:OD1	2:B:79:ASP:C	2.62	0.42
2:B:202:LEU:HD21	9:I:86:TYR:CG	2.53	0.42
3:C:127:ILE:HD11	3:C:175:VAL:HG21	2.02	0.42
4:D:348:LEU:HB3	18:Z:16:TYR:CD2	2.54	0.42
5:E:73:HIS:ND1	11:Q:166:TRP:CE2	2.88	0.42
5:E:174:GLU:O	5:E:175:CYS:C	2.63	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
6:F:114:VAL:HG21	6:F:235:VAL:HG21	2.01	0.42
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.42
6:F:300:ILE:HD13	6:F:307:VAL:CG2	2.50	0.42
7:G:36:VAL:O	7:G:37:ASP:C	2.63	0.42
7:G:246:ARG:NH1	11:Q:106:ARG:HE	2.17	0.42
8:H:86:TRP:CE3	8:H:89:LEU:HD22	2.54	0.42
8:H:114:TYR:O	8:H:115:SER:C	2.61	0.42
8:H:215:TYR:HD2	8:H:219:PRO:HB3	1.83	0.42
8:H:257:THR:O	8:H:260:MET:HB3	2.20	0.42
10:P:230:SER:C	10:P:232:GLY:N	2.77	0.42
11:Q:61:ILE:HG12	11:Q:140:LYS:HG2	2.01	0.42
13:S:62:GLN:O	13:S:64:LYS:HG3	2.20	0.42
15:V:11:LEU:H	15:V:11:LEU:HD12	1.84	0.42
17:X:16:GLU:O	17:X:64:ASN:ND2	2.53	0.42
18:Z:12:PRO:CD	18:Z:16:TYR:CZ	3.02	0.42
21:q:42:ASP:OD1	21:q:42:ASP:C	2.63	0.42
21:q:66:THR:HG23	21:q:74:PHE:HD1	1.83	0.42
4:D:141:TYR:HB2	4:D:222:MET:CE	2.49	0.42
4:D:184:ILE:HD12	4:D:210:MET:HE1	2.02	0.42
4:D:312:ASP:OD1	4:D:313:GLN:HG3	2.20	0.42
4:D:345:GLU:OE2	18:Z:18:PRO:HA	2.20	0.42
6:F:44:ASN:O	6:F:45:LEU:C	2.62	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:300:ILE:CG2	6:F:306:GLY:CA	2.95	0.42
8:H:97:ASN:HD22	19:a:38:VAL:HG13	1.84	0.42
8:H:283:ASP:N	8:H:283:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:36:TYR:HB3	22:r:104:TRP:HE3	1.85	0.42
14:T:90:TYR:OH	14:T:92:LYS:HD3	2.20	0.42
15:V:114:TRP:O	15:V:114:TRP:CE3	2.72	0.42
16:W:23:ILE:HD12	16:W:80:ARG:O	2.19	0.42
17:X:31:HIS:CB	17:X:70:PHE:HZ	2.31	0.42
17:X:75:LYS:O	17:X:79:ALA:HB2	2.19	0.42
19:a:49:GLU:O	19:a:50:ARG:C	2.62	0.42
20:b:69:HIS:H	20:b:72:ASP:CG	2.28	0.42
21:q:3:LEU:HD13	33:q:201:CDL:C52	2.49	0.42
3:C:116:VAL:HG21	4:D:412:VAL:HG21	2.02	0.42
4:D:211:PHE:O	4:D:214:TYR:N	2.53	0.42
5:E:99:LYS:O	5:E:99:LYS:HD3	2.20	0.42
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:403:VAL:HG13	7:G:476:LEU:CD1	2.50	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
7:G:480:ALA:O	7:G:483:ARG:HG3	2.20	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
10:P:75:ARG:C	10:P:77:GLY:H	2.28	0.42
10:P:96:LEU:HD12	10:P:97:MET:CA	2.49	0.42
11:Q:57:GLU:CD	11:Q:58:LYS:H	2.27	0.42
14:T:107:ASP:C	14:T:108:LEU:HD12	2.45	0.42
15:V:37:HIS:HB2	15:V:95:LEU:HD11	2.01	0.42
17:X:32:TYR:CE1	17:X:67:ALA:HB2	2.55	0.42
17:X:84:GLU:HA	17:X:87:THR:CG2	2.50	0.42
21:q:44:TYR:CD1	21:q:68:MET:HE3	2.55	0.42
33:q:201:CDL:HB32	22:r:8:ILE:HG13	2.01	0.42
22:r:4:ALA:O	22:r:5:THR:C	2.63	0.42
1:A:56:PHE:O	1:A:57:LEU:C	2.63	0.41
2:B:140:LYS:CD	4:D:115:LEU:HD23	2.49	0.41
26:B:302:PC1:H142	21:q:77:VAL:HG12	2.02	0.41
3:C:114:THR:OG1	4:D:421:ARG:NH1	2.53	0.41
4:D:88:HIS:O	4:D:89:PRO:C	2.63	0.41
4:D:112:HIS:HE1	16:W:100:TRP:NE1	2.18	0.41
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.20	0.41
6:F:45:LEU:HG	6:F:46:TYR:CE1	2.54	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:475:VAL:HG22	7:G:514:ASN:OD1	2.20	0.41
7:G:652:ASN:HA	7:G:655:ARG:CZ	2.50	0.41
7:G:671:LEU:HD12	13:S:42:VAL:HG23	2.02	0.41
8:H:5:ASN:CG	8:H:95:LEU:HD13	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:47:GLN:HB3	8:H:48:PRO:HD3	2.00	0.41
8:H:190:LEU:CD1	8:H:195:ARG:O	2.68	0.41
10:P:72:HIS:O	10:P:73:LEU:C	2.61	0.41
10:P:237:LYS:HE2	10:P:322:ILE:O	2.20	0.41
13:S:63:PRO:HB2	13:S:79:LEU:CD1	2.50	0.41
19:a:52:ARG:HG3	19:a:57:VAL:O	2.19	0.41
21:q:69:ASN:CG	21:q:70:GLY:N	2.78	0.41
2:B:99:CYS:SG	4:D:223:HIS:NE2	2.92	0.41
2:B:141:MET:CE	4:D:115:LEU:HB3	2.36	0.41
4:D:240:LEU:HG	4:D:244:ILE:HD11	2.02	0.41
4:D:420:TYR:CD2	15:V:114:TRP:HH2	2.38	0.41
5:E:78:VAL:HG23	5:E:79:LEU:H	1.84	0.41
6:F:126:LYS:HG3	6:F:275:LEU:HB2	2.01	0.41
6:F:299:LEU:C	6:F:299:LEU:CD1	2.91	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
7:G:388:ASN:N	7:G:514:ASN:CB	2.69	0.41
7:G:670:GLU:HB2	13:S:42:VAL:HG23	2.01	0.41
10:P:113:LYS:O	10:P:114:ASP:CB	2.68	0.41
18:Z:134:SER:O	18:Z:138:PHE:N	2.54	0.41
20:b:72:ASP:HB3	20:b:74:LEU:HD12	2.02	0.41
1:A:8:PHE:HB2	24:A:202:3PE:H2D1	2.01	0.41
2:B:179:ARG:NH2	3:C:204:THR:OG1	2.54	0.41
3:C:202:PRO:HD3	11:Q:121:LEU:HD21	2.02	0.41
3:C:219:VAL:HG21	16:W:113:THR:HG21	2.01	0.41
4:D:201:PHE:CB	8:H:32:GLN:HB3	2.50	0.41
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.41
8:H:215:TYR:CZ	8:H:223:PHE:HE2	2.38	0.41
10:P:128:ASN:HD21	10:P:149:PRO:HB3	1.84	0.41
10:P:185:ALA:O	10:P:186:VAL:C	2.64	0.41
10:P:262:THR:HG22	10:P:263:PHE:N	2.35	0.41
15:V:5:LEU:O	15:V:6:LYS:C	2.64	0.41
1:A:87:MET:HE2	1:A:87:MET:HB3	1.74	0.41
2:B:108:ALA:CA	2:B:114:MET:HE3	2.50	0.41
4:D:386:THR:HG22	9:I:118:LEU:CD1	2.50	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
5:E:225:GLU:O	5:E:227:ALA:N	2.53	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	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:567:VAL:HG23	7:G:567:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.41
8:H:96:ILE:HD12	8:H:98:LEU:HD11	2.02	0.41
8:H:197:PRO:HD3	8:H:273:ILE:HG22	2.03	0.41
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.50	0.41
9:I:128:ILE:HG22	9:I:130:ILE:HG23	2.01	0.41
10:P:227:PRO:HB3	10:P:291:TYR:CZ	2.55	0.41
14:T:112:SER:O	14:T:116:VAL:HG23	2.20	0.41
17:X:69:ASN:O	17:X:70:PHE:C	2.63	0.41
20:b:72:ASP:HB3	20:b:74:LEU:CD1	2.50	0.41
1:A:5:THR:OG1	8:H:2:PHE:HE2	2.03	0.41
24:A:201:3PE:H332	20:b:19:LEU:HD21	2.01	0.41
4:D:132:ALA:O	4:D:133:LEU:C	2.64	0.41
4:D:235:ASP:OD2	18:Z:8:GLN:HG3	2.20	0.41
6:F:94:PRO:CG	6:F:97:LEU:HD12	2.45	0.41
6:F:227:PRO:HB3	7:G:95:PRO:HD3	2.02	0.41
6:F:315:LEU:HD22	6:F:363:ILE:HD13	2.02	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
8:H:308:PRO:O	8:H:312:ALA:N	2.53	0.41
9:I:182:GLU:HA	21:q:124:TYR:HD2	1.85	0.41
11:Q:160:TYR:CE2	11:Q:164:PHE:CE2	3.09	0.41
11:Q:160:TYR:CE2	11:Q:164:PHE:CZ	3.09	0.41
13:S:16:LEU:HD11	13:S:19:ILE:HG12	2.01	0.41
16:W:58:THR:O	16:W:59:VAL:C	2.62	0.41
18:Z:125:TYR:C	18:Z:126:GLY:O	2.62	0.41
4:D:158:LEU:HD23	4:D:158:LEU:HA	1.95	0.41
5:E:155:LEU:CD1	5:E:204:ILE:HD13	2.50	0.41
6:F:64:LYS:HE3	6:F:67:GLU:OE1	2.21	0.41
6:F:70:LEU:O	6:F:71:LYS:C	2.63	0.41
6:F:262:PHE:HA	6:F:265:PHE:CD2	2.56	0.41
6:F:379:CYS:SG	25:F:502:SF4:S2	3.19	0.41
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.41
8:H:200:LEU:HD13	8:H:282:TYR:CD1	2.53	0.41
8:H:302:MET:HE3	8:H:302:MET:HB2	1.92	0.41
10:P:357:ARG:NH2	10:P:364:SER:HB3	2.36	0.41
12:R:31:ILE:CG2	12:R:35:GLY:HA2	2.50	0.41
13:S:16:LEU:HD21	13:S:19:ILE:CD1	2.50	0.41
15:V:81:ILE:O	15:V:84:ALA:N	2.53	0.41
16:W:53:MET:O	16:W:103:ARG:HG2	2.20	0.41
17:X:13:LEU:HD13	18:Z:85:GLN:HB2	2.03	0.41
18:Z:116:TRP:CZ2	18:Z:119:PRO:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:55:SER:HB3	19:a:61:TYR:CE2	2.54	0.41
21:q:20:LEU:C	21:q:20:LEU:HD23	2.45	0.41
1:A:77:TRP:HZ2	8:H:100:LEU:HD11	1.86	0.41
2:B:155:PRO:HG2	8:H:58:LYS:HA	2.03	0.41
2:B:199:GLU:O	2:B:200:ALA:C	2.60	0.41
4:D:87:GLN:HG3	4:D:87:GLN:O	2.21	0.41
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.56	0.41
4:D:181:LEU:HD22	4:D:214:TYR:OH	2.21	0.41
4:D:265:ASN:HD21	8:H:277:TYR:HD1	1.68	0.41
4:D:381:HIS:HE1	9:I:161:ALA:O	2.03	0.41
6:F:39:ASP:HA	6:F:261:TRP:CZ2	2.56	0.41
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.41
6:F:329:LYS:HE3	6:F:329:LYS:HB3	1.93	0.41
7:G:160:VAL:CG1	7:G:161:GLU:N	2.83	0.41
7:G:251:ILE:HG22	7:G:252:ASP:N	2.35	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.41
8:H:35:LYS:HE2	9:I:83:THR:OG1	2.20	0.41
8:H:303:TRP:HA	20:b:29:ALA:HB2	2.03	0.41
10:P:270:ARG:O	10:P:375:VAL:N	2.37	0.41
10:P:286:ARG:NH1	10:P:358:THR:HG22	2.36	0.41
11:Q:78:ARG:O	11:Q:80:PHE:CD1	2.74	0.41
11:Q:112:MET:CE	21:q:126:PRO:HB3	2.51	0.41
14:T:104:PHE:O	14:T:110:LEU:HB2	2.20	0.41
14:T:122:MET:HG3	14:T:144:ILE:HG21	2.02	0.41
14:T:140:CYS:O	14:T:141:PRO:C	2.59	0.41
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.36	0.41
17:X:86:TRP:CZ2	19:a:64:LYS:CA	3.03	0.41
18:Z:23:ARG:CG	18:Z:25:LEU:HD13	2.51	0.41
18:Z:61:LEU:O	18:Z:65:LEU:N	2.47	0.41
18:Z:134:SER:C	18:Z:136:ALA:N	2.76	0.41
19:a:34:LYS:O	19:a:35:GLU:C	2.63	0.41
20:b:66:VAL:HG13	20:b:66:VAL:O	2.20	0.41
20:b:80:TRP:O	20:b:81:LEU:C	2.64	0.41
21:q:75:TRP:CE3	21:q:75:TRP:HA	2.55	0.41
22:r:58:ASP:OD1	22:r:58:ASP:O	2.39	0.41
1:A:87:MET:HE1	8:H:309:ILE:CD1	2.46	0.41
2:B:110:PRO:O	9:I:83:THR:HG22	2.21	0.41
2:B:137:LEU:HD21	2:B:145:LEU:HD23	2.02	0.41
3:C:151:PRO:HG2	16:W:23:ILE:HG23	2.03	0.41
4:D:128:THR:N	4:D:131:GLN:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:140:ASP:OD1	4:D:457:VAL:HG11	2.20	0.41
4:D:209:LYS:CE	22:r:25:GLN:O	2.69	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
7:G:50:LEU:HB2	7:G:91:ALA:O	2.21	0.41
7:G:62:ARG:HD2	7:G:65:TYR:CD2	2.29	0.41
10:P:76:MET:HE2	10:P:76:MET:HB3	1.92	0.41
10:P:110:ALA:HB1	10:P:148:ILE:HD12	2.02	0.41
10:P:227:PRO:HB2	10:P:298:TYR:CZ	2.56	0.41
11:Q:71:HIS:NE2	11:Q:120:PRO:HD2	2.36	0.41
12:R:40:GLU:HA	12:R:45:ARG:NH1	2.35	0.41
24:A:201:3PE:H391	20:b:23:PHE:CE1	2.51	0.41
2:B:101:ALA:O	2:B:102:VAL:C	2.64	0.41
2:B:170:TYR:HE2	4:D:135:TYR:N	2.19	0.41
3:C:110:LEU:HD22	3:C:155:ILE:HD11	2.02	0.41
4:D:128:THR:HG22	4:D:131:GLN:CD	2.45	0.41
4:D:236:LEU:HD22	4:D:240:LEU:CD2	2.41	0.41
4:D:305:THR:OG1	4:D:306:GLN:N	2.54	0.41
4:D:378:LEU:HD22	7:G:126:LEU:HB2	2.03	0.41
5:E:60:LYS:O	5:E:61:ARG:C	2.62	0.41
5:E:67:LYS:HB3	5:E:67:LYS:HE2	1.86	0.41
6:F:109:ARG:HH21	6:F:239:PRO:CD	2.33	0.41
6:F:209:GLU:N	28:F:501:FMN:O2'	2.53	0.41
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:403:VAL:O	7:G:476:LEU:HD12	2.21	0.41
7:G:409:PHE:O	7:G:694:PHE:HD1	2.04	0.41
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.41
7:G:545:LEU:HD21	7:G:547:LEU:CD2	2.50	0.41
8:H:69:SER:O	8:H:73:ILE:HB	2.21	0.41
8:H:121:TRP:CE3	8:H:121:TRP:C	2.99	0.41
9:I:96:ARG:NH1	9:I:208:ASP:OD1	2.50	0.41
9:I:117:LYS:HA	9:I:130:ILE:HD11	2.03	0.41
9:I:135:ARG:O	9:I:135:ARG:CG	2.69	0.41
9:I:197:TRP:O	9:I:201:ILE:N	2.51	0.41
10:P:88:VAL:HG12	10:P:92:MET:HE2	2.03	0.41
10:P:141:PHE:CD1	10:P:145:PHE:HE2	2.39	0.41
10:P:225:ALA:HB3	10:P:291:TYR:CE2	2.55	0.41
11:Q:69:GLU:C	11:Q:72:ILE:HG22	2.44	0.41
11:Q:126:LEU:CD1	11:Q:137:PHE:CE2	3.03	0.41
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.41
13:S:35:ASP:HA	13:S:38:VAL:HG22	2.03	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:111:ASP:O	14:T:112:SER:C	2.64	0.41
14:T:142:GLN:O	14:T:143:GLU:C	2.64	0.41
16:W:31:ALA:C	16:W:33:ARG:N	2.74	0.41
17:X:21:SER:O	17:X:24:VAL:HG22	2.21	0.41
17:X:130:LYS:HG3	20:b:59:ASP:HA	2.03	0.41
17:X:134:ASP:OD1	17:X:134:ASP:C	2.63	0.41
26:B:303:PC1:C38	8:H:57:MET:HE2	2.50	0.41
4:D:181:LEU:HD11	4:D:210:MET:HB3	2.02	0.41
4:D:253:LEU:HD23	4:D:254:ARG:HH22	1.86	0.41
4:D:341:LEU:O	18:Z:19:ILE:HD11	2.21	0.41
5:E:198:LYS:HA	5:E:201:GLU:HB3	2.02	0.41
6:F:169:LEU:O	6:F:173:ILE:N	2.49	0.41
7:G:82:ILE:HD13	7:G:100:TRP:CZ3	2.55	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:308:ARG:HG3	7:G:581:ASP:HA	2.02	0.41
7:G:330:LEU:HD12	7:G:544:MET:CE	2.50	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.02	0.41
7:G:506:VAL:CG2	7:G:510:TRP:HB3	2.51	0.41
7:G:611:THR:HG23	11:Q:104:ARG:O	2.20	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.20	0.41
8:H:17:MET:HG2	8:H:228:TYR:CB	2.50	0.41
8:H:304:HIS:O	8:H:308:PRO:CD	2.64	0.41
15:V:9:THR:OG1	15:V:14:LEU:O	2.39	0.41
15:V:24:LEU:HD23	15:V:24:LEU:HA	1.90	0.41
21:q:66:THR:O	21:q:67:GLU:HG3	2.21	0.41
3:C:87:ILE:HG21	3:C:95:THR:HG21	2.02	0.40
3:C:155:ILE:O	3:C:158:VAL:N	2.54	0.40
4:D:265:ASN:OD1	4:D:266:ARG:N	2.54	0.40
4:D:275:ILE:HG22	4:D:450:ILE:HD11	2.02	0.40
5:E:77:ALA:C	5:E:80:PRO:HD2	2.46	0.40
6:F:119:GLU:CD	6:F:127:ASP:OD2	2.65	0.40
6:F:313:ASN:O	6:F:358:ASP:HA	2.21	0.40
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.55	0.40
7:G:598:ASN:ND2	7:G:600:GLU:CD	2.79	0.40
8:H:201:THR:O	8:H:202:GLU:C	2.62	0.40
8:H:245:PRO:HG2	8:H:255:TYR:CZ	2.55	0.40
8:H:248:TYR:O	8:H:249:ILE:C	2.62	0.40
24:H:402:3PE:H322	9:I:63:TRP:HZ3	1.85	0.40
10:P:64:PHE:CE2	10:P:242:VAL:HG22	2.56	0.40
10:P:170:LEU:HG	10:P:171:ASN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:234:LYS:O	10:P:234:LYS:HG3	2.21	0.40
11:Q:85:ASN:C	11:Q:87:MET:N	2.77	0.40
17:X:28:ALA:HB3	17:X:71:PHE:HE1	1.86	0.40
17:X:89:LEU:HD21	17:X:95:GLN:HB3	2.02	0.40
19:a:41:VAL:O	19:a:42:GLN:C	2.64	0.40
24:A:202:3PE:H3H1	8:H:76:THR:OG1	2.22	0.40
2:B:110:PRO:HG3	8:H:32:GLN:O	2.22	0.40
2:B:122:ARG:HH22	4:D:90:ALA:CB	2.30	0.40
6:F:45:LEU:HD13	6:F:129:GLU:OE1	2.20	0.40
6:F:61:ASP:O	6:F:140:GLU:OE1	2.40	0.40
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.40
6:F:280:GLY:O	6:F:356:VAL:HB	2.21	0.40
28:F:501:FMN:HM73	28:F:501:FMN:HM81	1.92	0.40
7:G:49:VAL:HG11	7:G:80:VAL:HG21	2.02	0.40
7:G:557:ARG:HG3	7:G:579:MET:HB2	2.03	0.40
7:G:557:ARG:HD3	21:q:144:TYR:CE2	2.56	0.40
8:H:142:TYR:CE2	8:H:289:LEU:HD12	2.57	0.40
8:H:142:TYR:O	8:H:146:MET:HG3	2.22	0.40
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.21	0.40
11:Q:69:GLU:HG2	11:Q:73:LYS:HG3	2.02	0.40
11:Q:81:VAL:O	11:Q:81:VAL:CG1	2.69	0.40
11:Q:156:LYS:HE2	11:Q:156:LYS:HB3	1.84	0.40
12:R:54:GLU:O	21:q:127:TYR:OH	2.24	0.40
14:T:105:MET:HE3	14:T:139:MET:HE2	2.03	0.40
17:X:129:THR:HB	20:b:68:SER:O	2.21	0.40
18:Z:10:MET:O	18:Z:11:PRO:C	2.63	0.40
20:b:74:LEU:HD12	20:b:74:LEU:N	2.35	0.40
4:D:207:ARG:HA	4:D:210:MET:HE3	2.03	0.40
4:D:410:TYR:HB3	4:D:423:LYS:HB3	2.03	0.40
6:F:128:ARG:HA	6:F:131:MET:CE	2.51	0.40
6:F:293:SER:C	6:F:336:LEU:HD13	2.45	0.40
6:F:329:LYS:O	6:F:330:SER:C	2.65	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
6:F:425:CYS:SG	25:F:502:SF4:S4	3.20	0.40
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.40
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.40
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.40
7:G:386:LEU:O	7:G:388:ASN:ND2	2.54	0.40
7:G:546:PHE:N	7:G:546:PHE:CD1	2.89	0.40
8:H:52:ALA:C	8:H:54:LYS:N	2.78	0.40
8:H:103:LEU:O	8:H:106:LEU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:197:PRO:O	8:H:279:ARG:HA	2.22	0.40
10:P:41:ILE:O	10:P:42:PRO:C	2.64	0.40
16:W:60:LYS:HZ3	16:W:64:ASP:CG	2.30	0.40
1:A:7:ILE:O	1:A:11:ILE:HG13	2.20	0.40
1:A:76:PRO:HG2	8:H:160:TYR:CZ	2.57	0.40
5:E:70:PRO:O	5:E:73:HIS:HB2	2.21	0.40
5:E:110:ARG:CZ	6:F:219:LYS:HG2	2.51	0.40
6:F:258:GLY:O	6:F:262:PHE:HD1	2.03	0.40
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.55	0.40
8:H:65:THR:HG22	8:H:67:SER:N	2.37	0.40
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.50	0.40
8:H:199:ASP:O	8:H:279:ARG:HD2	2.22	0.40
8:H:314:VAL:HG23	8:H:314:VAL:O	2.22	0.40
9:I:76:TYR:HE1	9:I:79:ARG:CZ	2.34	0.40
14:T:126:PHE:CE1	14:T:148:ILE:HG21	2.56	0.40
15:V:51:ILE:H	15:V:51:ILE:HG13	1.77	0.40
15:V:114:TRP:CE3	15:V:114:TRP:HA	2.57	0.40
17:X:7:LEU:HD13	18:Z:87:LEU:HD12	2.03	0.40
17:X:56:CYS:C	17:X:58:LYS:N	2.78	0.40
19:a:31:ASN:CG	19:a:59:ARG:HH22	2.28	0.40
19:a:43:TYR:O	19:a:47:LEU:HD13	2.22	0.40
20:b:32:MET:N	20:b:33:PRO:CD	2.84	0.40
22:r:18:GLN:O	22:r:20:LEU:HG	2.22	0.40
1:A:105:GLU:O	1:A:109:LYS:N	2.55	0.40
2:B:137:LEU:CD2	2:B:145:LEU:HD23	2.51	0.40
2:B:170:TYR:CE1	4:D:127:LYS:HD3	2.57	0.40
2:B:219:LYS:HD2	2:B:223:ARG:NH2	2.37	0.40
5:E:247:GLY:O	6:F:79:GLU:CD	2.65	0.40
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.51	0.40
6:F:208:GLU:OE1	6:F:210:THR:N	2.53	0.40
6:F:424:ILE:CA	7:G:76:ARG:NH1	2.82	0.40
7:G:51:GLN:HE22	11:Q:158:LYS:HB2	1.85	0.40
24:H:402:3PE:H261	24:H:402:3PE:H232	1.94	0.40
10:P:175:LYS:HB3	10:P:175:LYS:HE2	1.89	0.40
14:T:132:ASP:HA	16:W:40:ARG:HH22	1.87	0.40
15:V:44:TYR:HE2	15:V:91:ALA:HA	1.87	0.40
16:W:62:GLY:O	16:W:65:LYS:N	2.54	0.40
21:q:65:THR:HG21	21:q:68:MET:HB3	2.03	0.40
23:s:94:GLN:HA	23:s:95:PRO:HD3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	86/115 (75%)	84 (98%)	2 (2%)	0	100	100
2	B	153/224 (68%)	142 (93%)	10 (6%)	1 (1%)	18	51
3	C	196/263 (74%)	188 (96%)	8 (4%)	0	100	100
4	D	380/463 (82%)	358 (94%)	22 (6%)	0	100	100
5	E	208/248 (84%)	192 (92%)	16 (8%)	0	100	100
6	F	424/464 (91%)	403 (95%)	21 (5%)	0	100	100
7	G	685/727 (94%)	637 (93%)	48 (7%)	0	100	100
8	H	308/318 (97%)	280 (91%)	28 (9%)	0	100	100
9	I	168/212 (79%)	152 (90%)	16 (10%)	0	100	100
10	P	337/377 (89%)	311 (92%)	26 (8%)	0	100	100
11	Q	114/175 (65%)	102 (90%)	12 (10%)	0	100	100
12	R	81/116 (70%)	72 (89%)	9 (11%)	0	100	100
13	S	81/99 (82%)	72 (89%)	9 (11%)	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
17	X	140/172 (81%)	124 (89%)	16 (11%)	0	100	100
18	Z	136/144 (94%)	127 (93%)	8 (6%)	1 (1%)	18	51
19	a	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
20	b	78/84 (93%)	70 (90%)	8 (10%)	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	4153/5036 (82%)	3851 (93%)	300 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	82/104 (79%)	81 (99%)	1 (1%)	63	73
2	B	131/185 (71%)	129 (98%)	2 (2%)	57	71
3	C	181/227 (80%)	181 (100%)	0	100	100
4	D	332/395 (84%)	331 (100%)	1 (0%)	86	83
5	E	182/206 (88%)	180 (99%)	2 (1%)	65	74
6	F	341/370 (92%)	340 (100%)	1 (0%)	86	83
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	275/280 (98%)	274 (100%)	1 (0%)	84	81
9	I	146/178 (82%)	146 (100%)	0	100	100
10	P	296/325 (91%)	295 (100%)	1 (0%)	86	83
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	71
14	T	69/135 (51%)	69 (100%)	0	100	100
15	V	100/102 (98%)	98 (98%)	2 (2%)	48	67
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	r	76/96 (79%)	75 (99%)	1 (1%)	61	72
23	s	23/95 (24%)	23 (100%)	0	100	100
All	All	3654/4292 (85%)	3638 (100%)	16 (0%)	81	81

All (16) 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	127	LYS
5	E	99	LYS
5	E	200	ILE
6	F	137	LYS
7	G	271	MET
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
22	r	91	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) 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	92	HIS
4	D	112	HIS
4	D	117	HIS
4	D	147	ASN
4	D	149	GLN

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Mol	Chain	Res	Type
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
5	E	68	ASN
5	E	132	GLN
5	E	152	GLN
5	E	188	ASN
5	E	245	GLN
6	F	116	ASN
6	F	168	ASN
6	F	244	ASN
6	F	270	ASN
6	F	277	ASN
6	F	346	GLN
6	F	393	ASN
6	F	436	GLN
7	G	51	GLN
7	G	66	HIS
7	G	74	ASN
7	G	101	ASN
7	G	140	GLN
7	G	365	ASN
7	G	388	ASN
7	G	495	ASN
7	G	571	HIS
7	G	572	HIS
7	G	605	GLN
7	G	652	ASN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	171	HIS
8	H	194	ASN
8	H	284	GLN
8	H	287	HIS
8	H	292	ASN
9	I	180	HIS
10	P	71	ASN

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Mol	Chain	Res	Type
10	P	79	GLN
10	P	166	HIS
10	P	251	ASN
10	P	285	HIS
10	P	323	HIS
11	Q	88	GLN
13	S	22	HIS
13	S	31	GLN
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	143	HIS
18	Z	24	ASN
18	Z	90	ASN
20	b	46	ASN
21	q	17	HIS
21	q	59	HIS
21	q	91	HIS
21	q	135	HIS
22	r	18	GLN
22	r	21	GLN
22	r	29	GLN
23	s	76	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	3PE	H	402	-	50,50,50	0.91	2 (4%)	53,55,55	1.03	2 (3%)
26	PC1	B	303	-	42,42,53	1.05	2 (4%)	48,50,61	1.01	3 (6%)
28	FMN	F	501	-	33,33,33	1.41	5 (15%)	48,50,50	1.19	6 (12%)
33	CDL	q	201	-	56,56,99	1.19	4 (7%)	62,68,111	1.20	6 (9%)
25	SF4	F	502	6	0,12,12	-	-	-	-	-
26	PC1	B	302	-	34,34,53	1.13	2 (5%)	40,42,61	1.11	3 (7%)
27	FES	E	301	5	0,4,4	-	-	-	-	-
29	UQ9	H	401	-	35,35,58	0.79	2 (5%)	42,45,73	0.47	0
32	EHZ	W	201	-	30,34,37	1.80	7 (23%)	40,44,47	1.41	5 (12%)
25	SF4	G	801	7	0,12,12	-	-	-	-	-
24	3PE	A	201	-	41,41,50	1.00	2 (4%)	44,46,55	1.09	2 (4%)
25	SF4	I	301	9	0,12,12	-	-	-	-	-
25	SF4	I	302	9	0,12,12	-	-	-	-	-
24	3PE	A	202	-	47,47,50	0.93	2 (4%)	50,52,55	1.11	3 (6%)
30	NDP	P	401	-	49,52,52	1.20	6 (12%)	66,80,80	1.68	12 (18%)
25	SF4	G	802	7	0,12,12	-	-	-	-	-
25	SF4	B	301	2	0,12,12	-	-	-	-	-
27	FES	G	803	7	0,4,4	-	-	-	-	-

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
24	3PE	H	402	-	-	17/54/54/54	-
26	PC1	B	303	-	-	14/46/46/57	-
28	FMN	F	501	-	-	4/18/18/18	0/3/3/3
33	CDL	q	201	-	-	18/67/67/110	-
25	SF4	F	502	6	-	-	0/6/5/5
26	PC1	B	302	-	-	13/38/38/57	-
29	UQ9	H	401	-	-	16/30/54/81	0/1/1/1
27	FES	E	301	5	-	-	0/1/1/1
32	EHZ	W	201	-	-	26/42/42/45	-
25	SF4	G	801	7	-	-	0/6/5/5
24	3PE	A	201	-	-	12/45/45/54	-
25	SF4	I	301	9	-	-	0/6/5/5
25	SF4	I	302	9	-	-	0/6/5/5
24	3PE	A	202	-	-	13/51/51/54	-
30	NDP	P	401	-	-	6/34/77/77	0/5/5/5
25	SF4	G	802	7	-	-	0/6/5/5
25	SF4	B	301	2	-	-	0/6/5/5
27	FES	G	803	7	-	-	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	201	EHZ	C15-N2	5.44	1.45	1.33
32	W	201	EHZ	C12-N1	5.25	1.45	1.33
28	F	501	FMN	C9A-C5A	4.81	1.49	1.41
33	q	201	CDL	OA8-CA7	4.27	1.45	1.33
24	A	201	3PE	O31-C31	4.27	1.45	1.33
30	P	401	NDP	C5A-C4A	4.22	1.46	1.39
26	B	303	PC1	O31-C31	4.19	1.45	1.33
26	B	303	PC1	O21-C21	4.18	1.46	1.34
33	q	201	CDL	OB8-CB7	4.16	1.45	1.33
26	B	302	PC1	O31-C31	4.16	1.45	1.33
24	H	402	3PE	O21-C21	4.14	1.46	1.34
24	A	202	3PE	O31-C31	4.13	1.45	1.33
24	H	402	3PE	O31-C31	4.11	1.45	1.33
24	A	202	3PE	O21-C21	4.09	1.45	1.34
33	q	201	CDL	OA6-CA5	4.02	1.45	1.34
24	A	201	3PE	O21-C21	4.00	1.45	1.34
26	B	302	PC1	O21-C21	3.95	1.45	1.34
33	q	201	CDL	OB6-CB5	3.89	1.45	1.34
30	P	401	NDP	C6N-C5N	3.25	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	501	FMN	C8-C7	3.13	1.48	1.40
28	F	501	FMN	C4-N3	-2.76	1.33	1.38
32	W	201	EHZ	P1-O7	2.66	1.65	1.54
29	H	401	UQ9	C3-C2	-2.63	1.41	1.48
29	H	401	UQ9	C4-C5	-2.52	1.41	1.48
30	P	401	NDP	C5A-N7A	-2.46	1.34	1.39
32	W	201	EHZ	O4-C15	-2.41	1.18	1.23
32	W	201	EHZ	O3-C12	-2.40	1.18	1.23
30	P	401	NDP	C8A-N7A	2.39	1.36	1.31
30	P	401	NDP	C5A-C6A	2.38	1.47	1.41
28	F	501	FMN	C5A-N5	-2.33	1.35	1.39
32	W	201	EHZ	C9-S1	2.27	1.81	1.76
32	W	201	EHZ	P1-OP3	-2.25	1.46	1.54
28	F	501	FMN	C4A-N5	2.11	1.34	1.30
30	P	401	NDP	C4A-N9A	-2.02	1.33	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	P	401	NDP	C5A-C4A-N3A	-5.96	118.98	126.75
32	W	201	EHZ	C8-C9-S1	4.97	119.77	113.63
30	P	401	NDP	N3A-C4A-N9A	4.74	134.90	127.08
33	q	201	CDL	OA6-CA5-C11	4.21	120.58	111.50
24	H	402	3PE	O21-C21-C22	4.13	120.41	111.50
30	P	401	NDP	PN-O3-PA	-4.03	118.99	132.83
24	A	202	3PE	O21-C21-C22	4.02	120.16	111.50
26	B	303	PC1	O21-C21-C22	3.96	120.03	111.50
24	A	201	3PE	O21-C21-C22	3.92	119.95	111.50
30	P	401	NDP	C2A-N3A-C4A	3.80	120.73	111.75
26	B	302	PC1	O21-C21-C22	3.67	119.41	111.50
33	q	201	CDL	OB6-CB5-C51	3.53	119.11	111.50
30	P	401	NDP	N3A-C2A-N1A	-3.18	123.62	128.60
30	P	401	NDP	C4A-C5A-N7A	-3.15	106.78	110.62
30	P	401	NDP	C4A-N9A-C8A	2.94	108.92	105.73
24	A	202	3PE	O31-C31-C32	2.87	120.91	111.91
26	B	302	PC1	O31-C31-C32	2.82	120.77	111.91
33	q	201	CDL	OA8-CA7-C31	2.80	120.68	111.91
30	P	401	NDP	C5A-N7A-C8A	2.76	107.42	103.51
26	B	302	PC1	C2-O21-C21	-2.66	111.24	117.79
24	A	201	3PE	O31-C31-C32	2.64	120.19	111.91
28	F	501	FMN	C4A-C10-N1	-2.52	118.88	124.73
24	H	402	3PE	O31-C31-C32	2.50	119.76	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	F	501	FMN	O4-C4-C4A	-2.50	119.97	126.60
32	W	201	EHZ	C10-S1-C9	2.45	109.50	101.87
32	W	201	EHZ	OP3-P1-O9	-2.44	101.12	110.68
33	q	201	CDL	OB8-CB7-C71	2.44	119.56	111.91
26	B	303	PC1	O31-C31-C32	2.38	119.37	111.91
30	P	401	NDP	C2B-C1B-N9A	-2.34	109.58	113.53
28	F	501	FMN	C4-C4A-N5	2.32	121.54	118.23
30	P	401	NDP	N9A-C8A-N7A	-2.31	110.75	113.91
32	W	201	EHZ	O2-C9-S1	-2.31	119.62	122.61
30	P	401	NDP	C6A-C5A-N7A	2.20	136.11	132.02
33	q	201	CDL	CB4-OB6-CB5	-2.15	112.49	117.79
26	B	303	PC1	C2-O21-C21	-2.15	112.50	117.79
33	q	201	CDL	CA4-OA6-CA5	-2.10	112.62	117.79
30	P	401	NDP	C3D-C2D-C1D	2.09	105.39	101.43
28	F	501	FMN	C4A-C4-N3	2.06	118.43	113.19
28	F	501	FMN	C4A-C10-N10	2.06	119.48	116.48
28	F	501	FMN	C10-N1-C2	2.03	120.97	116.90
32	W	201	EHZ	C5-C6-C7	-2.03	109.00	114.85
24	A	202	3PE	O21-C21-O22	-2.01	118.84	123.70

There are no chirality outliers.

All (139) 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	A	202	3PE	C1-O11-P-O14
24	A	202	3PE	C11-O13-P-O14
24	A	202	3PE	O22-C21-O21-C2
24	A	202	3PE	C22-C21-O21-C2
24	H	402	3PE	C1-O11-P-O14
24	H	402	3PE	C11-O13-P-O12
26	B	302	PC1	C11-O13-P-O14
26	B	302	PC1	C22-C21-O21-C2
26	B	303	PC1	C1-O11-P-O14
26	B	303	PC1	C22-C21-O21-C2
28	F	501	FMN	C5'-O5'-P-O2P
28	F	501	FMN	C5'-O5'-P-O3P
29	H	401	UQ9	C22-C23-C24-C26
29	H	401	UQ9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
29	H	401	UQ9	C20-C19-C21-C22
29	H	401	UQ9	C18-C19-C21-C22
29	H	401	UQ9	C15-C14-C16-C17
29	H	401	UQ9	C13-C14-C16-C17
29	H	401	UQ9	C12-C13-C14-C16
29	H	401	UQ9	C12-C13-C14-C15
29	H	401	UQ9	C11-C12-C13-C14
30	P	401	NDP	C5D-O5D-PN-O1N
32	W	201	EHZ	O1-C7-C8-C9
32	W	201	EHZ	C15-C16-C17-C18
32	W	201	EHZ	C15-C16-C17-C19
32	W	201	EHZ	C15-C16-C17-C20
32	W	201	EHZ	O5-C16-C17-C18
32	W	201	EHZ	O5-C16-C17-C19
32	W	201	EHZ	O5-C16-C17-C20
32	W	201	EHZ	C16-C17-C20-O6
32	W	201	EHZ	C19-C17-C20-O6
33	q	201	CDL	CA2-OA2-PA1-OA4
33	q	201	CDL	OA7-CA5-OA6-CA4
33	q	201	CDL	C11-CA5-OA6-CA4
33	q	201	CDL	CB2-OB2-PB2-OB3
26	B	303	PC1	O32-C31-O31-C3
24	A	201	3PE	O22-C21-O21-C2
26	B	302	PC1	O22-C21-O21-C2
26	B	303	PC1	O22-C21-O21-C2
26	B	303	PC1	C32-C31-O31-C3
24	H	402	3PE	C32-C31-O31-C3
24	A	202	3PE	O32-C31-O31-C3
24	H	402	3PE	O32-C31-O31-C3
24	A	202	3PE	C32-C31-O31-C3
33	q	201	CDL	C31-CA7-OA8-CA6
24	H	402	3PE	C22-C21-O21-C2
24	H	402	3PE	O22-C21-O21-C2
33	q	201	CDL	OA9-CA7-OA8-CA6
29	H	401	UQ9	C9-C11-C12-C13
29	H	401	UQ9	C17-C18-C19-C20
29	H	401	UQ9	C17-C18-C19-C21
26	B	302	PC1	C11-C12-N-C13
29	H	401	UQ9	C19-C21-C22-C23
32	W	201	EHZ	C2-C3-C4-C5
24	H	402	3PE	C11-O13-P-O11
26	B	302	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
26	B	302	PC1	C1-O11-P-O13
33	q	201	CDL	CA2-OA2-PA1-OA5
26	B	302	PC1	C11-C12-N-C14
24	H	402	3PE	C32-C33-C34-C35
32	W	201	EHZ	C18-C17-C20-O6
32	W	201	EHZ	C13-C14-N2-C15
32	W	201	EHZ	C5-C6-C7-O1
32	W	201	EHZ	C1-C2-C3-C4
26	B	302	PC1	C11-C12-N-C15
33	q	201	CDL	C13-C14-C15-C16
24	H	402	3PE	C1-O11-P-O13
26	B	303	PC1	C1-O11-P-O13
33	q	201	CDL	C14-C15-C16-C17
32	W	201	EHZ	C21-C1-C2-C3
24	A	202	3PE	C3-C2-O21-C21
24	A	202	3PE	C2-C1-O11-P
28	F	501	FMN	C5'-O5'-P-O1P
24	H	402	3PE	C3B-C3C-C3D-C3E
32	W	201	EHZ	C5-C6-C7-C8
29	H	401	UQ9	C14-C16-C17-C18
26	B	302	PC1	C2-C1-O11-P
32	W	201	EHZ	C3-C4-C5-C6
24	A	201	3PE	C1-C2-C3-O31
24	A	202	3PE	C2B-C2C-C2D-C2E
32	W	201	EHZ	O2-C9-S1-C10
26	B	303	PC1	C38-C39-C3A-C3B
24	A	202	3PE	C2C-C2D-C2E-C2F
30	P	401	NDP	C2B-O2B-P2B-O1X
32	W	201	EHZ	C8-C9-S1-C10
32	W	201	EHZ	C12-C13-C14-N2
26	B	302	PC1	C31-C32-C33-C34
30	P	401	NDP	PN-O3-PA-O2A
30	P	401	NDP	O4D-C1D-N1N-C6N
33	q	201	CDL	CB4-CB3-OB5-PB2
24	H	402	3PE	C1-O11-P-O12
24	H	402	3PE	C11-O13-P-O14
26	B	302	PC1	C11-O13-P-O12
26	B	302	PC1	C1-O11-P-O14
26	B	303	PC1	C1-O11-P-O12
32	W	201	EHZ	C6-C7-C8-C9
28	F	501	FMN	N10-C1'-C2'-O2'
29	H	401	UQ9	C12-C11-C9-C10

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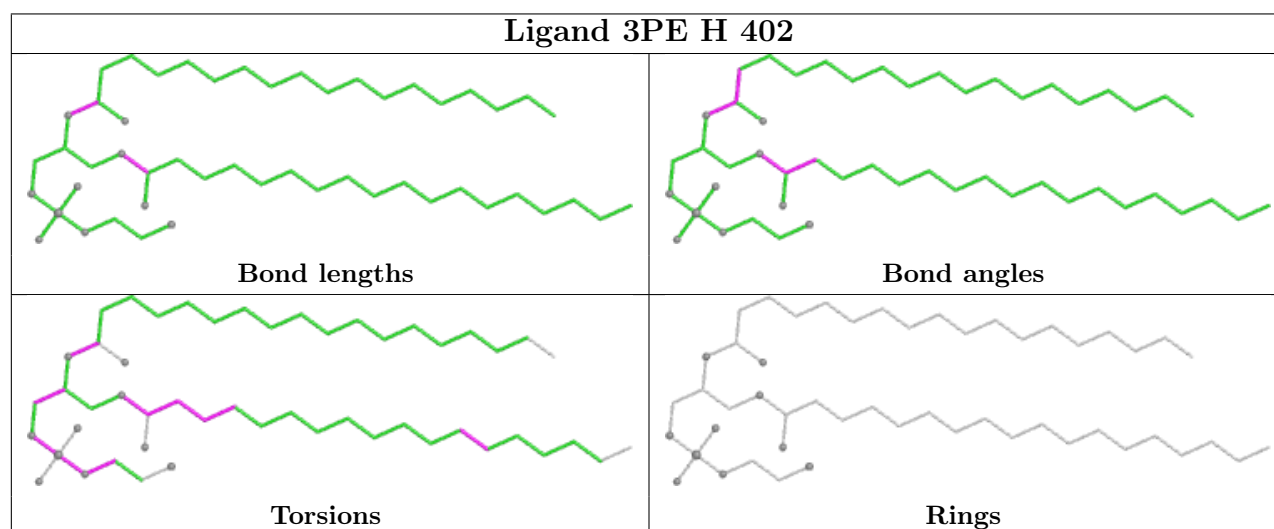
Mol	Chain	Res	Type	Atoms
26	B	303	PC1	C11-C12-N-C14
32	W	201	EHZ	O3-C12-C13-C14
24	A	201	3PE	O21-C2-C3-O31
24	A	201	3PE	C1-O11-P-O13
24	A	202	3PE	C11-O13-P-O11
33	q	201	CDL	CB3-OB5-PB2-OB2
32	W	201	EHZ	C2-C1-C21-C22
32	W	201	EHZ	N1-C12-C13-C14
29	H	401	UQ9	C12-C11-C9-C8
33	q	201	CDL	C71-CB7-OB8-CB6
24	A	202	3PE	C31-C32-C33-C34
26	B	303	PC1	C2-C1-O11-P
24	H	402	3PE	O11-C1-C2-C3
24	A	201	3PE	C23-C24-C25-C26
33	q	201	CDL	C15-C16-C17-C18
33	q	201	CDL	OB9-CB7-OB8-CB6
30	P	401	NDP	PN-O3-PA-O1A
24	A	201	3PE	C39-C3A-C3B-C3C
26	B	303	PC1	C11-C12-N-C13
24	A	201	3PE	C35-C36-C37-C38
24	H	402	3PE	C31-C32-C33-C34
32	W	201	EHZ	C10-C11-N1-C12
26	B	303	PC1	C3A-C3B-C3C-C3D
26	B	303	PC1	C11-C12-N-C15
30	P	401	NDP	C5D-O5D-PN-O3
24	A	202	3PE	C37-C38-C39-C3A
33	q	201	CDL	C18-C19-C20-C21
33	q	201	CDL	CB3-OB5-PB2-OB3
24	A	201	3PE	C25-C26-C27-C28
24	H	402	3PE	C12-C11-O13-P
33	q	201	CDL	C12-C11-CA5-OA6
32	W	201	EHZ	S1-C10-C11-N1
33	q	201	CDL	C12-C11-CA5-OA7
24	H	402	3PE	O31-C31-C32-C33
26	B	303	PC1	C3F-C3G-C3H-C3I
24	H	402	3PE	O32-C31-C32-C33
26	B	302	PC1	C33-C34-C35-C36

There are no ring outliers.

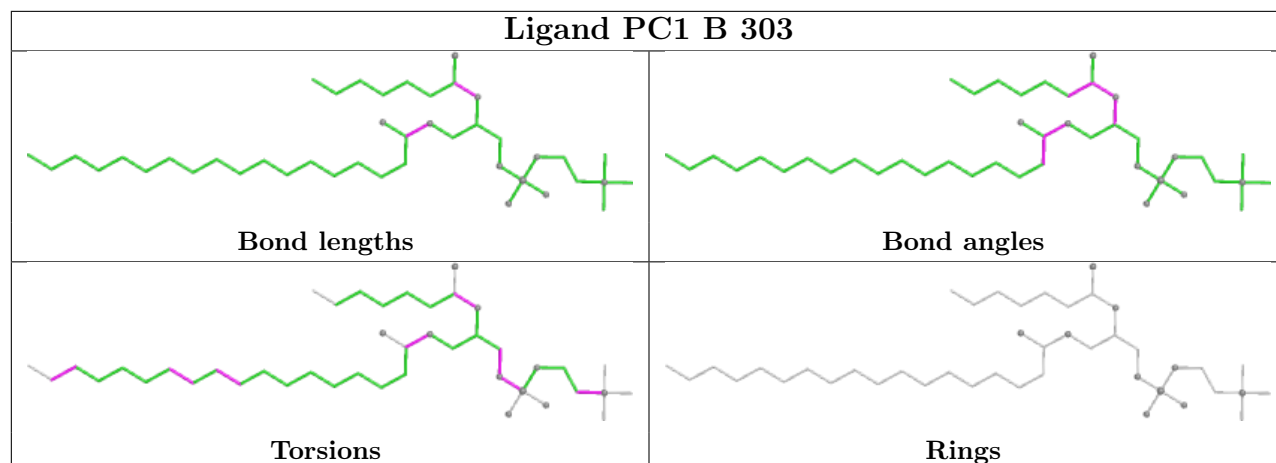
16 monomers are involved in 143 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	H	402	3PE	11	0
26	B	303	PC1	16	0
28	F	501	FMN	3	0
33	q	201	CDL	16	0
25	F	502	SF4	11	0
26	B	302	PC1	9	0
27	E	301	FES	3	0
29	H	401	UQ9	10	0
24	A	201	3PE	15	0
25	I	301	SF4	6	0
25	I	302	SF4	2	0
24	A	202	3PE	13	0
30	P	401	NDP	6	0
25	G	802	SF4	8	0
25	B	301	SF4	10	0
27	G	803	FES	4	0

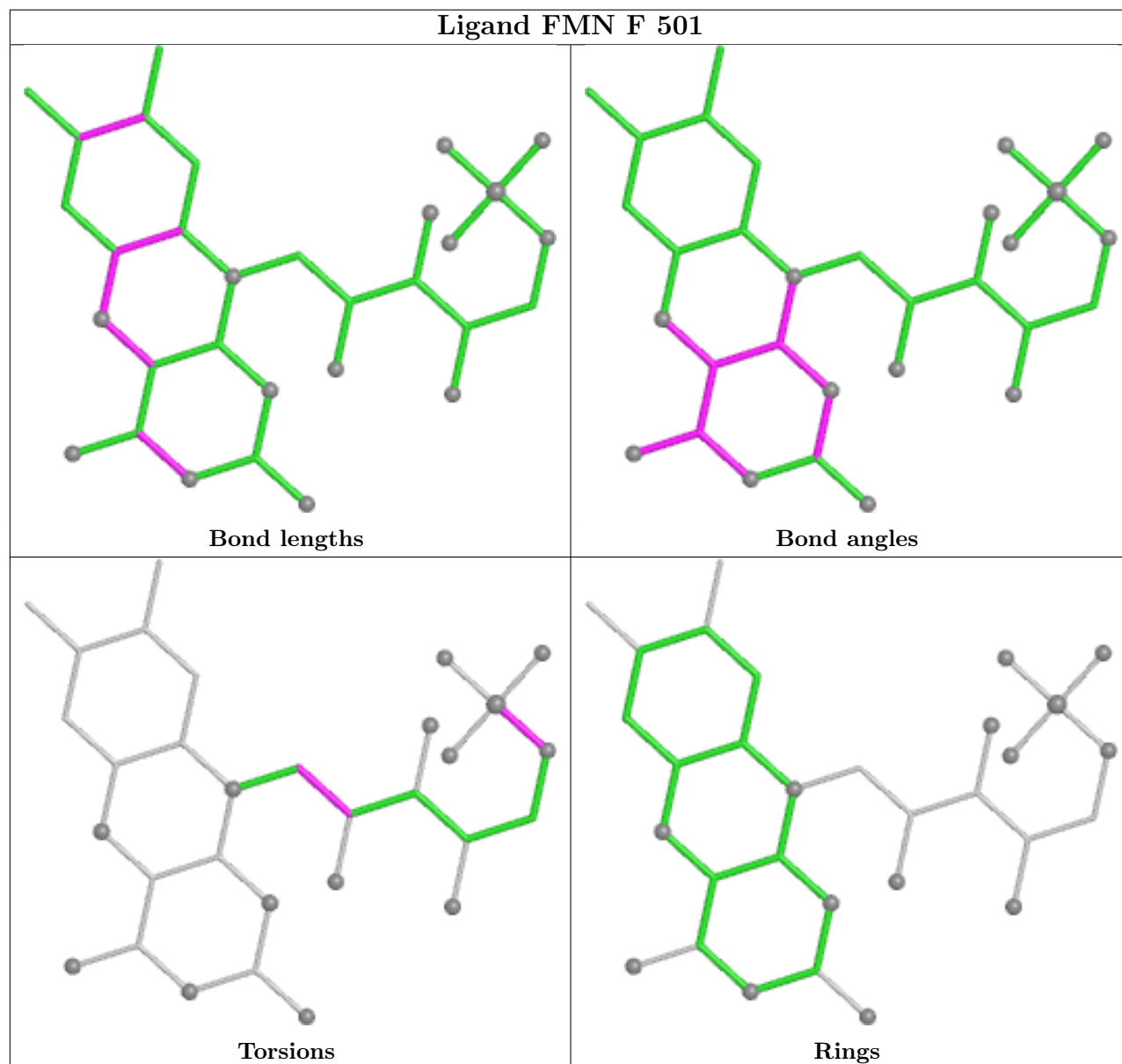
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

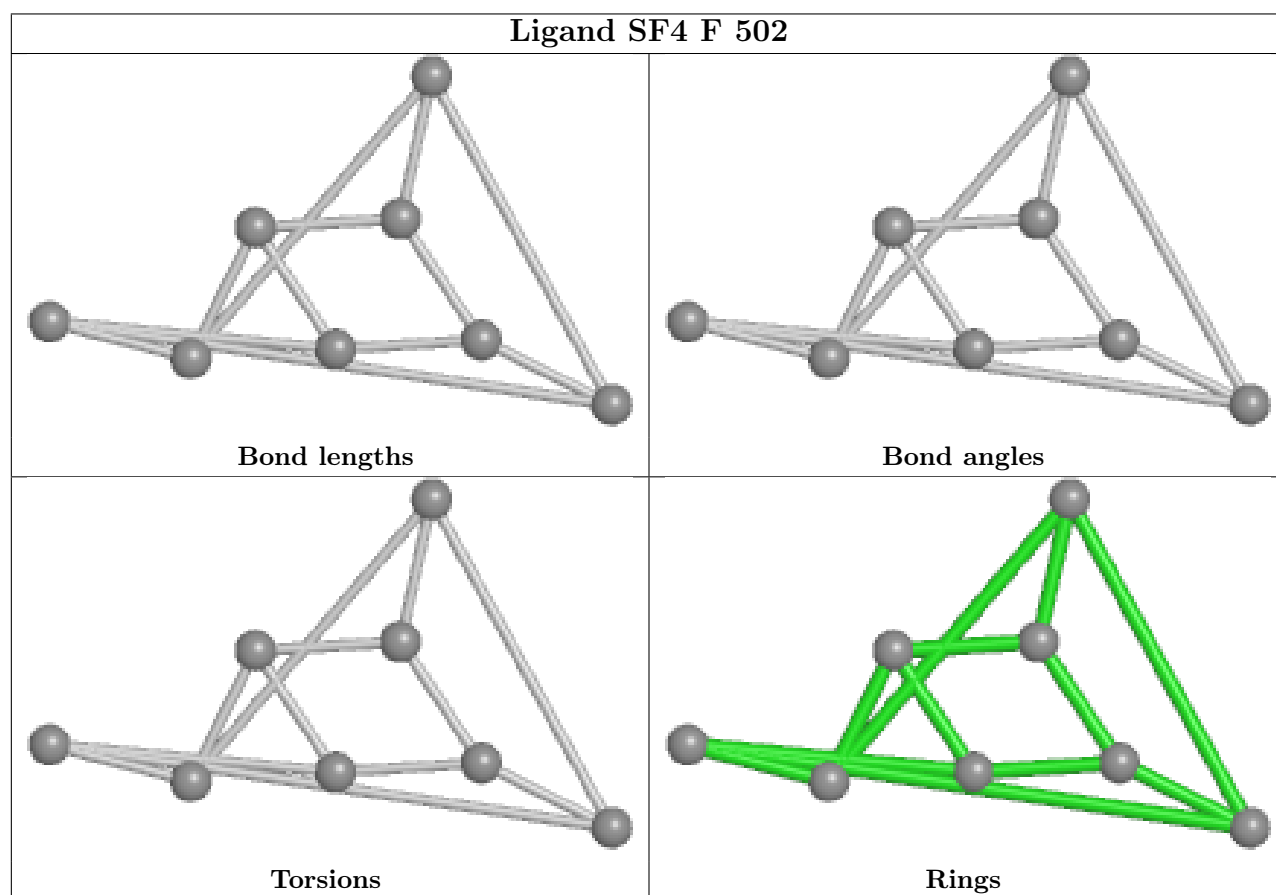
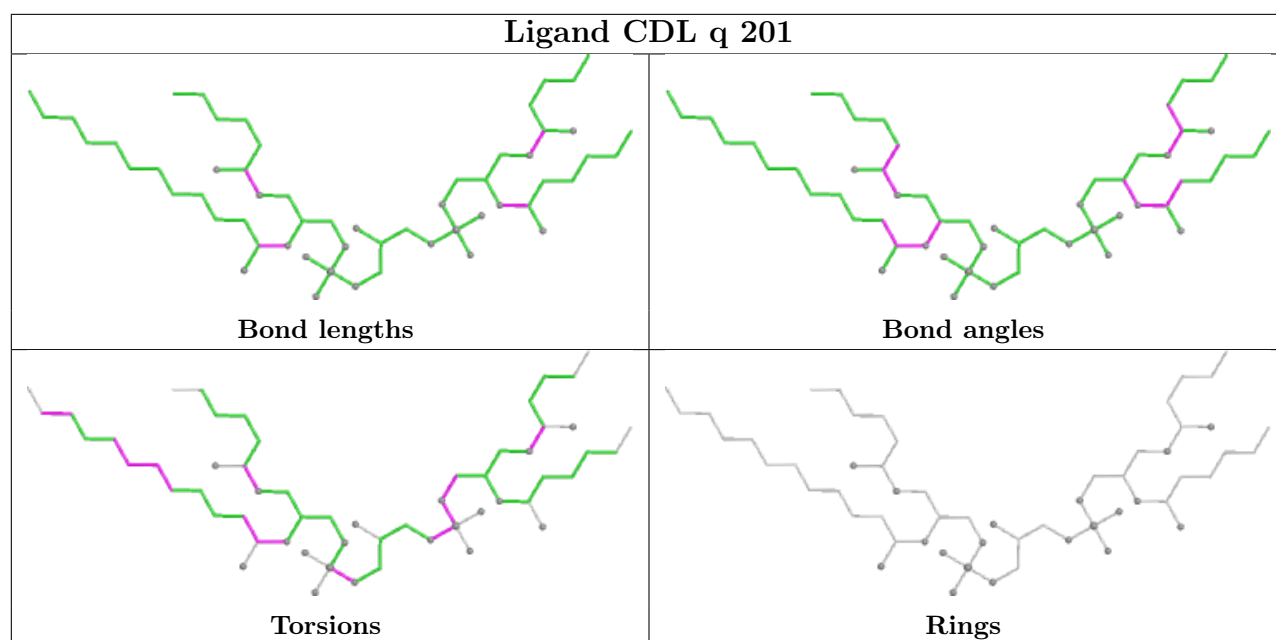


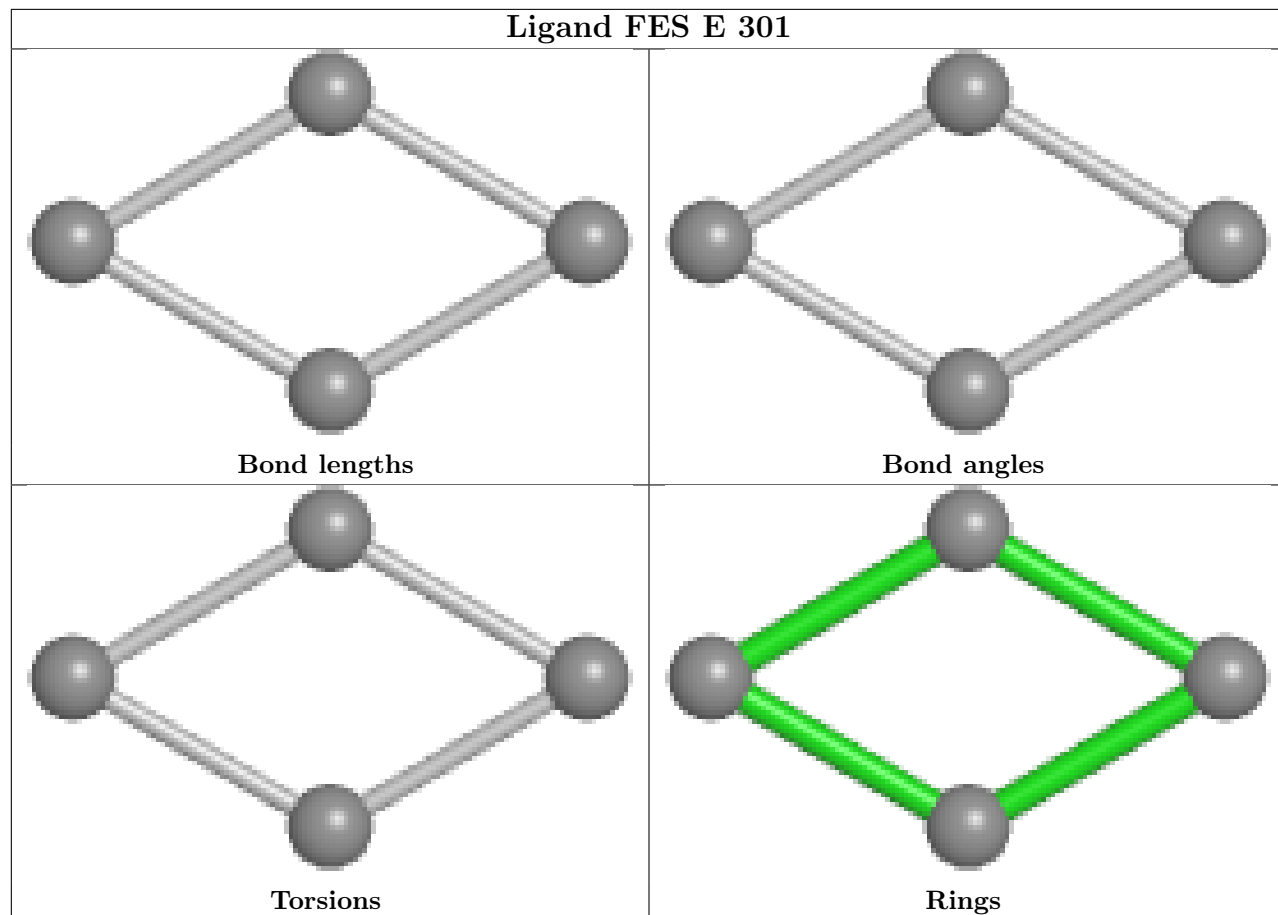
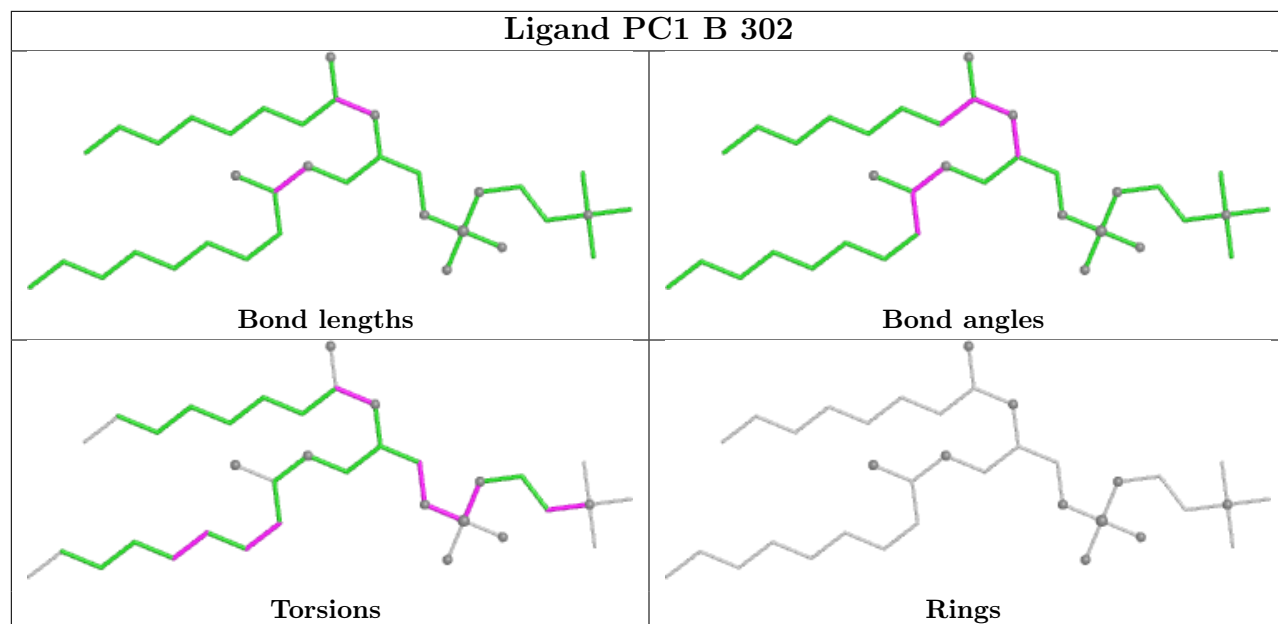
Ligand PC1 B 303

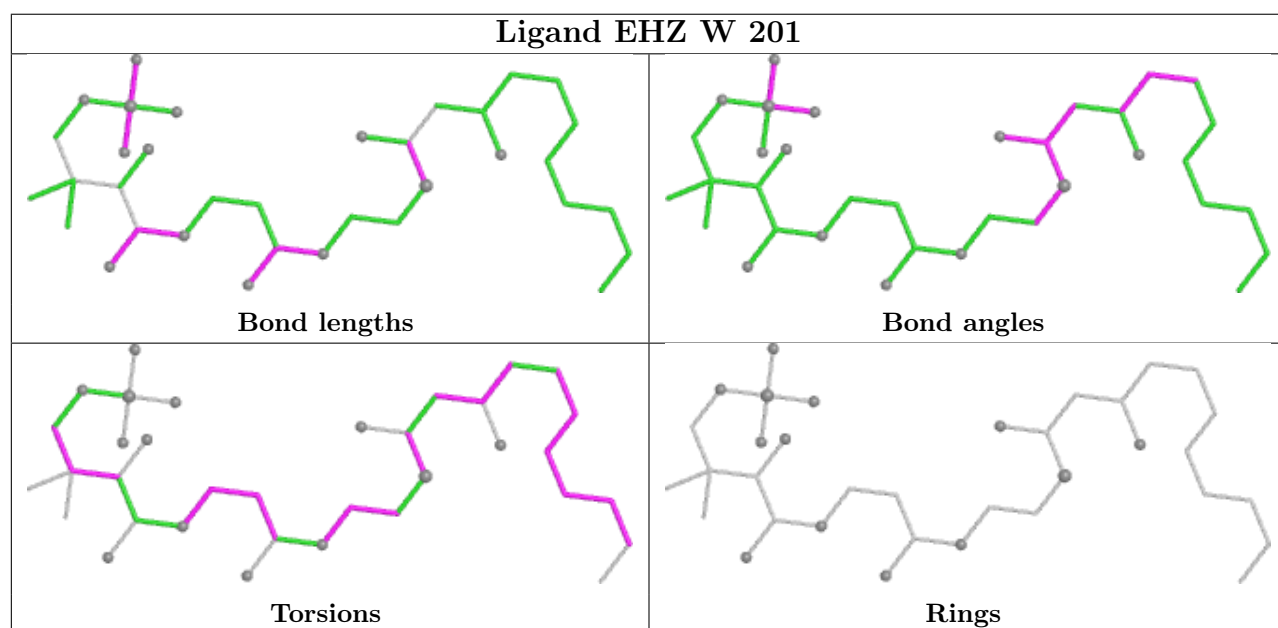
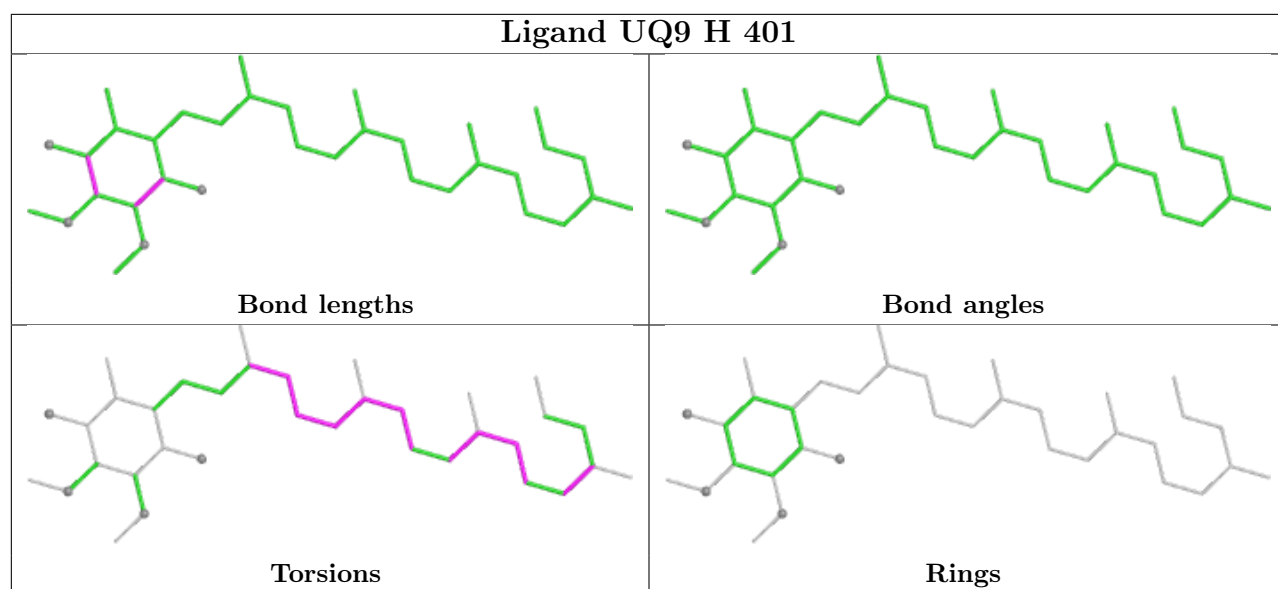


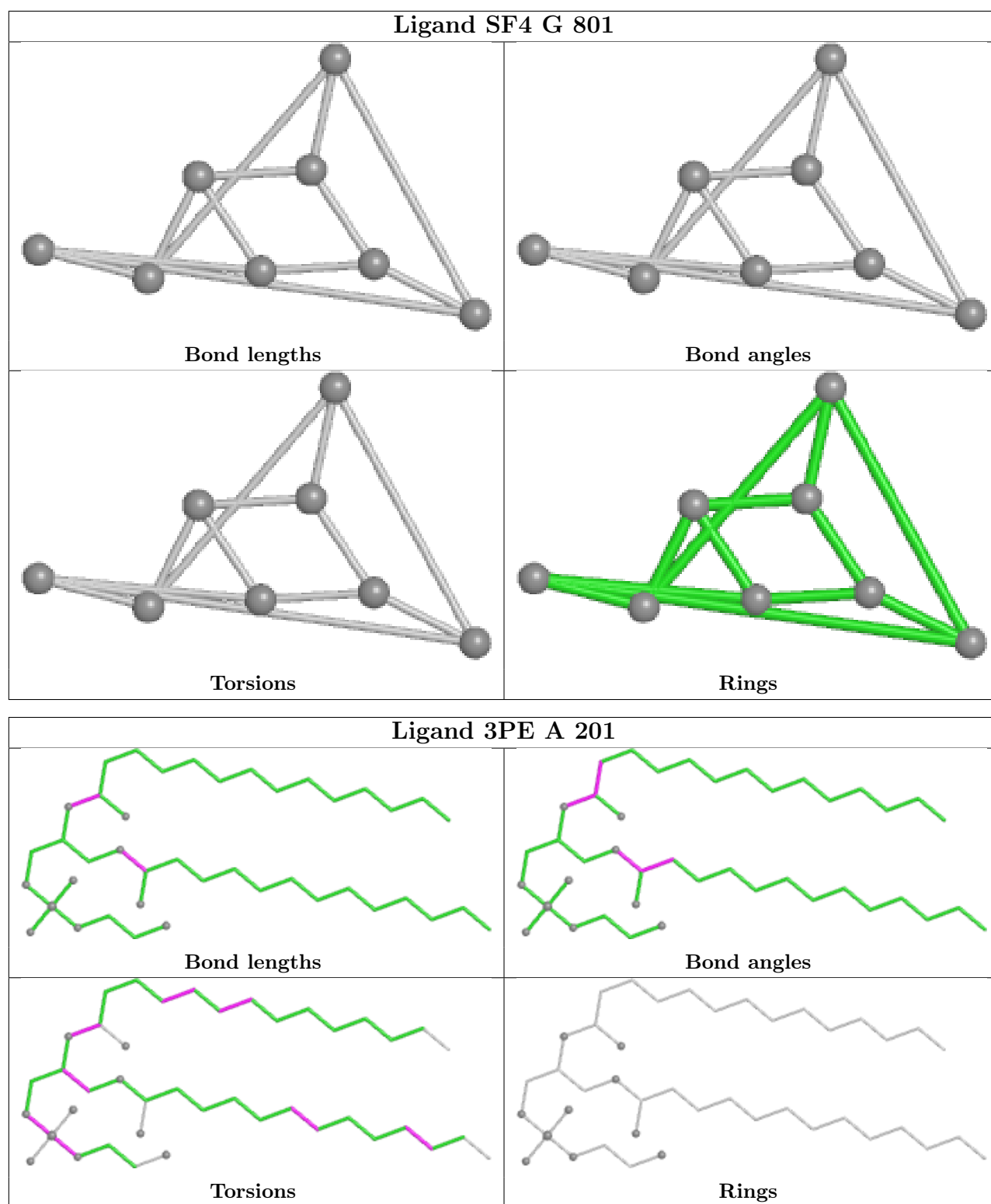
Ligand FMN F 501

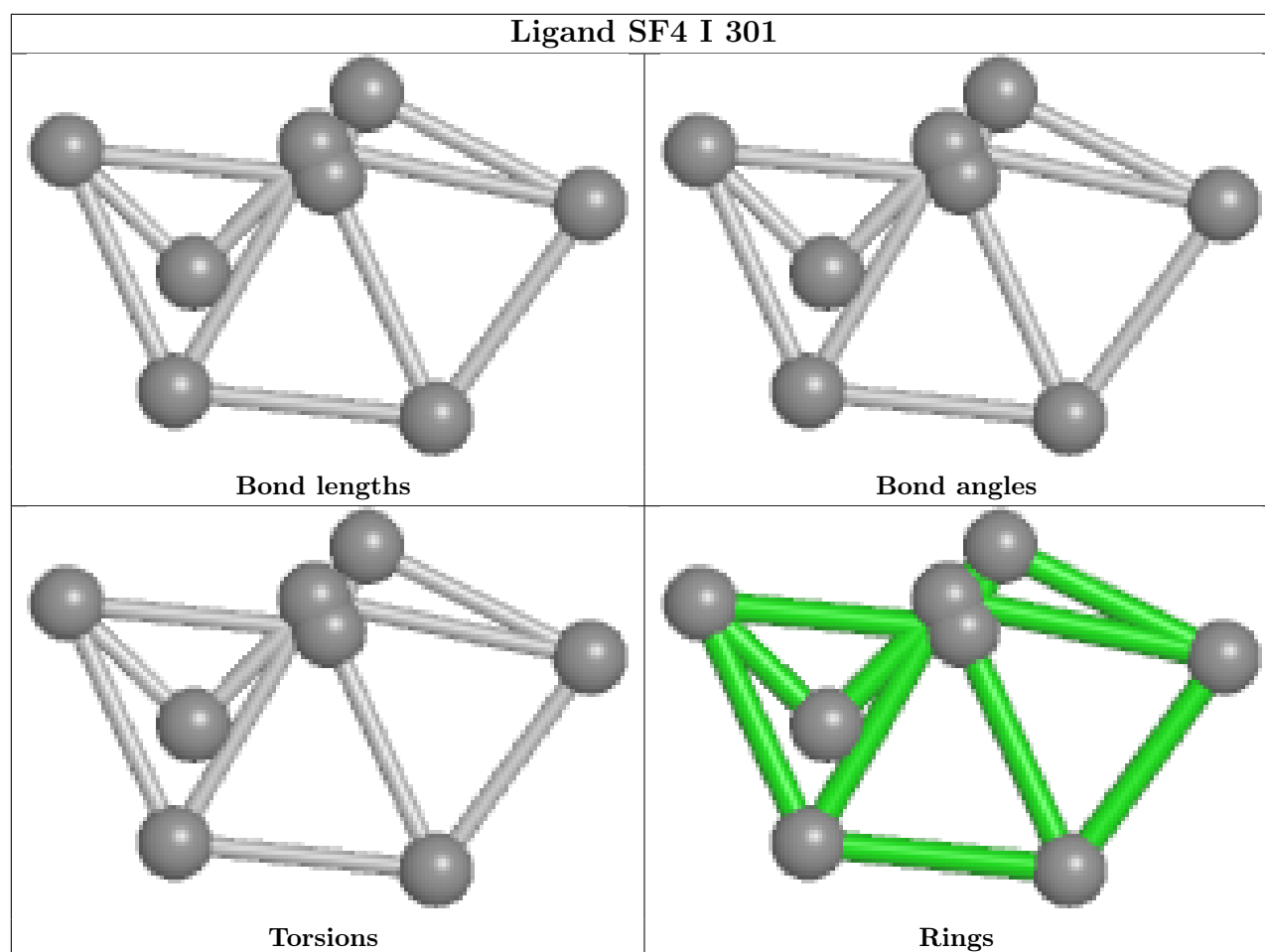


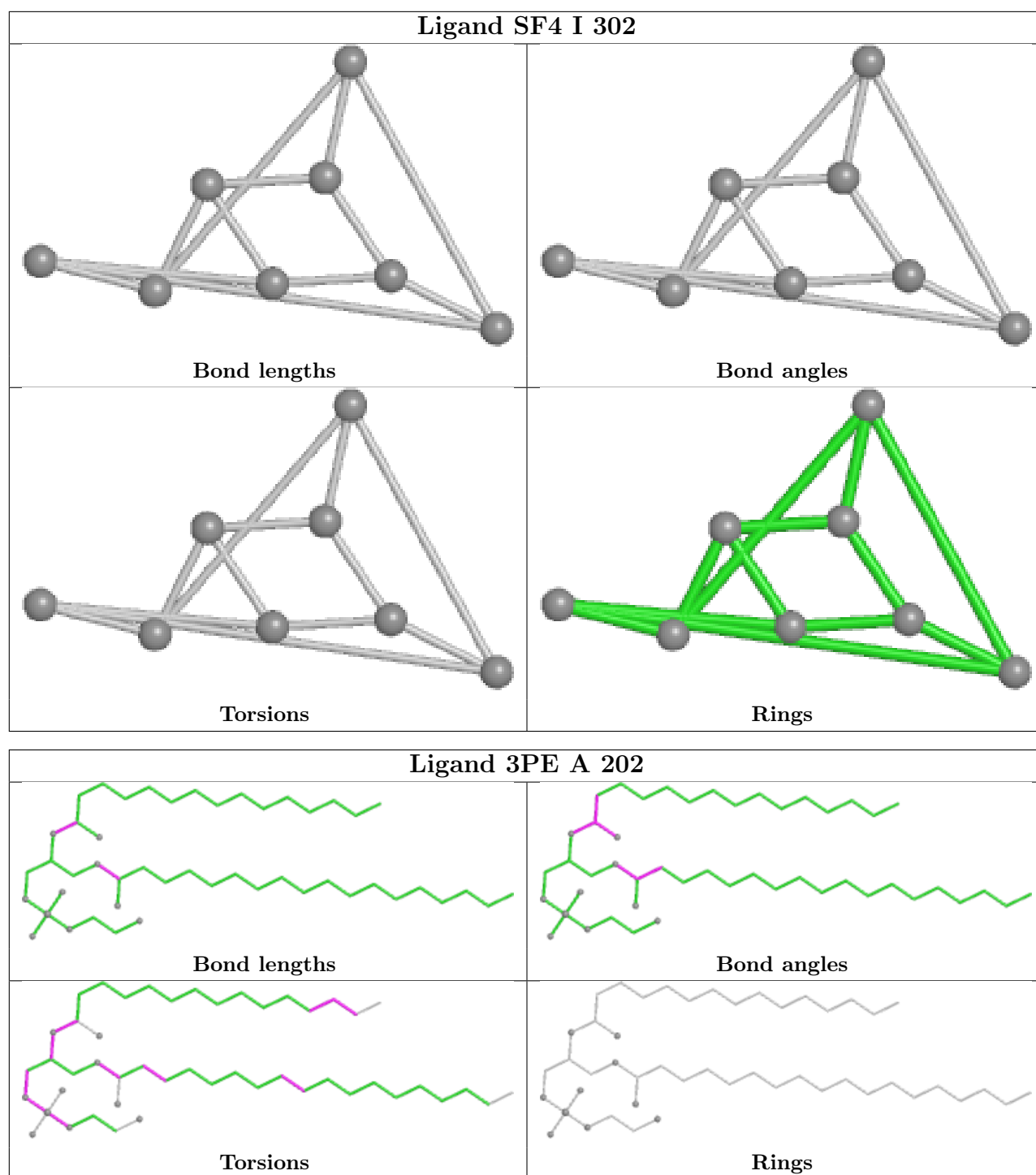


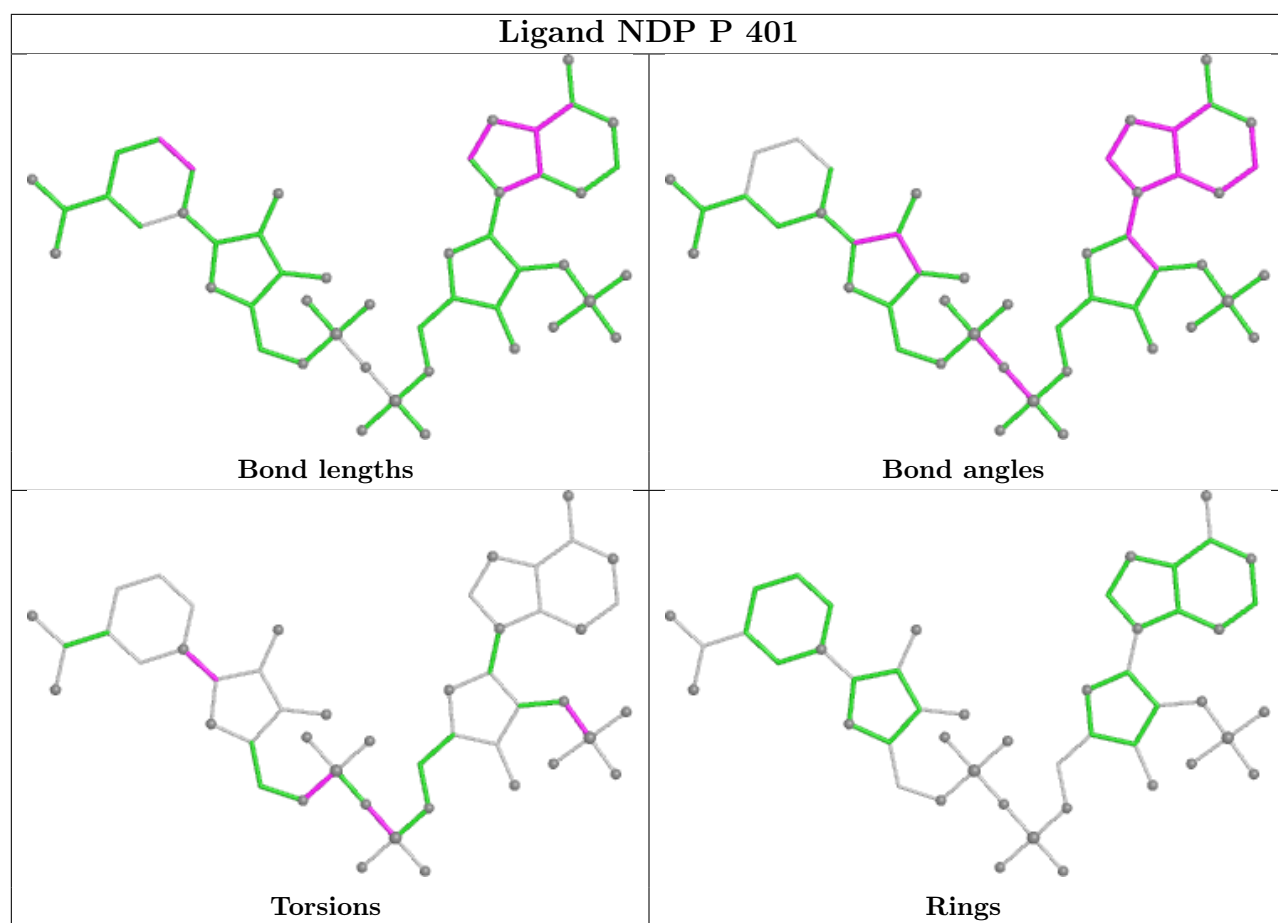




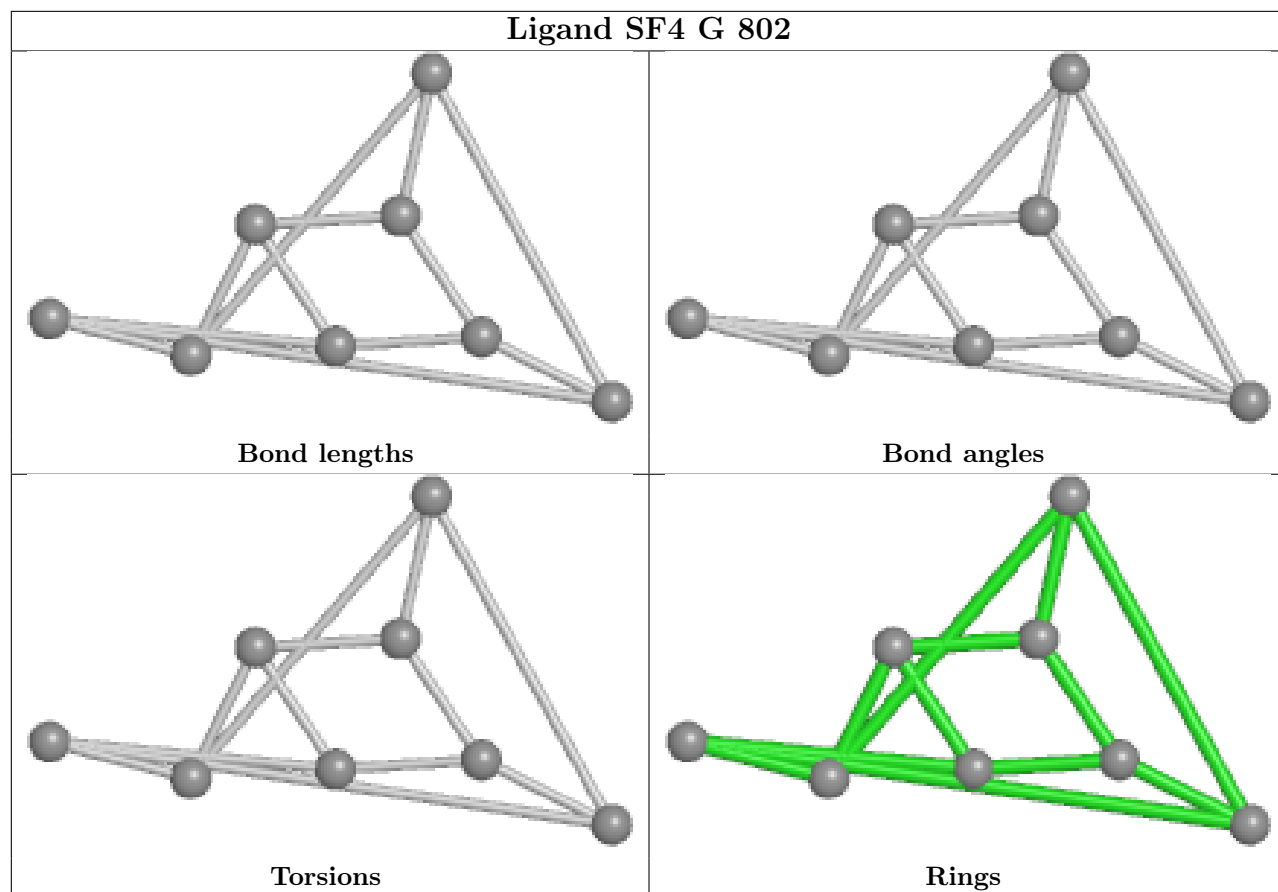




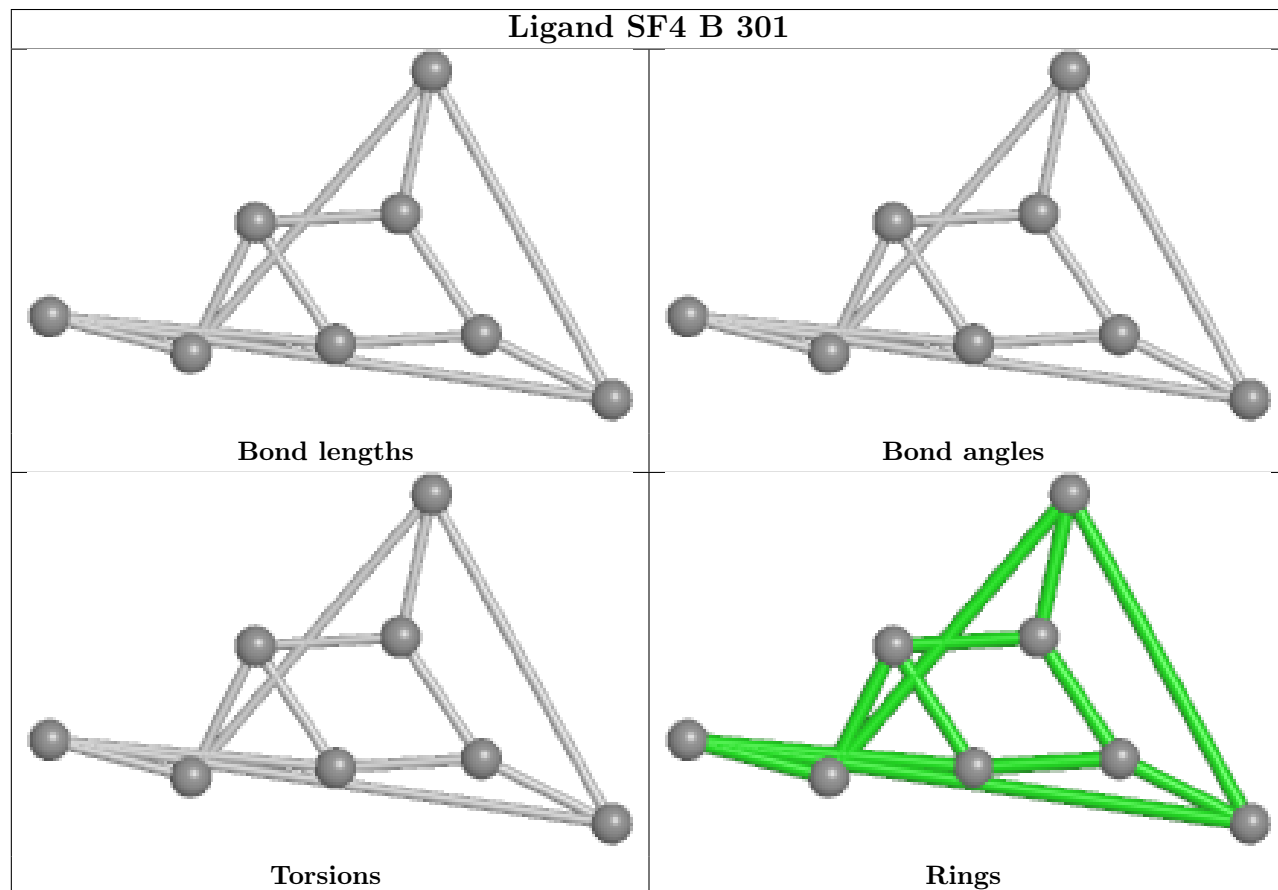


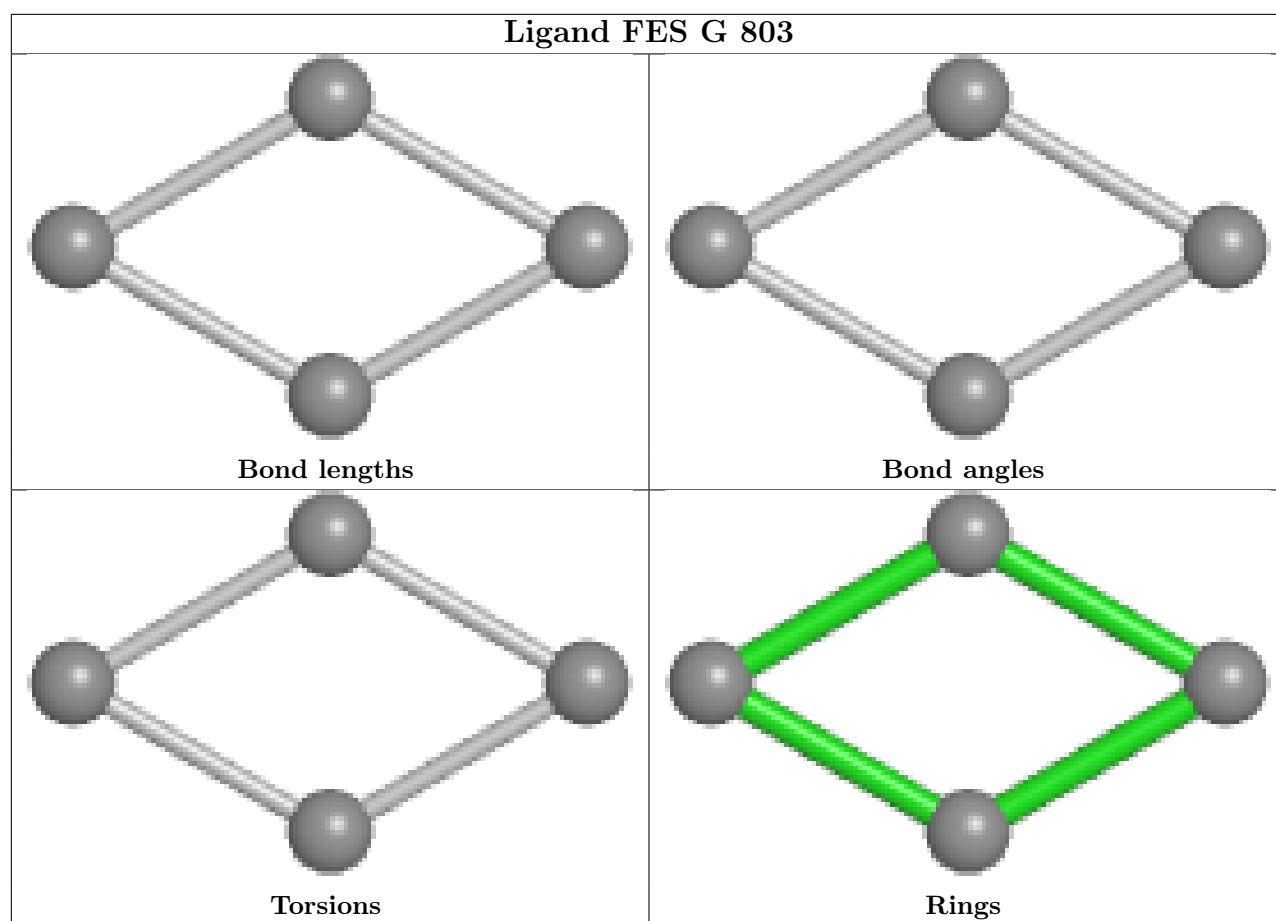


Ligand SF4 G 802



Ligand SF4 B 301





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.

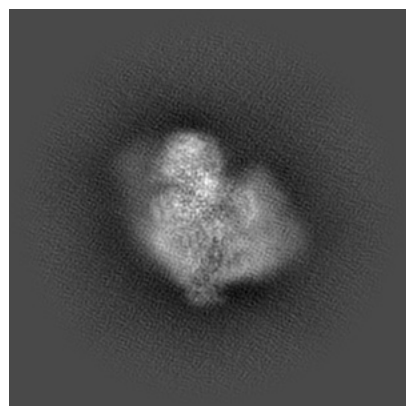
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38518. These allow visual inspection of the internal detail of the map and identification of artifacts.

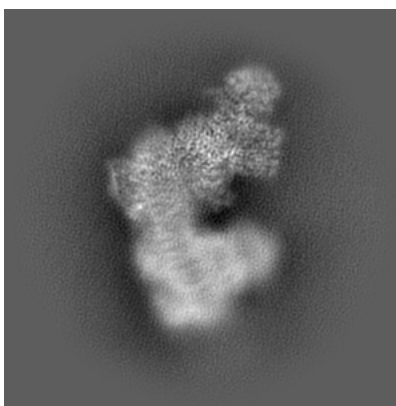
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

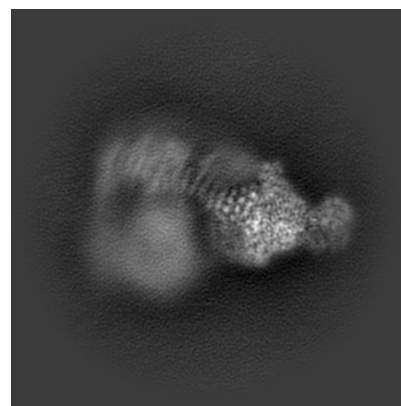
6.1.1 Primary map



X

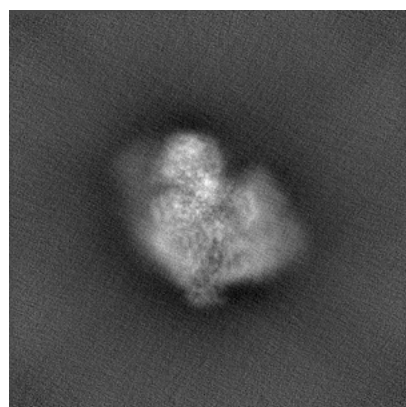


Y

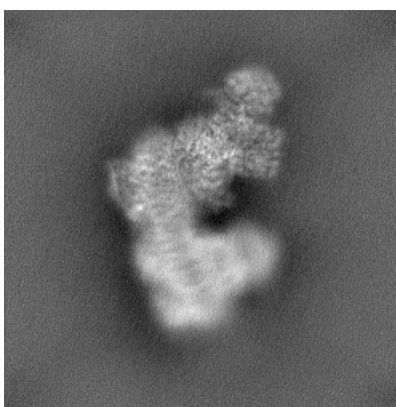


Z

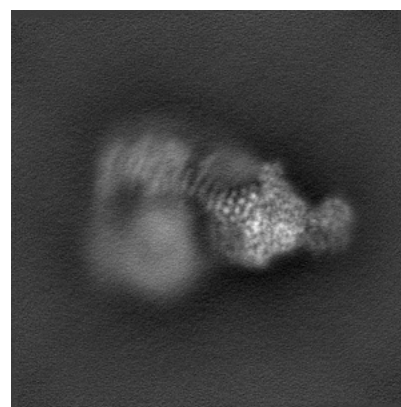
6.1.2 Raw map



X



Y

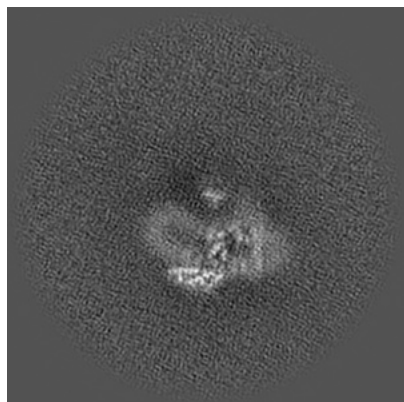


Z

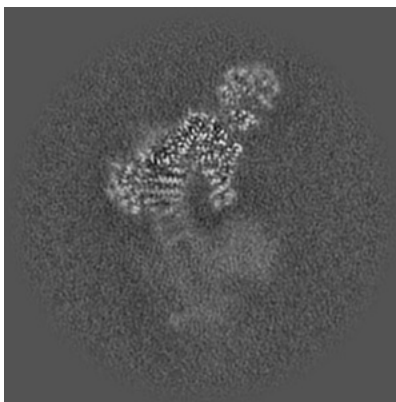
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

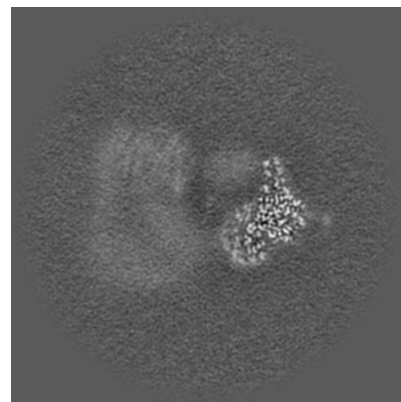
6.2.1 Primary map



X Index: 192

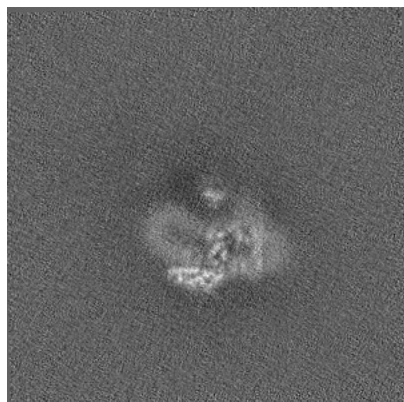


Y Index: 192



Z Index: 192

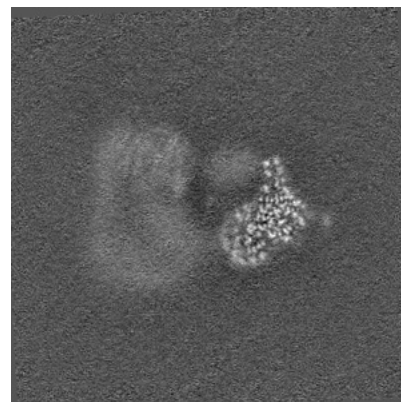
6.2.2 Raw map



X Index: 192



Y Index: 192

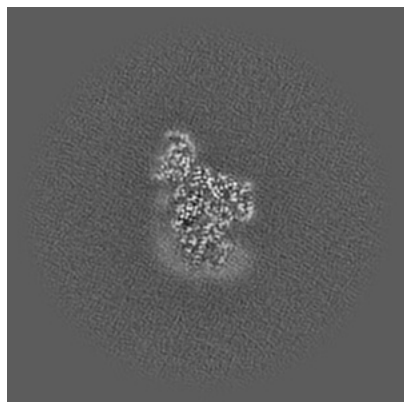


Z Index: 192

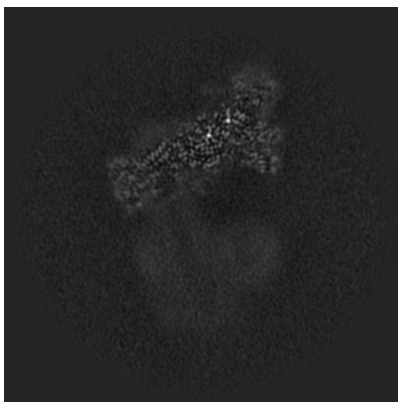
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

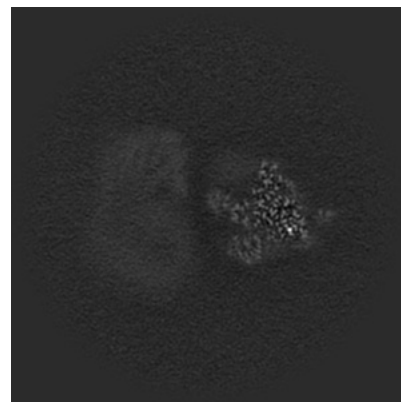
6.3.1 Primary map



X Index: 247

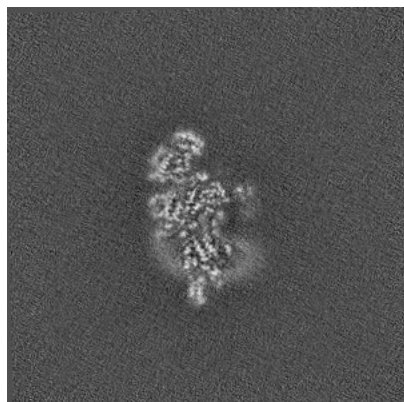


Y Index: 175

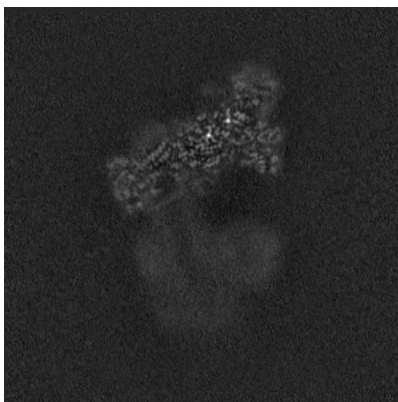


Z Index: 202

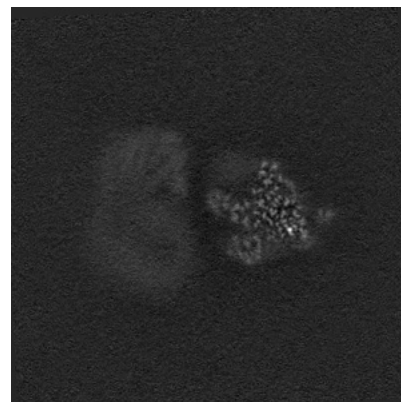
6.3.2 Raw map



X Index: 237



Y Index: 175

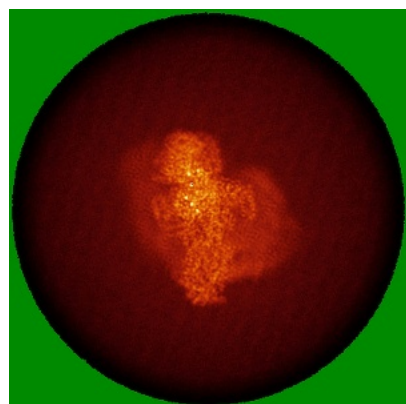


Z Index: 202

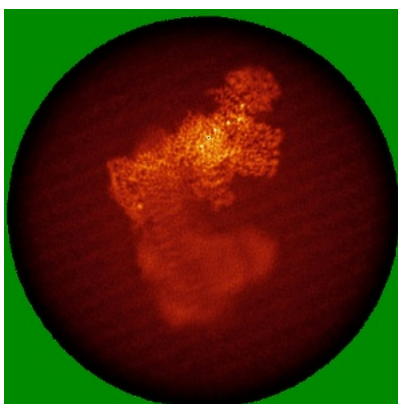
The images above show the largest variance slices of the map in three orthogonal directions.

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

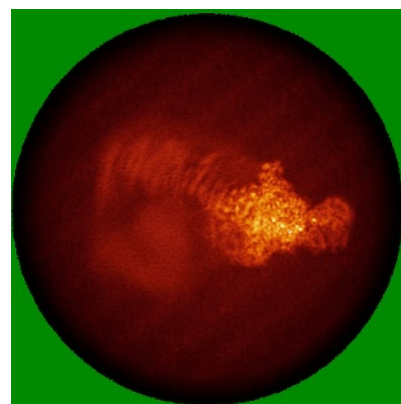
6.4.1 Primary map



X

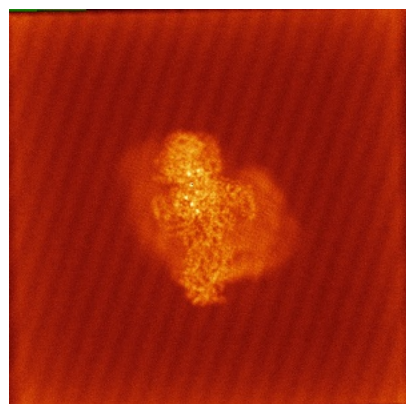


Y

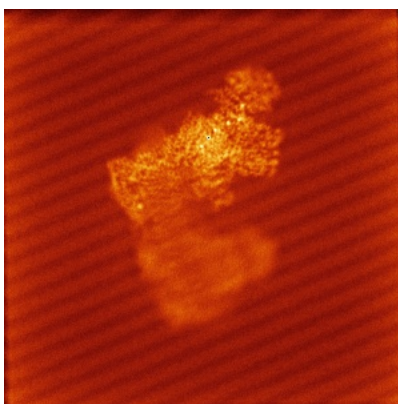


Z

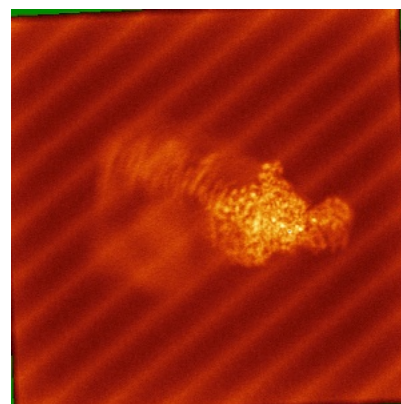
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

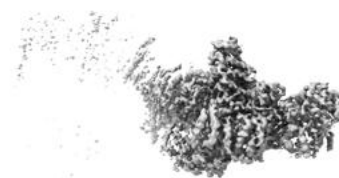
6.5.1 Primary map



X



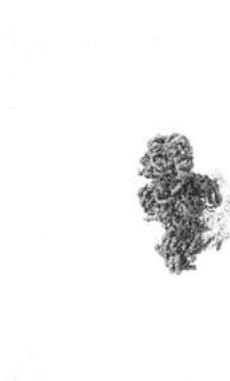
Y



Z

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



X



Y



Z

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

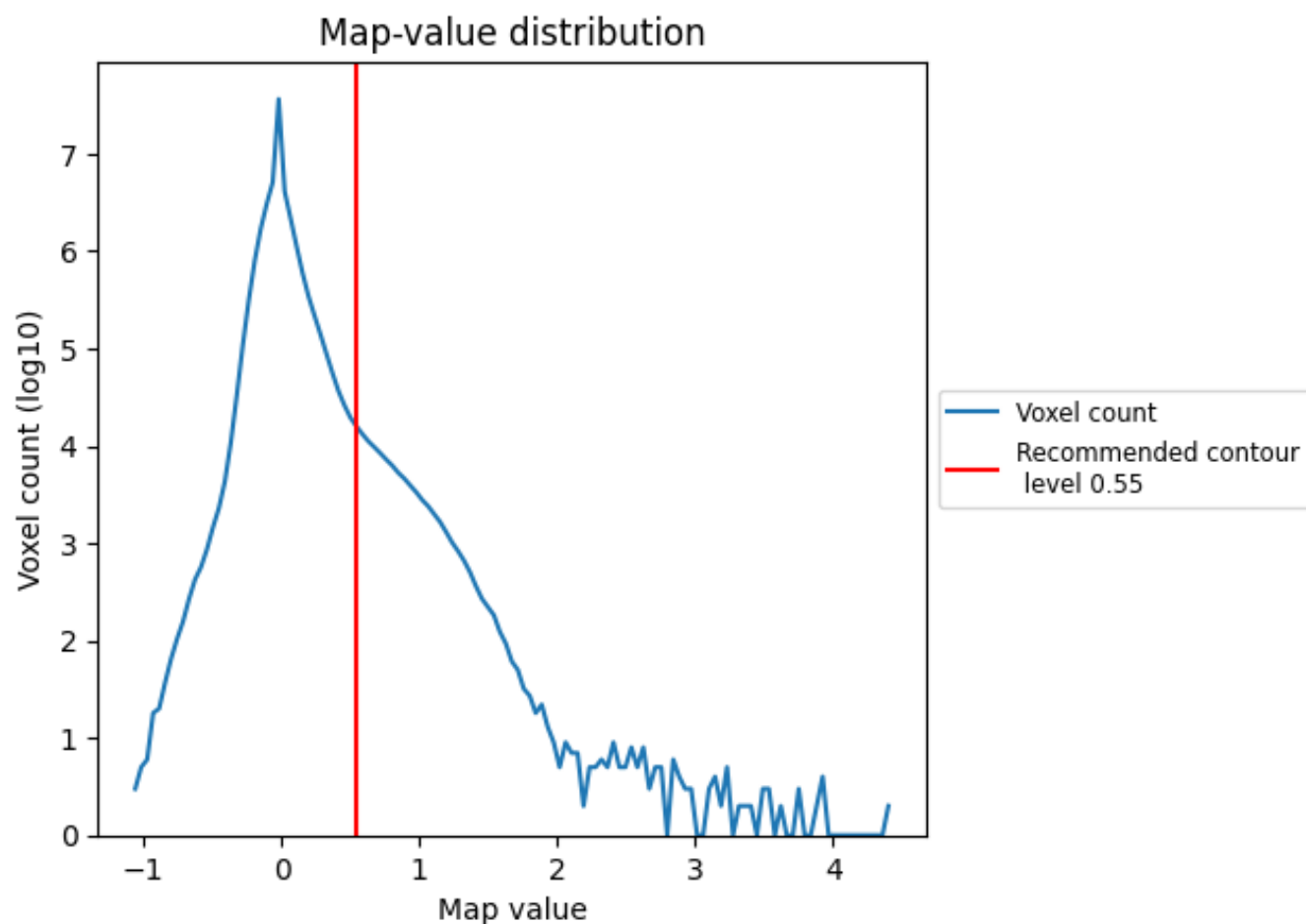
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

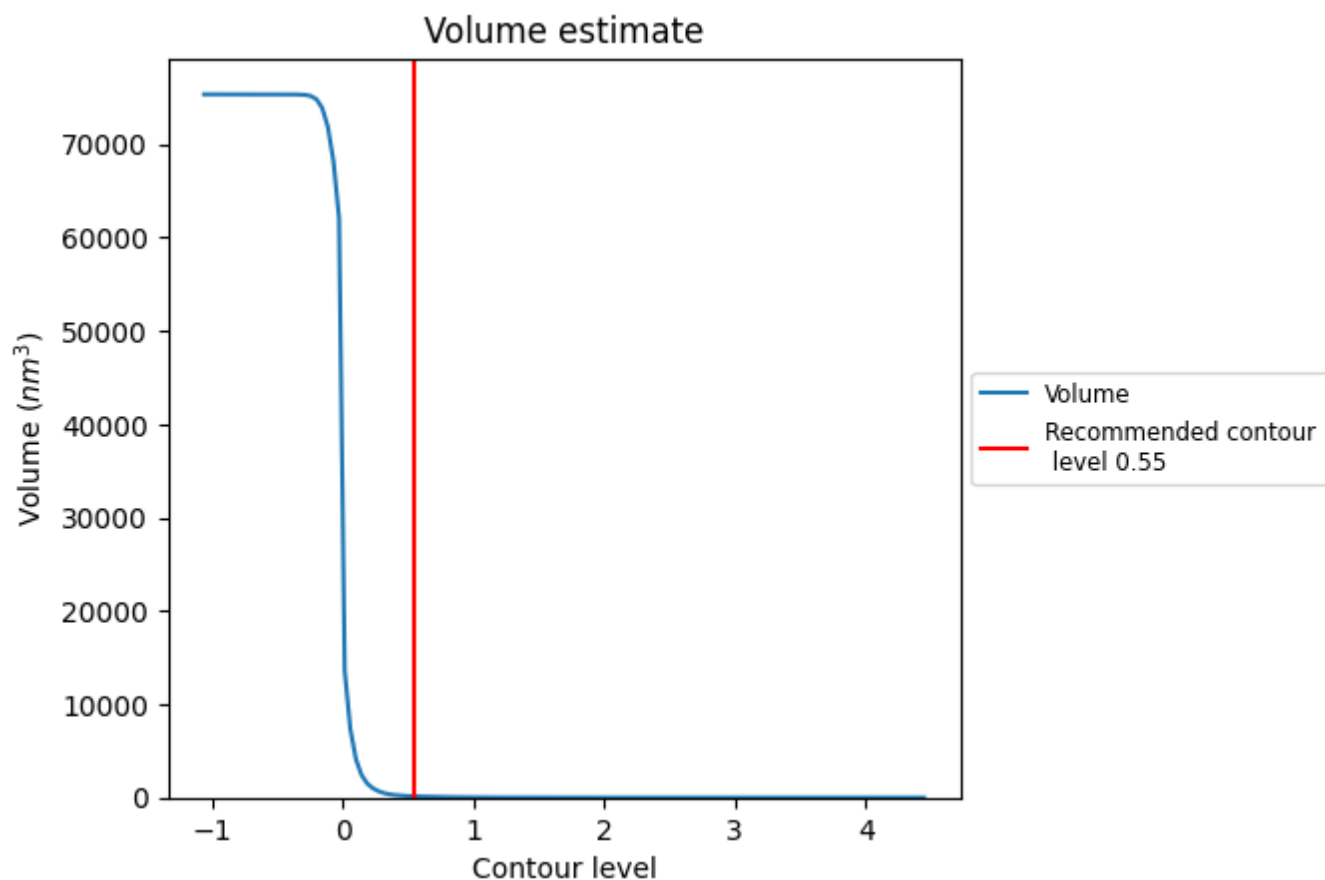
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

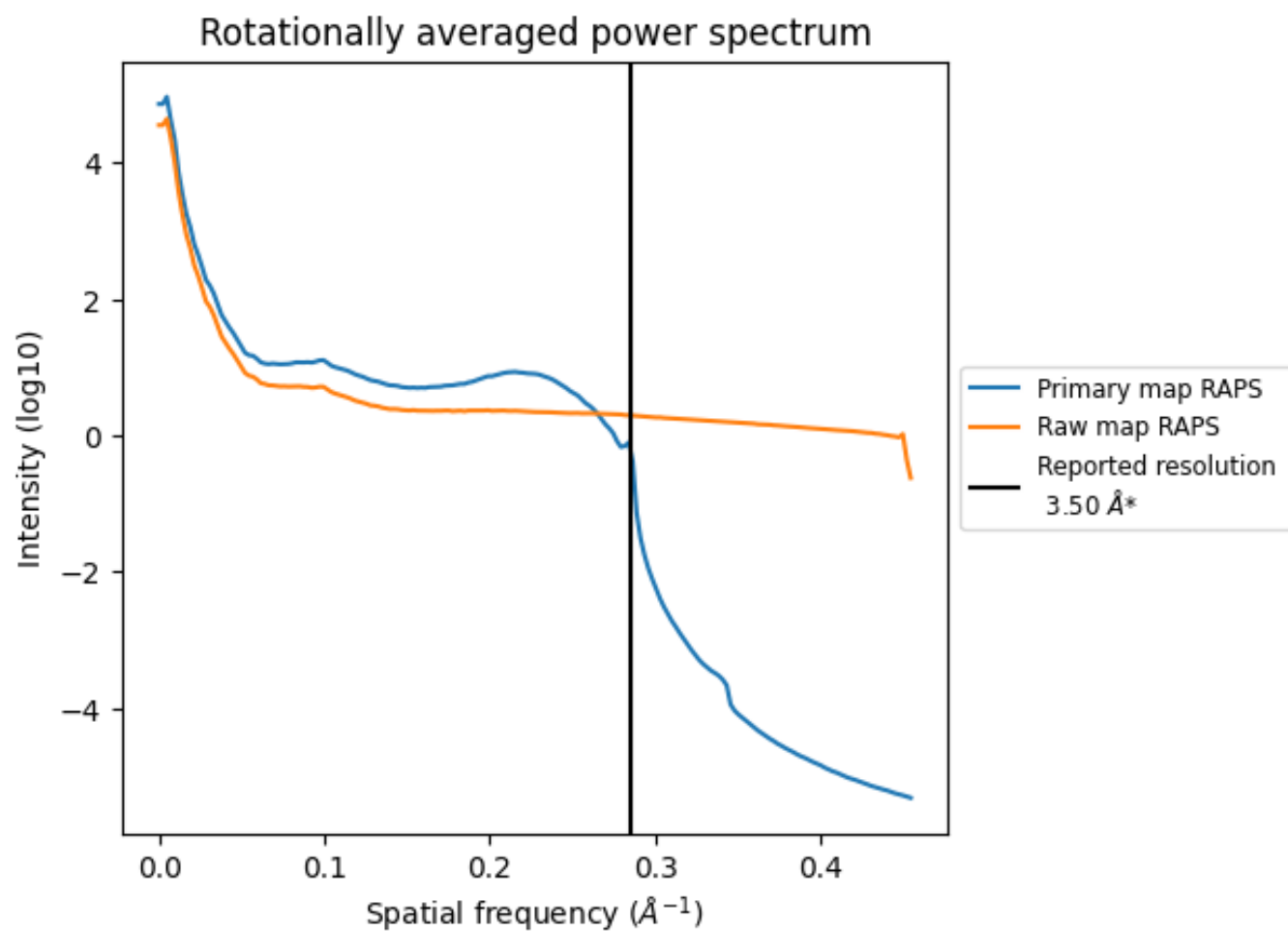
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136 nm³; this corresponds to an approximate mass of 123 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 ⓘ

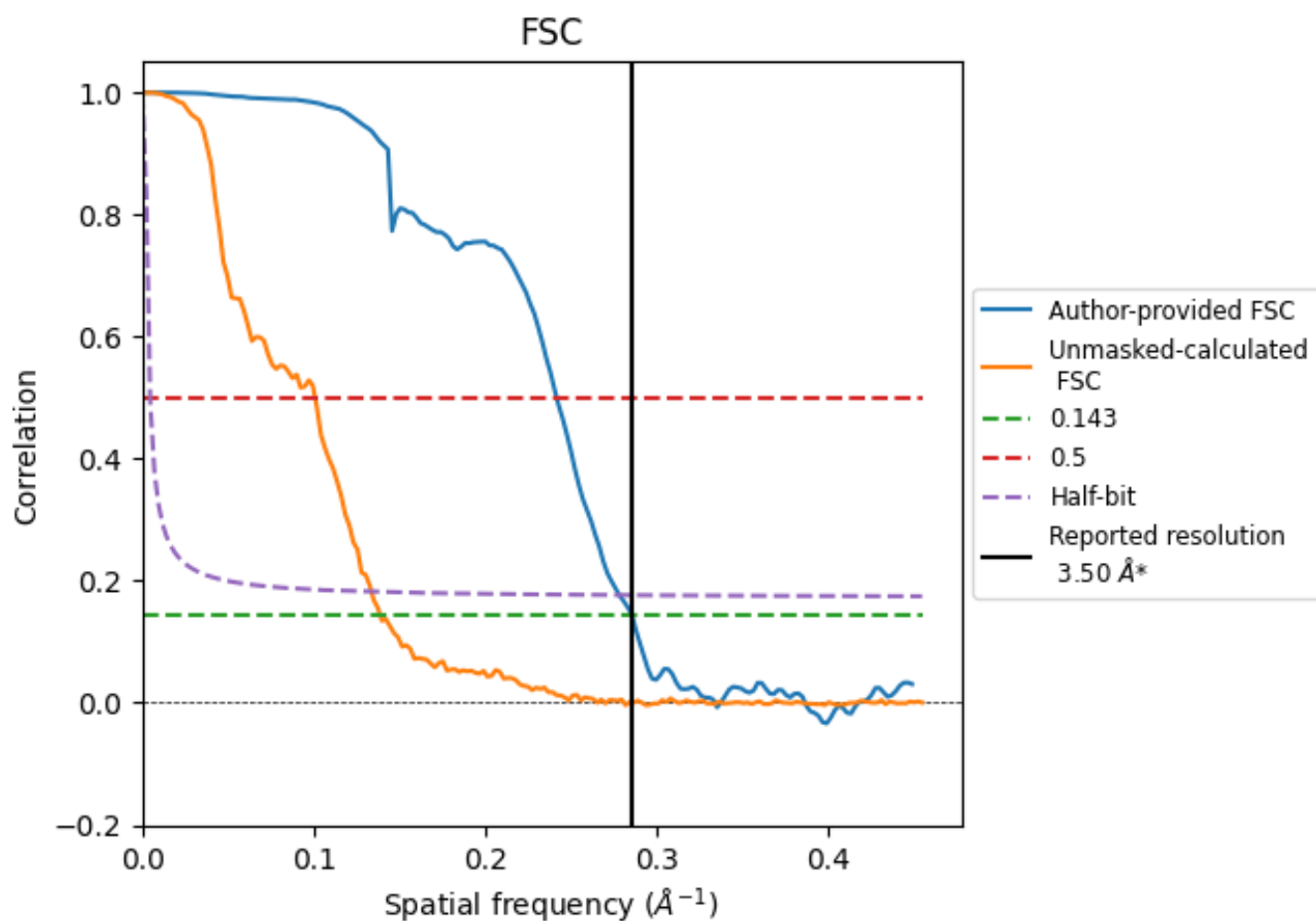


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

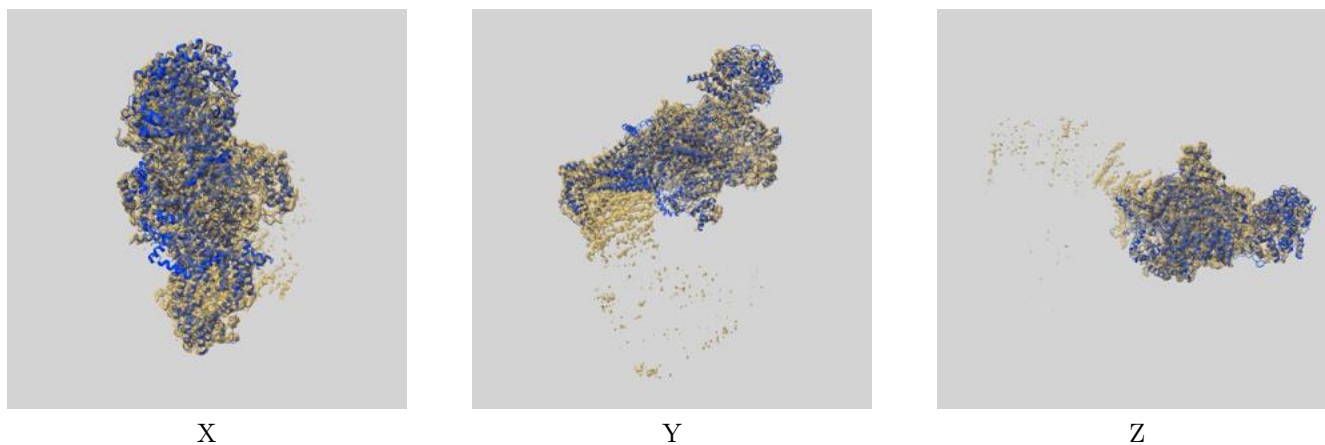
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	4.14	3.60
Unmasked-calculated*	7.21	9.92	7.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.21 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

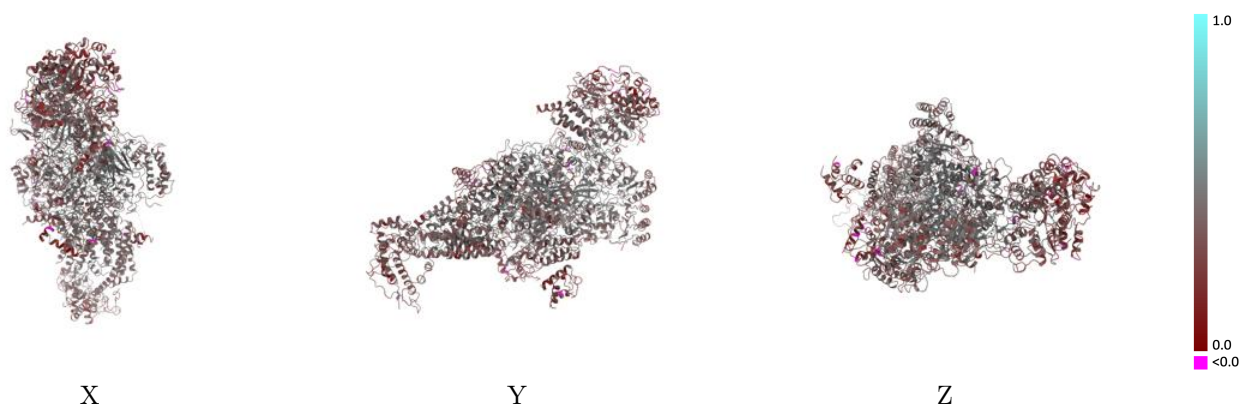
This section contains information regarding the fit between EMDB map EMD-38518 and PDB model 8XNX. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



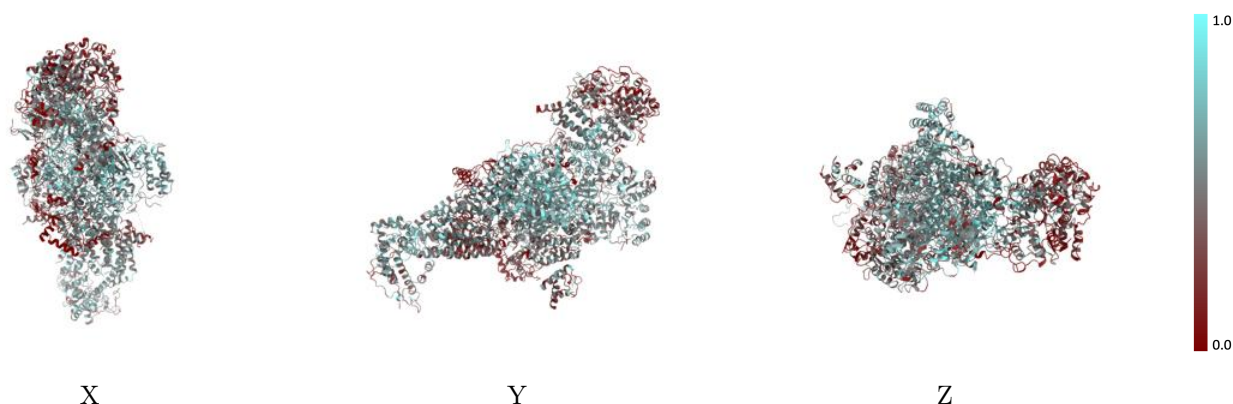
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



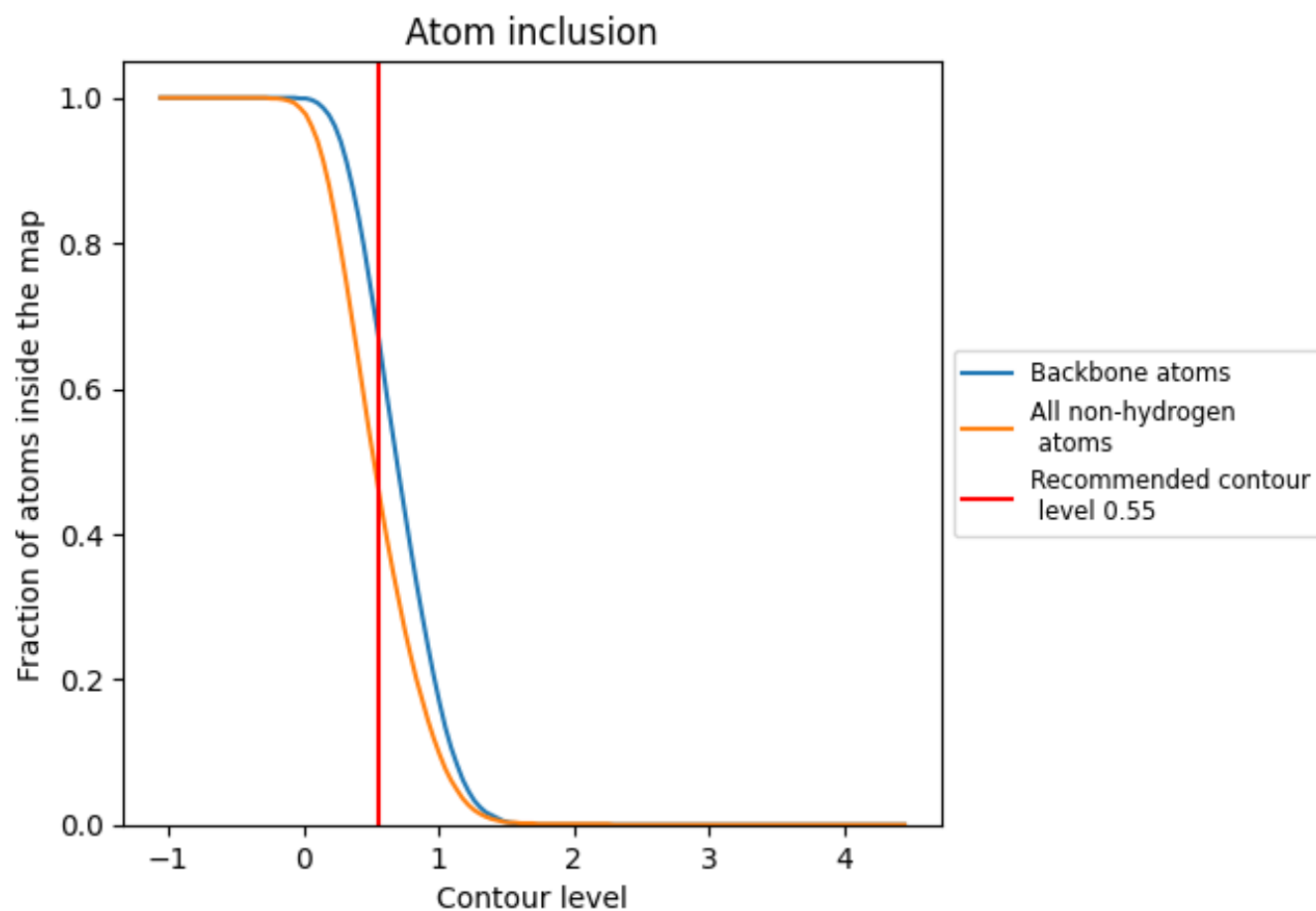
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



At the recommended contour level, 68% of all backbone atoms, 46% 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	 0.4650	 0.3720
A	 0.3400	 0.3650
B	 0.5850	 0.4300
C	 0.6200	 0.4440
D	 0.6140	 0.4460
E	 0.3010	 0.3030
F	 0.3660	 0.3170
G	 0.5740	 0.4070
H	 0.5070	 0.4180
I	 0.6550	 0.4360
P	 0.3120	 0.3100
Q	 0.4490	 0.4250
R	 0.2030	 0.3070
S	 0.5430	 0.3520
T	 0.3220	 0.2570
V	 0.5940	 0.3970
W	 0.4400	 0.3690
X	 0.4970	 0.3170
Z	 0.5070	 0.3370
a	 0.5800	 0.3860
b	 0.4750	 0.3360
q	 0.0640	 0.2910
r	 0.1490	 0.2790
s	 0.0370	 0.2310

