



Full wwPDB EM Validation Report ⓘ

Aug 7, 2026 – 12:38 AM JST

PDB ID : 8XNW / pdb_00008xnw
EMDB ID : EMD-38517
Title : Respiratory complex Peripheral Arm of CI, close form B, focus-refined map of type II, Wild type mouse under Cold Acclimation
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-12-30
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

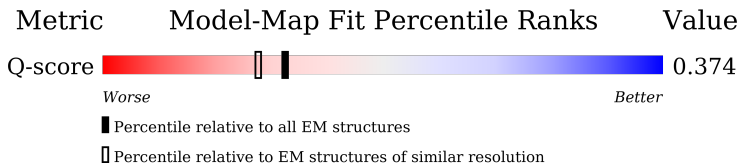
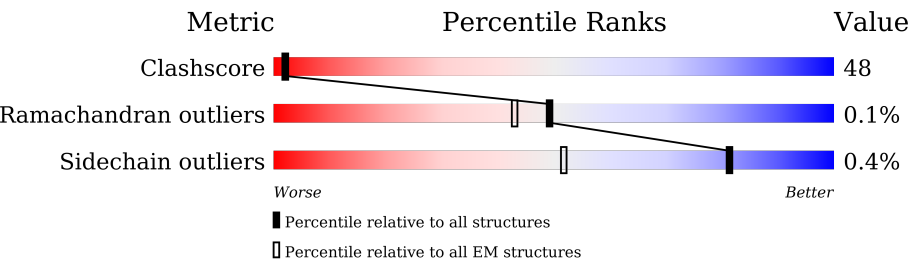
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

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

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	115	43% 21% 72% ...
2	B	224	8% 26% 38% 5% 30%
3	C	263	6% 37% 36% 25%
4	D	463	7% 35% 44% 17%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	SF4	B	301	-	-	X	-
24	SF4	F	502	-	-	X	-
24	SF4	G	802	-	-	X	-
24	SF4	I	302	-	-	X	-
24	SF4	I	303	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	FES	E	301	-	-	X	-
27	FES	G	803	-	-	X	-
29	3PE	I	301	-	-	X	-
33	CDL	q	201	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 33848 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	113	Total	C	N	O	S	0	0
			915	623	131	154	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	197	Total	C	N	O	S	0	0
			1636	1057	278	298	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	426	Total	C	N	O	S	0	0
			3288	2073	588	605	22		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	172	Total	C	N	O	S	0	0
			1380	869	237	262	12		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	116	Total	C	N	O	S	0	0
			940	598	161	177	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	138	Total	C	N	O	S	0	0
			1145	736	203	198	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	80	Total	C	N	O	S	0	0
			628	414	99	111	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	114	Total	C	N	O	S	0	0
			951	612	165	170	4		

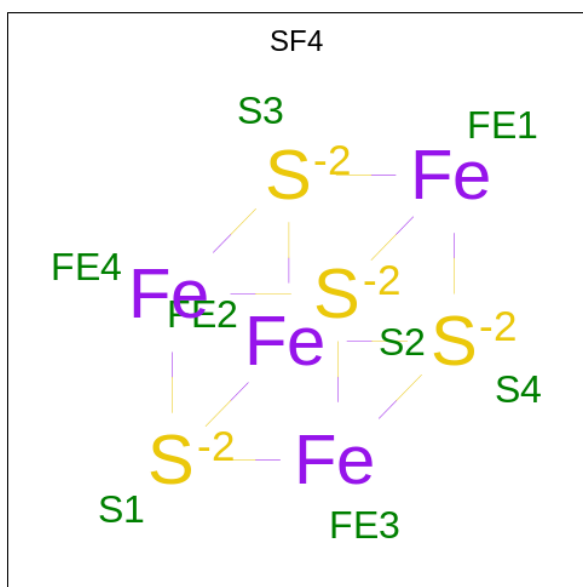
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	44	Total	C	N	O	S	0	0
			354	230	63	60	1		

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

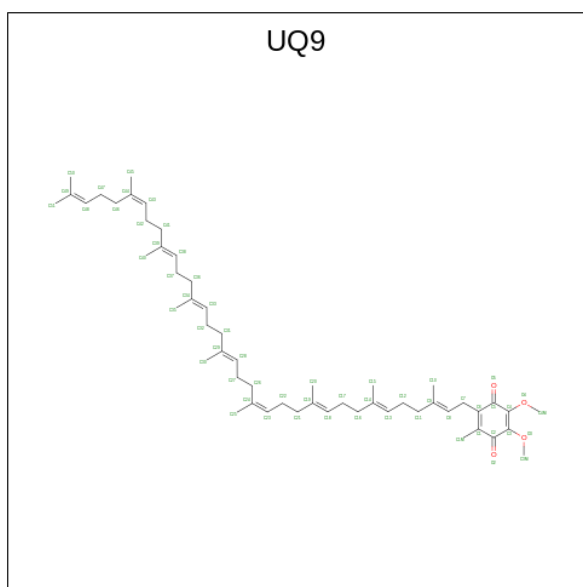
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	23	Total	C	N	O	0	0
			193	126	30	37		

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



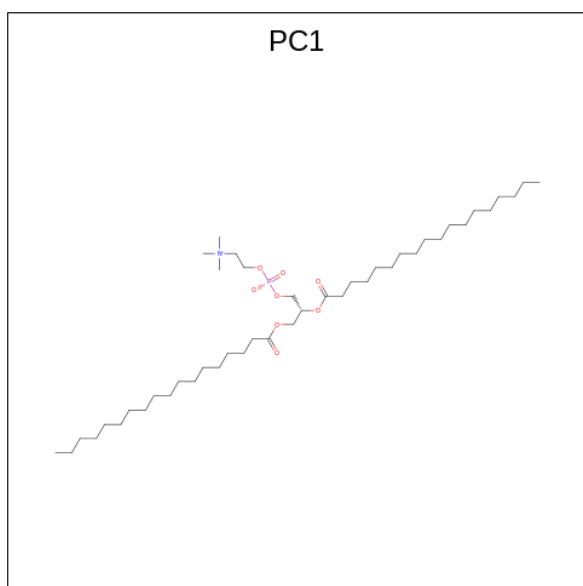
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	Fe	S	0
			8	4	4	
24	F	1	Total	Fe	S	0
			8	4	4	
24	G	1	Total	Fe	S	0
			8	4	4	
24	G	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 25 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



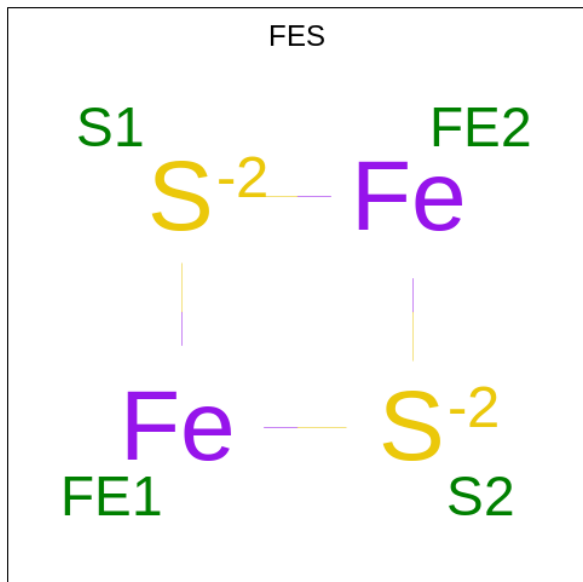
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			21	17	4	
25	H	1	Total	C	O	0
			35	31	4	

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



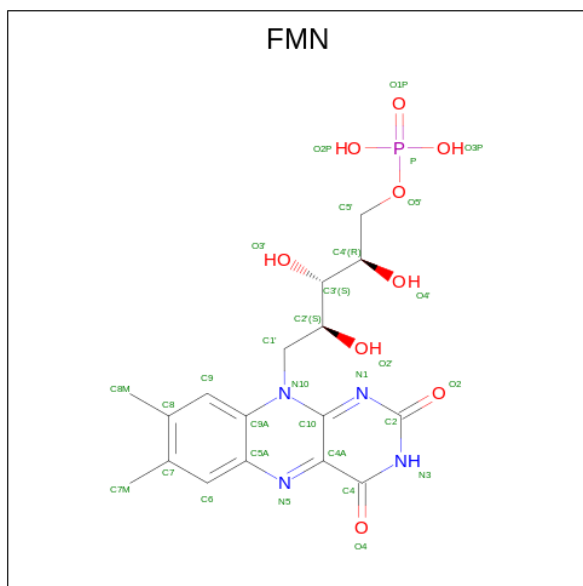
Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total	C	N	O	P	0
			35	25	1	8	1	

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



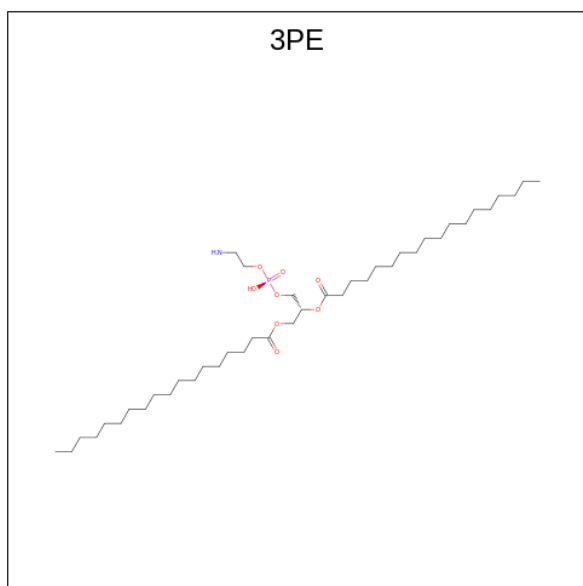
Mol	Chain	Residues	Atoms			AltConf
27	E	1	Total	Fe	S	0
			4	2	2	
27	G	1	Total	Fe	S	0
			4	2	2	

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



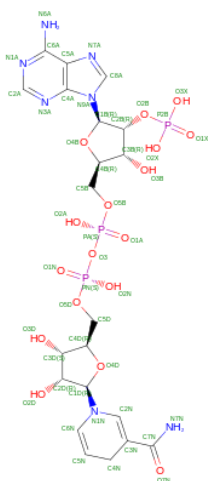
Mol	Chain	Residues	Atoms					AltConf
28	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 29 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	I	1	Total	C	N	O	P	0
			51	41	1	8	1	

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

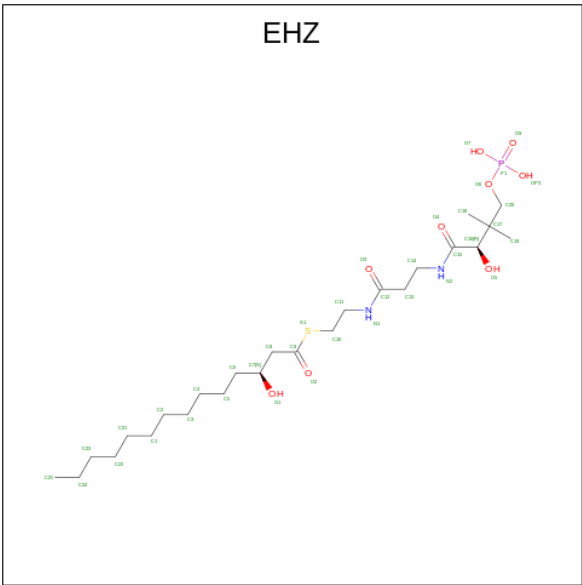


Mol	Chain	Residues	Atoms					AltConf
30	P	1	Total 48	C 21	N 7	O 17	P 3	0

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

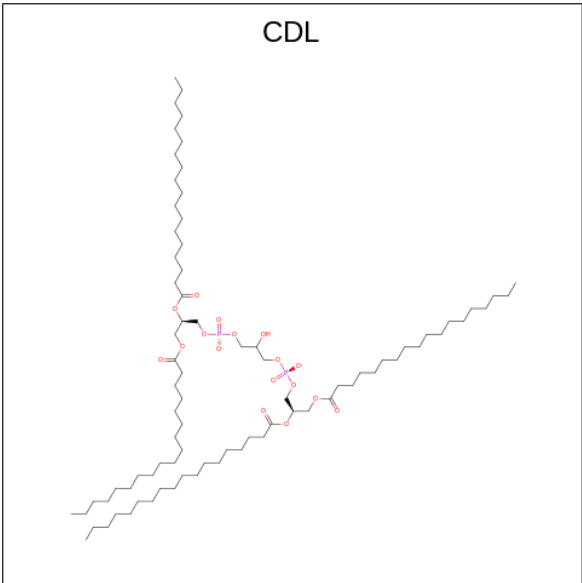
Mol	Chain	Residues	Atoms	AltConf
31	R	1	Total Zn 1 1	0

- 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).

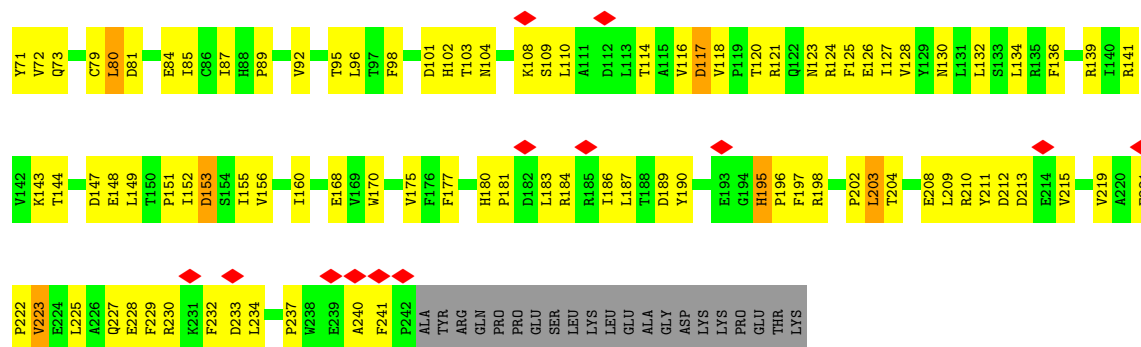


Mol	Chain	Residues	Atoms					AltConf	
32	W	1	Total	C	N	O	P	S	0
			35	22	2	9	1	1	

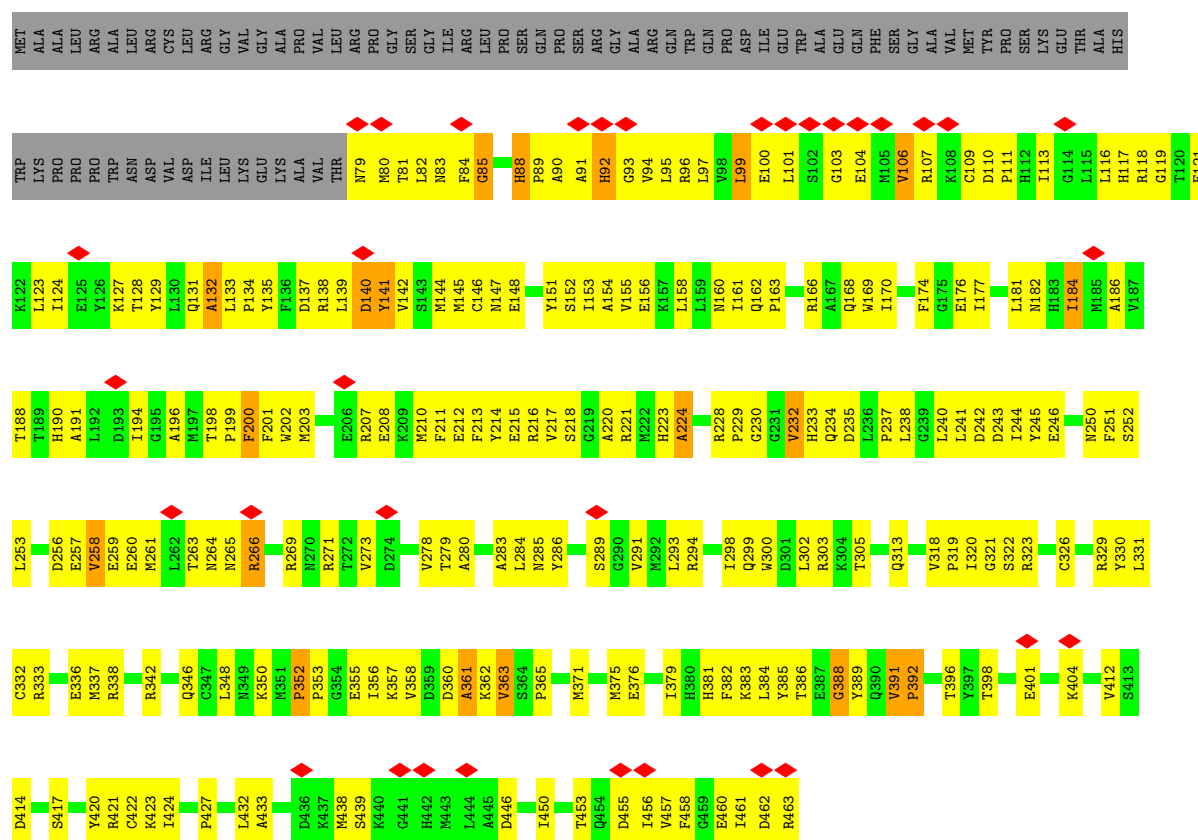
- Molecule 33 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



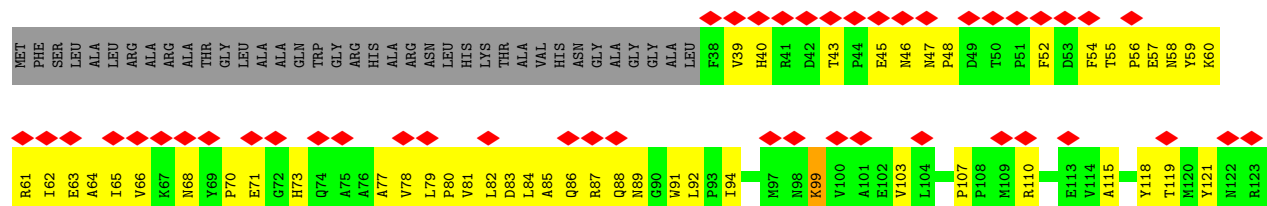
Mol	Chain	Residues	Atoms				AltConf
33	q	1	Total	C	O	P	0
			57	38	17	2	

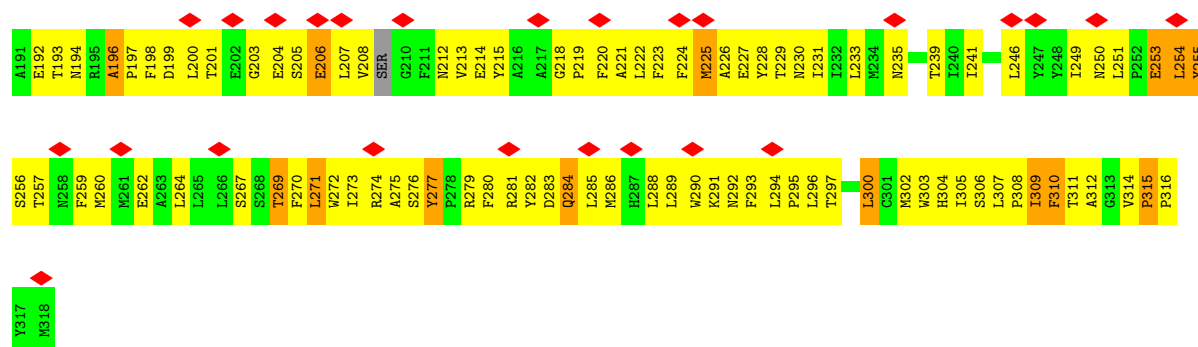


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

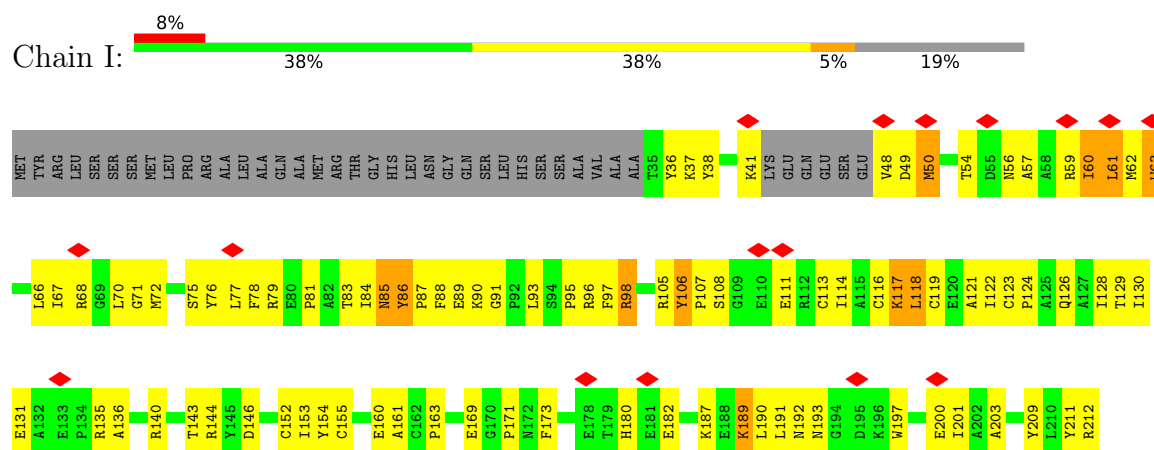


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

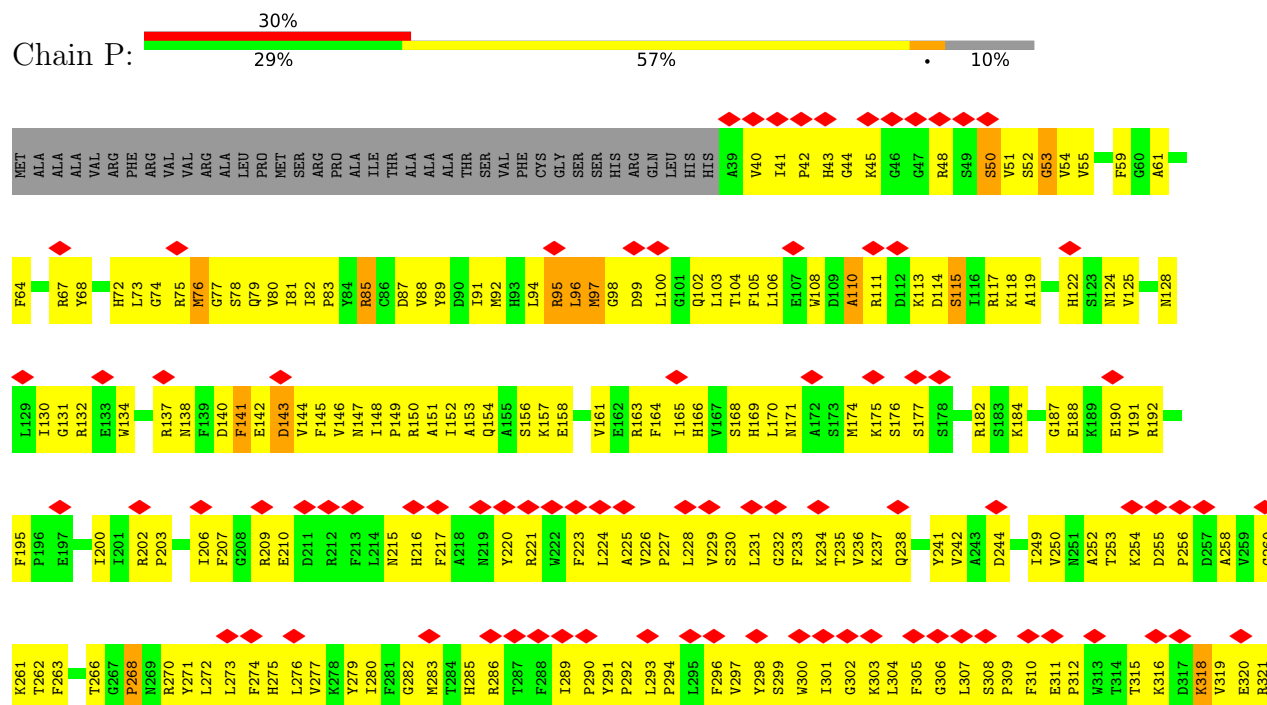




- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

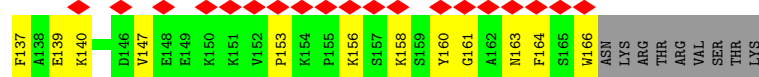
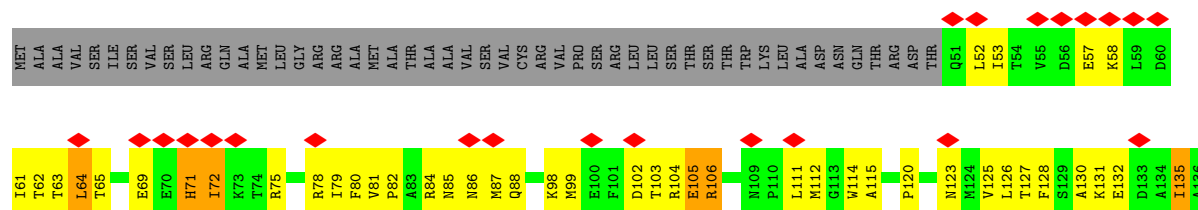


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

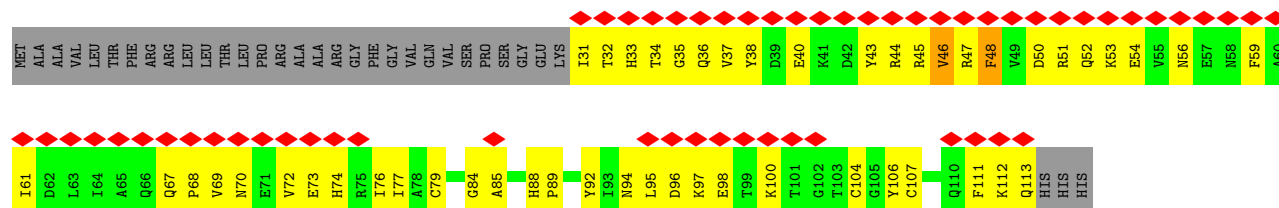




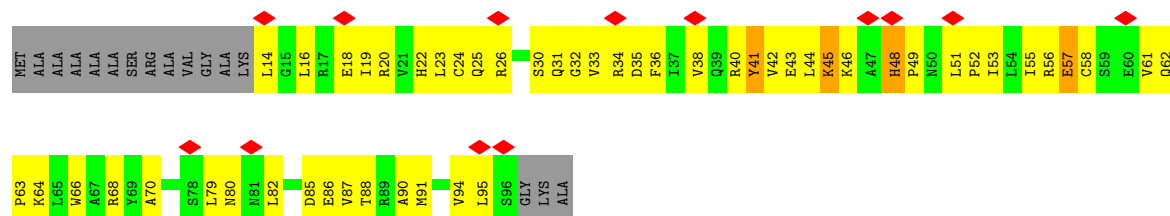
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



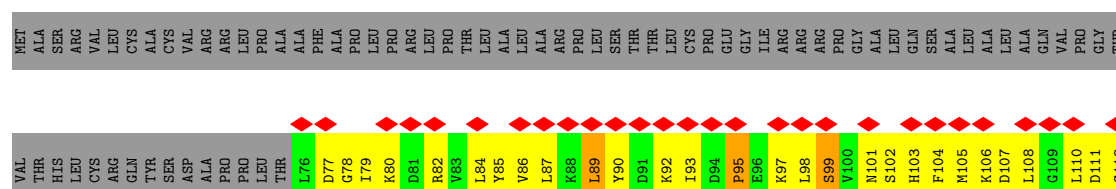
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

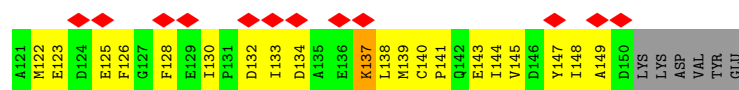


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

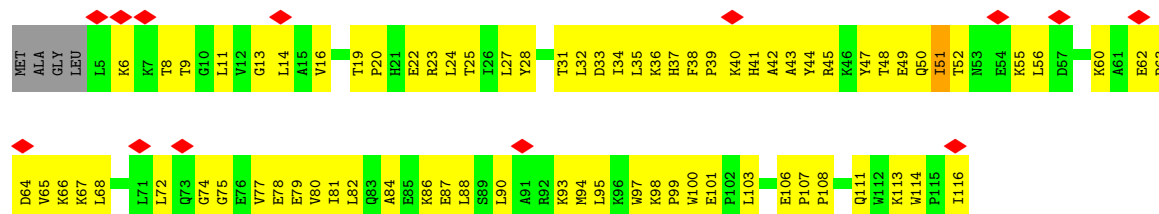


- Molecule 14: Acyl carrier protein, mitochondrial

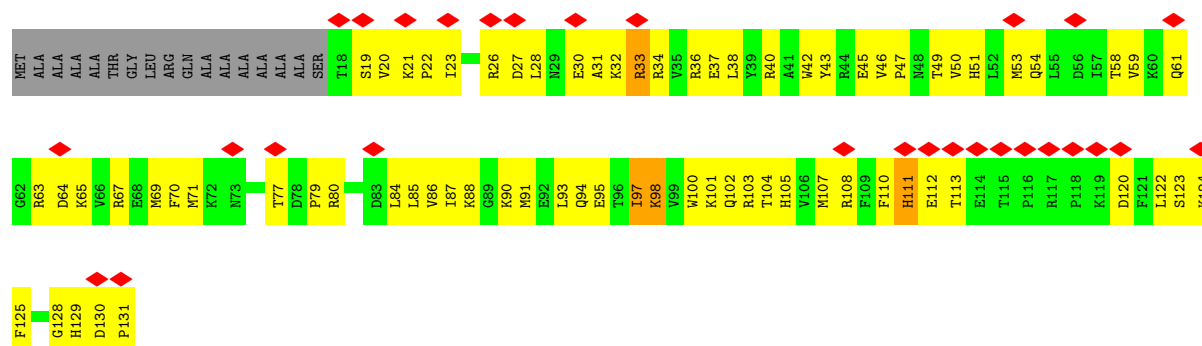




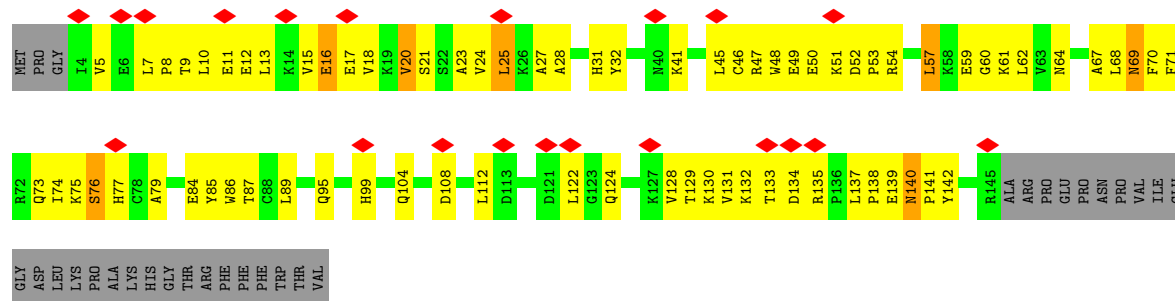
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



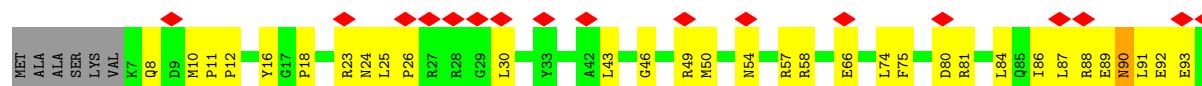
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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

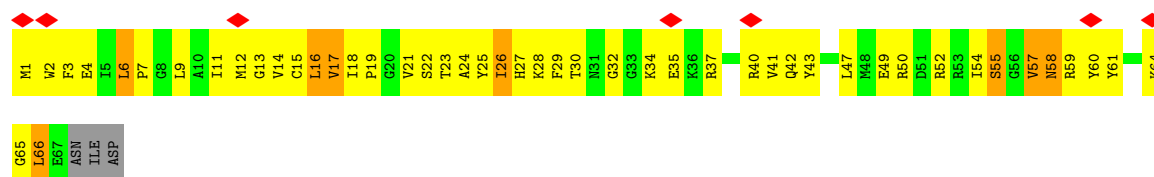


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

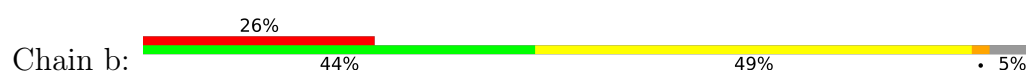




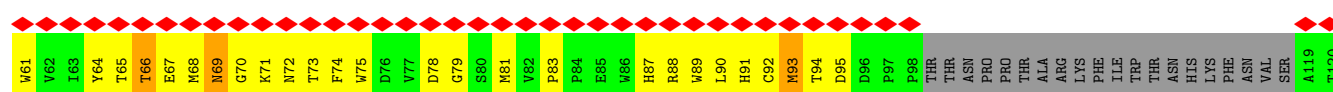
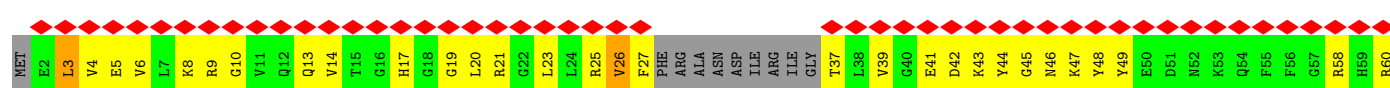
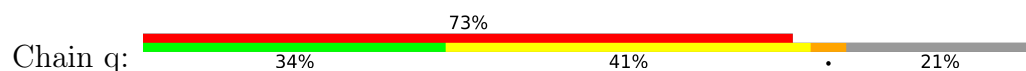
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



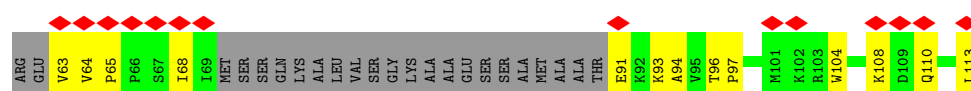
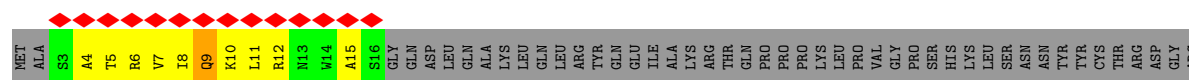
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



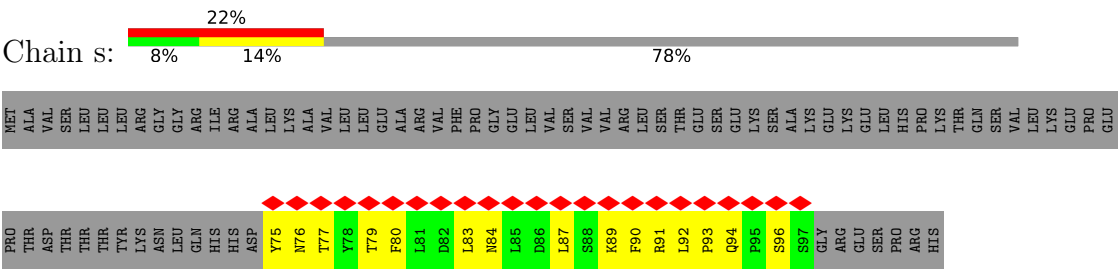
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17853	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	3.952	Depositor
Minimum map value	-1.031	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.55	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 3PE, PC1, EH2, NDP, FES, SF4, UQ9, CDL, FMN

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	0.99	0/941	1.24	10/1285 (0.8%)
2	B	1.01	1/1289 (0.1%)	1.40	15/1744 (0.9%)
3	C	1.02	1/1682 (0.1%)	1.37	18/2290 (0.8%)
4	D	0.96	6/3162 (0.2%)	1.33	28/4276 (0.7%)
5	E	0.74	0/1675	1.17	11/2282 (0.5%)
6	F	0.86	0/3363	1.47	58/4543 (1.3%)
7	G	0.91	5/5374 (0.1%)	1.49	86/7281 (1.2%)
8	H	0.90	1/2608 (0.0%)	1.46	49/3563 (1.4%)
9	I	0.75	2/1409 (0.1%)	1.22	20/1904 (1.1%)
10	P	0.75	0/2793	1.18	20/3787 (0.5%)
11	Q	0.91	1/963 (0.1%)	1.30	5/1302 (0.4%)
12	R	0.62	0/671	1.06	4/903 (0.4%)
13	S	0.79	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	0.71	1/1176 (0.1%)	1.10	7/1587 (0.4%)
19	a	0.88	0/561	1.41	12/755 (1.6%)
20	b	0.66	0/651	1.00	4/895 (0.4%)
21	q	0.66	1/983 (0.1%)	1.21	12/1336 (0.9%)
22	r	0.85	0/362	1.30	3/490 (0.6%)
23	s	0.76	0/198	1.10	0/269
All	All	0.85	20/34273 (0.1%)	1.31	393/46443 (0.8%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Q	106	ARG	C-O	9.02	1.34	1.24
18	Z	143	TYR	CA-C	-8.49	1.42	1.52
9	I	118	LEU	CA-C	8.20	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	31	LEU	CA-C	-7.27	1.43	1.52
7	G	127	ASP	CA-C	6.98	1.62	1.53
3	C	203	LEU	CA-C	-6.94	1.43	1.52
4	D	106	VAL	C-N	-6.54	1.24	1.33
4	D	140	ASP	C-N	-6.51	1.25	1.33
4	D	266	ARG	C-O	-6.32	1.16	1.24
2	B	110	PRO	C-O	-6.27	1.16	1.24
7	G	76	ARG	CA-C	6.20	1.61	1.53
7	G	192	VAL	CA-C	-6.04	1.47	1.53
4	D	392	PRO	C-O	-5.56	1.20	1.24
4	D	107	ARG	C-N	5.48	1.40	1.33
7	G	683	PRO	N-CD	-5.34	1.40	1.47
16	W	111	HIS	C-O	5.27	1.30	1.23
4	D	266	ARG	CA-C	-5.22	1.45	1.52
8	H	310	PHE	CA-C	5.06	1.59	1.52
21	q	4	VAL	CA-C	5.02	1.58	1.52
9	I	62	MET	C-O	-5.01	1.18	1.24

All (393) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	174	THR	N-CA-C	-16.87	89.00	114.64
6	F	125	CYS	N-CA-C	-15.63	93.47	113.17
7	G	77	MET	N-CA-C	-13.06	97.32	113.38
18	Z	143	TYR	N-CA-C	12.76	129.53	108.73
10	P	115	SER	N-CA-C	-12.62	97.35	113.12
6	F	171	VAL	N-CA-C	-11.93	99.32	110.53
6	F	449	ARG	N-CA-C	-11.61	98.70	111.36
9	I	118	LEU	N-CA-C	11.51	126.82	113.01
8	H	259	PHE	N-CA-C	-10.98	99.39	111.36
7	G	360	LYS	N-CA-C	-10.77	99.51	111.14
8	H	284	GLN	N-CA-C	-10.35	99.99	111.07
2	B	195	PRO	N-CA-C	-10.30	98.13	110.70
7	G	280	ASP	N-CA-C	10.24	122.45	111.28
4	D	337	MET	N-CA-C	-10.23	100.12	111.07
9	I	119	CYS	N-CA-C	10.15	126.92	113.72
7	G	414	PHE	N-CA-C	-10.08	101.48	113.88
7	G	325	ARG	N-CA-C	-9.92	100.16	110.97
6	F	178	GLU	N-CA-C	-9.85	99.29	111.11
6	F	144	VAL	N-CA-C	-9.85	101.27	110.53
9	I	50	MET	N-CA-C	9.81	121.92	111.03
6	F	141	GLY	N-CA-C	-9.77	101.17	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	103	ASN	N-CA-C	-9.76	101.06	113.16
7	G	35	PHE	N-CA-C	9.67	124.33	108.96
18	Z	144	THR	N-CA-CB	-9.65	95.10	111.50
7	G	694	PHE	N-CA-C	9.62	121.36	111.07
6	F	418	GLN	N-CA-C	-9.58	100.79	111.14
7	G	337	ALA	N-CA-C	-9.56	100.83	114.12
2	B	169	GLY	N-CA-C	-9.56	99.47	111.70
8	H	52	ALA	N-CA-C	-9.47	100.94	111.07
21	q	3	LEU	N-CA-C	-9.42	100.56	112.90
7	G	692	LYS	N-CA-C	-9.32	100.49	112.23
7	G	640	ASP	N-CA-C	-9.30	101.22	111.36
5	E	85	ALA	N-CA-C	-9.27	101.25	111.36
9	I	95	PRO	N-CA-C	-9.21	102.35	113.86
20	b	26	TRP	N-CA-C	-9.11	101.32	111.07
8	H	67	SER	N-CA-C	-9.09	98.54	110.53
3	C	180	HIS	N-CA-C	-8.92	95.73	109.64
7	G	212	LYS	N-CA-C	-8.81	94.54	108.90
19	a	66	LEU	N-CA-C	-8.72	102.42	113.23
7	G	133	GLN	N-CA-CB	8.71	121.42	110.45
21	q	66	THR	N-CA-C	-8.69	101.89	111.36
7	G	310	GLU	CB-CA-C	-8.68	106.55	116.54
4	D	88	HIS	N-CA-C	-8.55	96.93	109.50
7	G	452	LEU	N-CA-C	-8.34	102.19	111.28
18	Z	90	ASN	N-CA-C	-8.34	103.24	113.41
8	H	141	SER	N-CA-C	-8.32	102.17	111.07
21	q	64	TYR	N-CA-C	8.28	121.02	110.33
8	H	196	ALA	N-CA-C	8.25	128.04	109.81
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	-8.21	102.33	111.28
7	G	484	ASP	N-CA-C	8.20	121.14	111.71
10	P	143	ASP	N-CA-C	8.17	119.81	111.07
3	C	196	PRO	N-CA-C	8.15	124.86	113.53
2	B	110	PRO	N-CA-C	8.10	124.59	113.65
6	F	191	TYR	N-CA-C	8.09	121.64	110.24
7	G	664	TYR	N-CA-C	-8.03	97.58	109.62
22	r	10	LYS	N-CA-C	-8.03	102.94	112.89
7	G	534	VAL	N-CA-C	-8.01	104.78	111.91
7	G	361	VAL	N-CA-C	-7.97	101.36	110.05
8	H	271	LEU	N-CA-C	-7.96	102.55	111.14
6	F	364	VAL	N-CA-C	7.96	118.73	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	118	LEU	CA-C-O	7.84	129.25	119.05
8	H	253	GLU	N-CA-C	7.81	121.91	112.38
5	E	193	GLU	N-CA-C	7.80	120.58	108.96
11	Q	72	ILE	N-CA-C	-7.79	105.90	113.53
4	D	92	HIS	N-CA-C	-7.78	97.44	113.31
11	Q	139	GLU	N-CA-C	-7.75	102.78	111.07
7	G	56	VAL	N-CA-C	-7.73	102.91	110.72
10	P	95	ARG	N-CA-C	7.72	120.59	111.71
6	F	58	ARG	N-CA-C	-7.72	102.94	111.36
4	D	361	ALA	N-CA-C	-7.71	102.97	112.38
5	E	235	GLU	N-CA-C	-7.60	98.33	109.50
6	F	238	CYS	CA-C-N	-7.60	111.93	119.76
6	F	238	CYS	C-N-CA	-7.60	111.93	119.76
10	P	50	SER	N-CA-C	-7.59	98.32	109.63
9	I	190	LEU	N-CA-C	-7.55	104.68	114.04
7	G	569	GLN	N-CA-C	7.54	121.89	108.24
6	F	171	VAL	N-CA-CB	7.54	120.22	110.57
7	G	277	MET	N-CA-C	7.52	120.65	109.59
15	V	41	HIS	N-CA-CB	-7.51	101.94	110.35
7	G	497	VAL	N-CA-C	-7.50	103.22	110.42
12	R	74	HIS	N-CA-C	7.49	121.06	110.50
18	Z	142	TRP	N-CA-C	-7.49	99.20	110.28
7	G	467	LYS	N-CA-C	-7.47	102.29	111.33
6	F	430	GLY	N-CA-C	7.47	121.69	112.73
7	G	303	THR	N-CA-C	7.45	123.09	113.18
9	I	60	ILE	CB-CA-C	-7.44	103.36	110.65
4	D	99	LEU	N-CA-C	7.42	121.02	109.07
2	B	183	ARG	N-CA-C	-7.36	104.55	113.97
4	D	350	LYS	CB-CA-C	-7.35	101.05	111.85
17	X	69	ASN	N-CA-C	-7.31	102.92	111.03
8	H	309	ILE	N-CA-C	7.28	117.36	110.30
1	A	93	ILE	N-CA-C	-7.25	102.75	110.36
13	S	33	VAL	N-CA-C	-7.25	103.23	110.62
8	H	139	THR	N-CA-CB	7.23	120.50	110.01
13	S	57	GLU	N-CA-C	7.22	121.01	109.24
8	H	50	ALA	N-CA-C	7.22	118.80	111.07
14	T	99	SER	N-CA-C	-7.21	99.21	109.96
18	Z	102	PRO	N-CA-C	7.21	122.52	111.57
7	G	83	GLU	N-CA-C	7.15	120.58	110.50
7	G	465	VAL	N-CA-CB	7.14	118.44	110.51
6	F	73	PRO	N-CA-C	-7.14	103.83	113.40
8	H	254	LEU	N-CA-C	-7.11	103.58	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	97	MET	N-CA-CB	7.09	121.31	110.60
6	F	81	LYS	N-CA-C	-7.09	103.64	111.36
7	G	461	SER	N-CA-C	7.08	119.90	111.33
6	F	246	GLU	N-CA-C	-7.05	103.59	111.28
7	G	376	GLY	N-CA-C	-7.04	101.36	110.38
3	C	195	HIS	CB-CA-C	7.03	117.13	110.17
7	G	217	GLU	N-CA-C	-7.03	101.77	110.41
19	a	57	VAL	N-CA-C	-7.02	105.88	112.83
7	G	148	SER	N-CA-C	7.02	120.83	109.40
6	F	455	GLN	N-CA-C	7.01	118.57	111.07
6	F	78	GLY	N-CA-C	-7.01	104.32	112.73
6	F	169	LEU	N-CA-C	6.98	118.89	111.28
15	V	74	GLY	N-CA-C	-6.97	104.42	112.79
8	H	176	LEU	CA-C-N	-6.97	113.62	120.52
8	H	176	LEU	C-N-CA	-6.97	113.62	120.52
3	C	80	LEU	N-CA-C	-6.96	104.67	113.02
2	B	166	ASN	N-CA-C	-6.95	103.39	110.97
6	F	428	GLY	N-CA-C	-6.95	103.87	112.77
8	H	292	ASN	N-CA-C	6.95	118.94	111.36
7	G	582	VAL	N-CA-C	6.93	118.46	108.48
6	F	103	ASN	N-CA-CB	6.92	121.03	110.44
8	H	300	LEU	N-CA-C	-6.92	104.10	112.54
6	F	418	GLN	N-CA-CB	6.90	120.07	110.07
7	G	294	TYR	N-CA-C	-6.89	104.68	113.23
21	q	137	TRP	N-CA-C	-6.89	99.62	109.96
5	E	152	GLN	N-CA-C	-6.88	103.70	111.07
7	G	300	GLN	N-CA-CB	6.88	122.47	112.08
1	A	9	ILE	N-CA-C	-6.87	102.46	111.05
8	H	311	THR	N-CA-C	-6.87	104.47	112.92
6	F	148	ALA	N-CA-C	-6.85	103.89	111.36
7	G	133	GLN	N-CA-C	-6.85	101.16	110.68
12	R	46	VAL	N-CA-C	-6.85	103.63	110.62
5	E	235	GLU	N-CA-CB	6.84	122.20	109.68
8	H	305	ILE	N-CA-C	-6.81	103.38	113.39
3	C	233	ASP	CB-CA-C	-6.80	102.29	111.88
6	F	244	ASN	N-CA-C	-6.79	100.93	110.50
7	G	434	SER	N-CA-C	-6.76	100.97	110.29
9	I	119	CYS	N-CA-CB	-6.75	100.73	110.65
7	G	268	GLY	N-CA-C	6.74	124.67	115.30
18	Z	126	GLY	N-CA-C	-6.74	103.22	112.25
3	C	204	THR	N-CA-C	6.72	120.45	112.93
9	I	86	TYR	CB-CA-C	-6.71	101.28	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	104	GLN	N-CA-C	6.71	118.38	111.14
8	H	8	THR	N-CA-C	-6.70	101.24	110.35
6	F	344	GLN	N-CA-C	-6.70	103.98	111.28
4	D	85	GLY	N-CA-C	6.69	125.98	112.34
6	F	206	CYS	N-CA-C	-6.68	105.00	113.01
7	G	640	ASP	N-CA-CB	6.67	120.04	110.16
8	H	206	GLU	N-CA-C	-6.65	105.30	113.41
1	A	24	LEU	CA-C-N	-6.65	113.87	120.98
1	A	24	LEU	C-N-CA	-6.65	113.87	120.98
17	X	57	LEU	N-CA-C	-6.65	104.27	112.38
1	A	33	LYS	N-CA-C	-6.63	104.41	113.30
4	D	89	PRO	N-CA-C	-6.63	104.70	113.65
19	a	65	GLY	N-CA-C	-6.62	105.61	114.95
8	H	182	ALA	N-CA-C	-6.60	104.00	111.07
9	I	62	MET	N-CA-C	-6.60	97.97	108.73
9	I	98	ARG	N-CA-C	6.59	119.02	108.41
2	B	123	ALA	N-CA-C	6.59	118.26	111.14
7	G	189	ILE	N-CA-C	-6.59	105.29	111.48
8	H	93	HIS	CB-CA-C	6.58	117.77	108.76
7	G	287	SER	N-CA-C	6.58	119.21	110.53
4	D	184	ILE	N-CA-C	-6.56	103.93	110.62
16	W	98	LYS	N-CA-C	-6.55	102.06	110.19
7	G	605	GLN	N-CA-C	6.54	119.17	108.52
7	G	435	PRO	N-CA-C	-6.53	100.26	110.50
19	a	16	LEU	CA-C-N	-6.52	112.97	122.69
19	a	16	LEU	C-N-CA	-6.52	112.97	122.69
14	T	95	PRO	N-CA-C	-6.52	106.34	114.68
6	F	178	GLU	N-CA-CB	6.50	119.63	109.94
13	S	41	TYR	N-CA-C	-6.50	103.89	110.97
7	G	653	LEU	N-CA-CB	6.49	121.46	110.49
4	D	388	GLY	N-CA-C	6.49	119.59	110.38
6	F	234	GLY	N-CA-C	6.49	128.55	113.18
19	a	58	ASN	N-CA-C	6.48	119.28	108.73
10	P	119	ALA	N-CA-C	-6.47	104.16	111.14
8	H	267	SER	N-CA-C	-6.46	104.32	111.36
8	H	255	TYR	N-CA-CB	6.45	119.36	110.01
7	G	273	ILE	N-CA-C	-6.44	98.35	107.75
7	G	127	ASP	CA-C-O	6.43	128.99	121.78
7	G	190	ALA	N-CA-C	-6.43	99.15	109.96
8	H	177	PRO	N-CA-C	-6.43	101.54	111.13
7	G	250	SER	N-CA-C	6.42	116.75	108.34
5	E	166	LYS	N-CA-C	-6.41	105.88	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	370	LEU	N-CA-C	-6.41	104.38	111.36
10	P	224	LEU	CB-CA-C	-6.40	109.18	116.54
8	H	271	LEU	N-CA-CB	6.38	119.32	110.07
7	G	662	THR	N-CA-C	-6.37	96.52	107.61
6	F	226	LYS	CA-C-N	-6.36	113.83	120.38
6	F	226	LYS	C-N-CA	-6.36	113.83	120.38
11	Q	105	GLU	N-CA-C	6.33	119.39	109.96
6	F	144	VAL	N-CA-CB	6.31	118.65	110.57
7	G	176	CYS	N-CA-C	6.29	119.60	110.42
3	C	223	VAL	N-CA-C	6.25	117.09	108.84
8	H	269	THR	N-CA-C	6.23	118.07	111.28
9	I	86	TYR	N-CA-C	6.23	120.96	112.55
8	H	52	ALA	N-CA-CB	6.22	119.03	110.01
2	B	113	ASP	N-CA-CB	6.21	119.47	109.28
7	G	389	THR	N-CA-C	-6.21	101.22	110.23
7	G	451	ILE	N-CA-C	-6.21	104.93	113.00
6	F	415	ILE	N-CA-C	-6.21	104.45	110.72
19	a	26	ILE	N-CA-C	-6.20	104.64	113.07
7	G	356	ASP	N-CA-CB	6.20	119.23	110.12
6	F	101	PHE	N-CA-C	6.19	118.82	111.33
7	G	418	ILE	N-CA-C	-6.18	103.38	112.04
4	D	291	VAL	N-CA-C	-6.18	103.37	111.09
6	F	192	ASP	N-CA-C	6.16	118.99	109.07
21	q	5	GLU	N-CA-C	6.15	117.65	111.07
7	G	325	ARG	N-CA-CB	6.14	118.87	109.91
8	H	276	SER	N-CA-C	6.10	118.90	111.82
3	C	101	ASP	CB-CA-C	-6.09	102.89	111.85
11	Q	71	HIS	N-CA-C	-6.09	105.14	113.30
10	P	85	ARG	N-CA-C	-6.09	105.43	112.92
7	G	420	LYS	N-CA-C	6.08	118.69	111.33
10	P	361	TRP	N-CA-C	-6.07	106.86	114.56
11	Q	64	LEU	N-CA-C	-6.06	106.50	114.31
17	X	140	ASN	CA-C-N	-6.05	114.04	120.03
17	X	140	ASN	C-N-CA	-6.05	114.04	120.03
8	H	185	TRP	N-CA-C	-6.05	104.04	112.45
4	D	352	PRO	N-CA-C	6.04	118.07	110.70
10	P	268	PRO	N-CA-C	6.04	121.92	113.53
21	q	132	LYS	N-CA-CB	-6.03	107.30	114.17
8	H	7	LEU	N-CA-C	-6.03	104.34	111.03
9	I	63	TRP	N-CA-C	6.03	118.01	108.67
8	H	24	GLU	N-CA-C	-6.02	104.08	112.45
21	q	141	SER	N-CA-C	6.00	117.82	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	W	33	ARG	N-CA-C	-5.99	104.75	111.28
2	B	196	PRO	N-CA-C	-5.99	101.81	111.03
4	D	427	PRO	N-CA-C	-5.99	100.14	112.47
17	X	60	GLY	N-CA-C	-5.97	105.57	112.50
7	G	353	ALA	N-CA-C	-5.96	104.72	112.23
7	G	638	THR	N-CA-C	-5.96	100.24	109.24
7	G	651	PRO	N-CA-C	5.95	121.35	114.03
17	X	16	GLU	N-CA-C	-5.95	102.26	110.35
6	F	291	GLU	N-CA-C	5.94	118.21	110.43
8	H	315	PRO	O-C-N	5.93	123.94	121.15
8	H	103	LEU	N-CA-C	-5.93	104.90	111.36
7	G	639	LEU	N-CA-C	5.92	118.68	111.82
10	P	331	ASP	CB-CA-C	-5.92	103.37	111.95
10	P	76	MET	N-CA-C	-5.91	106.11	113.15
5	E	233	LEU	CB-CA-C	-5.91	101.60	111.23
6	F	127	ASP	N-CA-C	5.89	118.48	111.71
4	D	258	VAL	N-CA-C	-5.88	103.92	110.62
17	X	76	SER	N-CA-C	-5.87	101.94	111.04
8	H	116	ILE	N-CA-C	-5.82	104.83	110.42
9	I	85	ASN	N-CA-C	-5.82	100.78	109.15
19	a	55	SER	N-CA-C	5.82	118.13	108.13
14	T	77	ASP	N-CA-C	-5.80	107.20	114.56
7	G	672	ALA	N-CA-C	-5.79	104.96	111.28
7	G	289	LYS	N-CA-C	5.78	117.58	111.28
8	H	225	MET	N-CA-C	-5.78	104.33	111.33
16	W	97	ILE	N-CA-C	-5.78	104.87	110.42
9	I	60	ILE	N-CA-C	5.78	119.19	113.53
10	P	375	VAL	N-CA-C	5.78	118.00	108.99
2	B	135	GLY	CA-C-O	-5.76	117.97	122.52
6	F	299	LEU	N-CA-C	5.76	118.50	111.82
6	F	393	ASN	N-CA-C	-5.76	104.91	111.07
18	Z	26	PRO	N-CA-C	5.76	120.30	110.74
5	E	119	THR	N-CA-C	-5.75	105.76	112.89
4	D	414	ASP	N-CA-C	-5.75	101.45	110.36
20	b	61	GLY	N-CA-C	-5.75	107.74	115.21
10	P	44	GLY	N-CA-C	5.73	119.50	110.96
9	I	106	TYR	N-CA-C	-5.72	101.89	109.84
6	F	102	MET	CB-CA-C	-5.71	101.53	110.94
3	C	117	ASP	CA-C-N	-5.68	116.37	122.85
3	C	117	ASP	C-N-CA	-5.68	116.37	122.85
7	G	181	ARG	N-CA-C	-5.68	104.70	111.69
8	H	126	LYS	N-CA-C	5.67	117.46	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	183	PRO	N-CA-C	-5.66	102.25	110.80
6	F	176	ALA	N-CA-C	5.66	118.18	111.33
2	B	112	TYR	N-CA-C	5.65	122.83	110.80
7	G	59	GLN	N-CA-C	5.65	117.98	107.99
7	G	615	LEU	N-CA-C	-5.64	106.17	113.16
6	F	416	SER	N-CA-C	5.62	117.85	111.11
6	F	409	ILE	N-CA-C	5.62	116.35	110.62
9	I	189	LYS	N-CA-C	-5.62	106.09	113.17
2	B	71	ALA	N-CA-CB	-5.62	101.27	110.14
7	G	475	VAL	N-CA-C	5.62	115.95	107.75
2	B	201	LEU	N-CA-C	-5.61	105.16	111.28
7	G	530	TYR	N-CA-C	-5.61	101.97	110.28
6	F	304	ALA	CB-CA-C	-5.60	110.10	116.54
22	r	108	LYS	N-CA-C	5.60	117.38	111.28
6	F	457	HIS	N-CA-CB	-5.59	100.99	110.50
20	b	24	SER	N-CA-C	-5.59	107.10	114.31
8	H	76	THR	N-CA-C	-5.58	104.57	111.33
5	E	233	LEU	N-CA-C	5.58	119.91	113.38
10	P	177	SER	CB-CA-C	-5.55	103.69	111.80
2	B	167	GLY	N-CA-C	-5.55	100.03	113.18
10	P	110	ALA	N-CA-CB	-5.52	101.72	110.28
19	a	25	TYR	N-CA-C	-5.50	107.81	114.75
10	P	141	PHE	N-CA-C	-5.50	104.71	111.75
6	F	118	ASP	N-CA-C	-5.50	102.14	110.28
20	b	25	VAL	N-CA-C	-5.48	107.01	113.42
4	D	132	ALA	N-CA-C	-5.47	106.60	113.72
4	D	200	PHE	CA-CB-CG	5.47	119.27	113.80
8	H	141	SER	N-CA-CB	5.47	117.94	110.01
3	C	153	ASP	N-CA-C	5.46	117.13	110.41
7	G	82	ILE	N-CA-C	-5.45	104.06	110.21
14	T	78	GLY	N-CA-C	-5.44	106.20	112.73
4	D	141	TYR	CA-C-N	-5.44	113.71	120.56
4	D	141	TYR	C-N-CA	-5.44	113.71	120.56
7	G	420	LYS	N-CA-CB	-5.43	101.91	110.06
3	C	228	GLU	N-CA-C	-5.39	103.36	110.43
4	D	391	VAL	CA-C-N	-5.39	115.78	119.66
4	D	391	VAL	C-N-CA	-5.39	115.78	119.66
6	F	294	VAL	CA-C-N	-5.39	114.20	119.76
6	F	294	VAL	C-N-CA	-5.39	114.20	119.76
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
8	H	94	PRO	N-CA-C	5.39	118.76	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	411	SER	N-CA-C	-5.38	105.49	111.36
22	r	9	GLN	N-CA-C	5.38	118.07	111.82
10	P	53	GLY	N-CA-C	5.38	121.34	113.48
1	A	110	GLY	N-CA-C	-5.38	104.37	112.60
6	F	199	ARG	N-CA-C	5.37	117.48	109.59
7	G	652	ASN	CB-CA-C	-5.35	102.14	111.23
7	G	654	VAL	N-CA-C	-5.34	105.81	113.07
4	D	201	PHE	N-CA-C	-5.33	105.56	111.36
12	R	48	PHE	N-CA-C	5.33	119.53	113.19
8	H	46	LEU	N-CA-C	-5.29	106.59	113.16
1	A	101	GLY	N-CA-C	-5.27	106.39	112.50
7	G	356	ASP	N-CA-C	-5.27	105.54	111.28
7	G	682	ASP	CA-C-N	-5.27	114.34	119.76
7	G	682	ASP	C-N-CA	-5.27	114.34	119.76
19	a	17	VAL	CB-CA-C	-5.26	104.67	111.20
8	H	146	MET	N-CA-C	-5.26	105.44	111.07
17	X	25	LEU	N-CA-C	-5.26	105.55	111.28
6	F	412	LEU	N-CA-C	-5.25	105.73	111.82
4	D	363	VAL	N-CA-C	5.24	116.32	111.81
10	P	96	LEU	CB-CA-C	-5.24	99.65	109.72
7	G	277	MET	N-CA-CB	-5.24	101.64	109.71
7	G	435	PRO	CB-CA-C	-5.24	105.85	111.56
7	G	63	PHE	CA-C-O	-5.23	115.00	121.06
6	F	300	ILE	N-CA-CB	5.21	119.27	110.56
21	q	93	MET	N-CA-C	-5.21	105.77	111.82
14	T	137	LYS	N-CA-C	5.20	117.86	111.82
21	q	26	VAL	N-CA-CB	5.20	119.81	111.23
9	I	96	ARG	N-CA-C	5.20	119.47	113.18
8	H	310	PHE	N-CA-C	5.20	119.24	113.01
3	C	240	ALA	N-CA-CB	-5.19	102.22	110.06
17	X	20	VAL	N-CA-C	-5.18	100.74	108.46
7	G	458	GLY	N-CA-C	-5.17	108.18	115.32
6	F	131	MET	N-CA-C	-5.17	105.80	112.68
13	S	45	LYS	N-CA-C	-5.17	105.54	111.07
3	C	109	SER	N-CA-C	5.16	118.23	109.76
1	A	48	ARG	N-CA-C	-5.15	106.53	114.16
4	D	391	VAL	N-CA-C	5.15	113.81	109.02
21	q	87	HIS	N-CA-C	-5.15	105.75	111.36
7	G	172	ILE	N-CA-C	-5.14	98.65	109.34
7	G	569	GLN	CB-CA-C	-5.14	104.24	112.05
2	B	153	PRO	N-CA-C	5.13	118.41	111.22
7	G	192	VAL	CB-CA-C	-5.13	105.26	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	277	TYR	N-CA-C	5.13	117.95	110.10
8	H	90	PRO	CA-C-O	-5.12	117.44	121.38
21	q	8	LYS	N-CA-C	-5.12	105.61	111.14
7	G	713	ALA	N-CA-C	-5.11	105.60	111.07
6	F	60	GLY	N-CA-C	-5.11	106.00	114.48
8	H	101	GLY	N-CA-C	5.11	118.42	112.50
8	H	196	ALA	CA-C-N	-5.11	113.55	119.47
8	H	196	ALA	C-N-CA	-5.11	113.55	119.47
3	C	241	PHE	CB-CA-C	5.10	118.05	109.69
4	D	88	HIS	CA-C-N	-5.09	113.68	119.28
4	D	88	HIS	C-N-CA	-5.09	113.68	119.28
15	V	87	GLU	N-CA-CB	5.09	117.60	110.12
17	X	139	GLU	N-CA-C	-5.09	102.25	110.14
7	G	150	ARG	N-CA-CB	-5.09	101.89	110.49
14	T	89	LEU	N-CA-C	-5.09	105.73	111.28
3	C	181	PRO	CB-CA-C	-5.08	105.31	111.46
1	A	66	ASP	N-CA-C	-5.08	105.65	111.14
4	D	224	ALA	CA-C-O	-5.08	115.47	120.90
9	I	61	LEU	N-CA-C	-5.08	104.73	112.04
21	q	69	ASN	CB-CA-C	-5.07	110.71	116.54
3	C	139	ARG	N-CA-CB	-5.07	102.15	111.37
12	R	53	LYS	N-CA-C	5.07	116.67	108.41
8	H	254	LEU	N-CA-CB	5.05	118.11	110.28
7	G	660	GLU	N-CA-C	5.05	118.04	109.76
4	D	106	VAL	O-C-N	-5.04	116.78	122.94
10	P	52	SER	N-CA-C	-5.04	106.37	112.88
6	F	366	ALA	N-CA-C	-5.04	105.47	110.97
7	G	280	ASP	N-CA-CB	-5.04	102.72	110.12
19	a	6	LEU	CA-C-N	-5.04	113.58	119.32
19	a	6	LEU	C-N-CA	-5.04	113.58	119.32
3	C	108	LYS	N-CA-C	5.03	116.77	111.28
5	E	213	PRO	CB-CA-C	-5.03	106.30	112.89
9	I	117	LYS	N-CA-C	-5.02	103.06	113.31
2	B	94	THR	N-CA-C	5.01	117.14	109.62
1	A	69	ILE	N-CA-C	-5.01	105.10	110.36
14	T	149	ALA	N-CA-C	5.01	116.43	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	915	0	957	199	0
2	B	1258	0	1270	190	0
3	C	1636	0	1591	148	0
4	D	3088	0	3059	347	0
5	E	1635	0	1625	183	0
6	F	3288	0	3243	380	0
7	G	5287	0	5322	542	0
8	H	2532	0	2621	522	0
9	I	1380	0	1339	176	0
10	P	2720	0	2740	268	0
11	Q	940	0	930	85	0
12	R	660	0	639	72	0
13	S	667	0	685	73	0
14	T	604	0	596	72	0
15	V	915	0	954	82	0
16	W	970	0	991	97	0
17	X	1164	0	1150	113	0
18	Z	1145	0	1139	104	0
19	a	548	0	562	126	0
20	b	628	0	628	79	0
21	q	951	0	904	68	0
22	r	354	0	375	40	0
23	s	193	0	187	35	0
24	B	8	0	0	7	0
24	F	8	0	0	10	0
24	G	16	0	0	8	0
24	I	16	0	0	8	0
25	B	21	0	20	12	0
25	H	35	0	43	13	0
26	B	35	0	44	6	0
27	E	4	0	0	3	0
27	G	4	0	0	4	0
28	F	31	0	19	4	0
29	I	51	0	82	23	0
30	P	48	0	26	6	0
31	R	1	0	0	0	0
32	W	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	q	57	0	58	21	0
All	All	33848	0	33799	3241	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 48.

All (3241) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:HD1	4:D:80:MET:SD	1.36	1.47
1:A:18:ILE:CD1	8:H:222:LEU:HD22	1.47	1.43
1:A:51:PHE:CE1	4:D:80:MET:HE1	1.55	1.42
4:D:104:GLU:HG3	8:H:130:PHE:CZ	1.55	1.40
8:H:249:ILE:HD13	17:X:99:HIS:ND1	1.38	1.37
1:A:17:LEU:CD2	8:H:222:LEU:HD11	1.60	1.30
4:D:160:ASN:ND2	22:r:63:VAL:HB	1.48	1.29
1:A:17:LEU:HD22	8:H:222:LEU:CD1	1.63	1.28
1:A:51:PHE:CD1	4:D:80:MET:SD	2.26	1.28
3:C:234:LEU:HD12	3:C:234:LEU:O	1.36	1.25
1:A:2:ASN:HB2	18:Z:143:TYR:CE1	1.72	1.24
1:A:33:LYS:HG2	8:H:61:MET:CE	1.68	1.22
2:B:170:TYR:CE2	9:I:153:ILE:HD13	1.75	1.22
10:P:293:LEU:HB2	10:P:298:TYR:CE2	1.74	1.21
7:G:571:HIS:HD2	7:G:572:HIS:CD2	1.59	1.20
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.19
8:H:15:ILE:HG22	19:a:15:CYS:SG	1.82	1.19
8:H:224:PHE:CE2	8:H:228:TYR:HE2	1.61	1.18
8:H:251:LEU:HD12	8:H:251:LEU:O	1.42	1.17
3:C:87:ILE:HG13	3:C:144:THR:HG22	1.25	1.17
1:A:51:PHE:HZ	8:H:130:PHE:CE1	1.62	1.17
3:C:229:PHE:CE1	9:I:126:GLN:HG3	1.80	1.17
8:H:172:MET:HE1	18:Z:46:GLY:CA	1.75	1.17
7:G:544:MET:HE3	7:G:546:PHE:CZ	1.78	1.16
1:A:33:LYS:CG	8:H:61:MET:HE2	1.74	1.16
3:C:223:VAL:CG2	3:C:225:LEU:CD1	2.22	1.16
1:A:51:PHE:CZ	8:H:130:PHE:CE1	2.33	1.15
8:H:63:PRO:HB2	8:H:66:THR:HB	1.18	1.15
8:H:249:ILE:HG21	17:X:99:HIS:CE1	1.82	1.14
3:C:186:ILE:HG13	4:D:113:ILE:CD1	1.78	1.14
8:H:260:MET:HE1	19:a:16:LEU:HB2	1.15	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:ILE:HG22	19:a:15:CYS:HG	0.99	1.13
6:F:266:GLY:CA	6:F:271:SER:HA	1.79	1.12
7:G:358:LEU:HD12	7:G:366:LEU:CD2	1.77	1.13
6:F:293:SER:HA	6:F:336:LEU:HD13	1.22	1.12
9:I:152:CYS:SG	24:I:302:SF4:FE1	1.41	1.12
8:H:249:ILE:HD13	17:X:99:HIS:CE1	1.85	1.11
13:S:95:LEU:HD12	13:S:95:LEU:O	1.46	1.11
8:H:135:ALA:CB	8:H:201:THR:HG21	1.79	1.11
4:D:94:VAL:O	4:D:94:VAL:HG22	1.49	1.10
8:H:1:MET:HB2	19:a:30:THR:HG21	1.10	1.09
3:C:186:ILE:HG13	4:D:113:ILE:HD11	1.21	1.09
18:Z:120:LEU:HD23	18:Z:122:GLY:H	1.14	1.09
3:C:229:PHE:HE1	9:I:126:GLN:HG3	0.99	1.09
8:H:96:ILE:HG12	18:Z:143:TYR:OH	1.52	1.09
8:H:172:MET:CE	18:Z:46:GLY:HA2	1.83	1.09
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.09
1:A:18:ILE:CD1	8:H:222:LEU:CD2	2.30	1.09
8:H:1:MET:CB	19:a:30:THR:HG21	1.83	1.09
1:A:27:MET:CG	8:H:59:GLU:HG3	1.83	1.08
7:G:355:LYS:HA	7:G:366:LEU:CD1	1.82	1.08
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.12	1.08
8:H:303:TRP:HE3	20:b:29:ALA:HB2	1.10	1.08
10:P:171:ASN:HB3	10:P:327:VAL:HB	1.26	1.08
6:F:266:GLY:HA3	6:F:271:SER:CA	1.84	1.08
8:H:135:ALA:HB2	8:H:201:THR:CG2	1.82	1.08
8:H:1:MET:HB2	19:a:30:THR:CG2	1.83	1.07
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.08	1.07
3:C:187:LEU:HD23	4:D:113:ILE:CD1	1.83	1.07
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.07
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.15	1.06
5:E:131:ILE:HD11	5:E:185:VAL:HB	1.37	1.06
6:F:379:CYS:SG	24:F:502:SF4:FE4	1.46	1.06
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.36	1.06
8:H:224:PHE:CD2	25:H:400:UQ9:H15B	1.89	1.06
3:C:120:THR:HG21	15:V:116:ILE:HG21	1.36	1.06
7:G:571:HIS:CD2	7:G:572:HIS:CD2	2.44	1.06
1:A:62:PHE:CE1	8:H:144:VAL:CG2	2.39	1.05
7:G:358:LEU:HD12	7:G:366:LEU:HD21	1.06	1.05
8:H:249:ILE:CD1	17:X:99:HIS:ND1	2.20	1.05
4:D:99:LEU:HD13	4:D:101:LEU:HD13	1.38	1.05
2:B:100:CYS:SG	24:B:301:SF4:FE4	1.48	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.35	1.05
7:G:355:LYS:HA	7:G:366:LEU:HD11	1.09	1.04
8:H:1:MET:CB	19:a:30:THR:CG2	2.36	1.04
3:C:186:ILE:HG23	3:C:187:LEU:HG	1.35	1.03
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.03
8:H:142:TYR:CD1	8:H:289:LEU:HD12	1.94	1.03
10:P:350:ILE:HD11	10:P:366:ILE:HB	1.35	1.03
1:A:18:ILE:HD13	8:H:222:LEU:CD2	1.87	1.03
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.03
2:B:82:ILE:HG23	8:H:57:MET:SD	1.99	1.03
8:H:15:ILE:CG2	19:a:15:CYS:SG	2.47	1.03
1:A:51:PHE:CE1	4:D:80:MET:CE	2.42	1.02
21:q:71:LYS:HB3	21:q:73:THR:HG23	1.40	1.02
1:A:27:MET:SD	8:H:60:PRO:HD2	1.99	1.02
2:B:170:TYR:CE2	9:I:153:ILE:CD1	2.41	1.02
1:A:27:MET:HG2	8:H:59:GLU:CG	1.89	1.02
6:F:300:ILE:HG23	6:F:305:GLY:O	1.58	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.38	1.01
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	1.01
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.01
6:F:382:CYS:SG	24:F:502:SF4:FE3	1.50	1.01
8:H:19:PHE:CE2	19:a:11:ILE:HG21	1.95	1.01
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.41	1.00
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.99
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.43	0.99
3:C:160:ILE:HD12	4:D:285:ASN:HD21	1.24	0.99
8:H:224:PHE:CE2	8:H:228:TYR:CE2	2.49	0.99
9:I:61:LEU:HD11	29:I:301:3PE:H381	1.44	0.99
9:I:48:VAL:HG21	20:b:11:ASN:HB3	1.46	0.98
3:C:223:VAL:HG22	3:C:225:LEU:CD1	1.90	0.97
6:F:118:ASP:HA	6:F:159:ARG:HG3	1.45	0.97
8:H:96:ILE:HG23	18:Z:143:TYR:CZ	1.98	0.97
21:q:78:ASP:HB2	21:q:81:MET:HG3	1.42	0.97
8:H:1:MET:CG	19:a:30:THR:HG22	1.94	0.97
8:H:316:PRO:HG3	18:Z:57:ARG:CB	1.91	0.97
6:F:382:CYS:HG	24:F:502:SF4:FE3	0.76	0.97
8:H:1:MET:HG3	19:a:30:THR:HG22	1.43	0.97
8:H:99:ASN:HD21	19:a:40:ARG:HA	1.27	0.97
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.99	0.97
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.96
3:C:152:ILE:HD11	3:C:177:PHE:CE2	1.99	0.96
3:C:223:VAL:CG2	3:C:225:LEU:HD11	1.92	0.96
9:I:171:PRO:CB	21:q:93:MET:HE1	1.96	0.96
4:D:348:LEU:O	18:Z:11:PRO:HG3	1.65	0.96
7:G:75:CYS:SG	27:G:803:FES:FE1	1.57	0.96
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.96
8:H:260:MET:CE	19:a:16:LEU:HB2	1.94	0.96
9:I:123:CYS:HG	24:I:302:SF4:FE2	0.67	0.96
1:A:62:PHE:CD1	8:H:144:VAL:HG21	2.00	0.96
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.96
2:B:93:MET:HE1	2:B:131:MET:HE2	1.47	0.96
19:a:58:ASN:HD22	19:a:60:TYR:HE1	1.10	0.96
1:A:62:PHE:CD1	8:H:144:VAL:CG2	2.48	0.96
2:B:82:ILE:HG12	8:H:57:MET:CE	1.94	0.96
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.96
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.28	0.96
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.96
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.95
10:P:220:TYR:HD2	10:P:226:VAL:HG13	1.29	0.95
14:T:138:LEU:HD12	14:T:138:LEU:O	1.66	0.95
6:F:300:ILE:HG22	6:F:306:GLY:HA2	1.47	0.95
8:H:303:TRP:CE3	20:b:29:ALA:HB2	2.00	0.95
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.95
7:G:611:THR:HG21	11:Q:105:GLU:CA	1.95	0.95
8:H:260:MET:HE1	19:a:16:LEU:CB	1.97	0.95
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.32	0.95
3:C:186:ILE:HG13	4:D:113:ILE:CG1	1.95	0.95
10:P:306:GLY:HA2	10:P:312:PRO:HB3	1.48	0.94
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.48	0.94
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.94
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.94
1:A:27:MET:HG2	8:H:59:GLU:HG3	0.96	0.94
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.94
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.94
7:G:544:MET:HE3	7:G:546:PHE:CE1	2.03	0.94
7:G:674:LEU:HD11	13:S:46:LYS:HE2	1.49	0.94
9:I:61:LEU:HD21	29:I:301:3PE:H391	1.50	0.94
7:G:338:VAL:CG1	7:G:546:PHE:HE1	1.81	0.94
8:H:1:MET:HG3	19:a:30:THR:CG2	1.98	0.94
3:C:160:ILE:HD12	4:D:285:ASN:ND2	1.84	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:293:SER:CA	6:F:336:LEU:HD13	1.97	0.93
4:D:160:ASN:ND2	22:r:63:VAL:CB	2.31	0.93
7:G:661:GLU:O	7:G:661:GLU:HG2	1.68	0.93
1:A:39:CYS:HB3	4:D:85:GLY:HA3	1.51	0.93
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.51	0.93
1:A:51:PHE:CZ	8:H:130:PHE:CD1	2.57	0.93
1:A:17:LEU:HB3	8:H:222:LEU:HD21	1.50	0.93
18:Z:97:ILE:HG23	18:Z:98:MET:HG3	1.51	0.92
4:D:104:GLU:HG3	8:H:130:PHE:CE1	2.03	0.92
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.32	0.92
5:E:134:CYS:HG	27:E:301:FES:FE1	0.66	0.92
7:G:541:PRO:HB2	7:G:561:PRO:HD3	1.52	0.92
3:C:187:LEU:HD23	4:D:113:ILE:HD12	1.51	0.92
7:G:611:THR:CG2	11:Q:105:GLU:HA	1.99	0.92
7:G:358:LEU:CD1	7:G:366:LEU:HD21	1.99	0.92
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.92
9:I:113:CYS:HG	24:I:303:SF4:FE3	0.63	0.92
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.92
3:C:160:ILE:CD1	4:D:285:ASN:ND2	2.33	0.92
14:T:99:SER:HB2	14:T:102:SER:HB3	1.48	0.91
7:G:182:CYS:SG	24:G:802:SF4:FE2	1.62	0.91
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.91
8:H:1:MET:HE3	19:a:26:ILE:HG23	1.50	0.91
3:C:87:ILE:HG13	3:C:144:THR:CG2	2.00	0.91
7:G:404:GLY:HA2	7:G:684:LEU:HD13	1.52	0.91
1:A:51:PHE:CD1	4:D:80:MET:CE	2.52	0.91
7:G:176:CYS:HG	24:G:802:SF4:FE4	0.62	0.91
6:F:379:CYS:HG	24:F:502:SF4:FE4	0.62	0.91
10:P:168:SER:O	10:P:202:ARG:HA	1.71	0.91
1:A:25:PRO:HB3	8:H:57:MET:O	1.69	0.91
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.52	0.90
2:B:170:TYR:HE2	9:I:153:ILE:CD1	1.78	0.90
8:H:16:ALA:HB2	19:a:15:CYS:HB3	1.53	0.90
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.86	0.90
19:a:64:LYS:HE2	19:a:66:LEU:HB2	1.51	0.90
4:D:232:VAL:HG12	4:D:356:ILE:HD13	1.53	0.90
3:C:234:LEU:O	3:C:234:LEU:CD1	2.20	0.90
8:H:1:MET:CG	19:a:30:THR:CG2	2.49	0.90
10:P:268:PRO:HG3	10:P:342:PRO:HB2	1.54	0.90
1:A:51:PHE:CZ	8:H:130:PHE:HE1	1.81	0.90
11:Q:57:GLU:OE1	11:Q:58:LYS:HG2	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
1:A:18:ILE:HD13	8:H:222:LEU:HD22	0.91	0.89
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.89
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.89
3:C:160:ILE:CD1	4:D:285:ASN:HD21	1.84	0.89
1:A:51:PHE:CD1	4:D:80:MET:HE1	2.08	0.89
8:H:16:ALA:HB2	19:a:15:CYS:CB	2.03	0.89
1:A:51:PHE:HZ	8:H:130:PHE:HE1	0.95	0.89
6:F:213:ILE:HG23	6:F:235:VAL:HG22	1.54	0.89
7:G:662:THR:HG23	7:G:662:THR:O	1.71	0.89
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.85	0.88
1:A:52:SER:O	4:D:103:GLY:HA3	1.72	0.88
2:B:81:LEU:HG	26:B:303:PC1:H261	1.52	0.88
8:H:249:ILE:HG21	17:X:99:HIS:HE1	1.32	0.88
17:X:20:VAL:HG23	17:X:25:LEU:CD1	2.03	0.88
7:G:355:LYS:CA	7:G:366:LEU:HD11	2.02	0.88
9:I:152:CYS:HG	24:I:302:SF4:FE1	0.61	0.88
3:C:229:PHE:HE1	9:I:126:GLN:CG	1.86	0.88
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.37	0.88
4:D:101:LEU:HD11	4:D:106:VAL:HG22	1.56	0.88
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.56	0.88
8:H:135:ALA:HB2	8:H:201:THR:HG21	1.40	0.88
10:P:293:LEU:HB2	10:P:298:TYR:CZ	2.07	0.88
3:C:223:VAL:HG21	3:C:225:LEU:HD11	1.56	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
1:A:51:PHE:HE1	4:D:80:MET:HE1	0.93	0.88
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.88	0.88
19:a:58:ASN:HB3	19:a:60:TYR:CD1	2.08	0.88
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.38	0.88
5:E:68:ASN:ND2	23:s:84:ASN:HD21	1.71	0.87
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.09	0.87
1:A:62:PHE:HD1	8:H:144:VAL:HG21	1.35	0.87
10:P:293:LEU:HB2	10:P:298:TYR:HE2	1.34	0.87
1:A:37:TYR:HE2	8:H:208:VAL:HG21	1.40	0.87
4:D:93:GLY:O	4:D:94:VAL:CG1	2.22	0.87
6:F:110:PRO:HB3	6:F:152:ARG:HE	1.39	0.87
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.87
7:G:615:LEU:HG	10:P:41:ILE:HG23	1.57	0.87
17:X:130:LYS:HD2	20:b:59:ASP:OD1	1.74	0.87
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.86
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:129:GLU:OE2	6:F:287:THR:HB	1.75	0.86
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.74	0.86
10:P:293:LEU:CB	10:P:298:TYR:CE2	2.59	0.86
7:G:608:VAL:HG23	11:Q:103:THR:HB	1.57	0.86
1:A:18:ILE:HD11	8:H:222:LEU:HD22	1.55	0.86
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.39	0.86
11:Q:52:LEU:HD22	16:W:19:SER:HB3	1.58	0.86
6:F:45:LEU:HD11	6:F:129:GLU:CD	2.01	0.86
10:P:55:VAL:HG21	12:R:43:TYR:HB2	1.58	0.86
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.86
18:Z:120:LEU:HD23	18:Z:122:GLY:N	1.90	0.86
2:B:95:PHE:CZ	2:B:141:MET:HE2	2.09	0.85
2:B:95:PHE:HZ	2:B:141:MET:HE2	1.39	0.85
8:H:59:GLU:CD	8:H:61:MET:SD	2.58	0.85
3:C:87:ILE:CG1	3:C:144:THR:HG22	2.05	0.85
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.85
8:H:135:ALA:HB2	8:H:201:THR:HG22	1.58	0.85
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.58	0.85
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.58	0.85
10:P:220:TYR:CD2	10:P:226:VAL:HG13	2.12	0.85
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.85
7:G:126:LEU:O	7:G:126:LEU:CD1	2.24	0.85
7:G:662:THR:O	7:G:662:THR:CG2	2.25	0.85
7:G:388:ASN:H	7:G:514:ASN:CB	1.90	0.85
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.07	0.85
1:A:62:PHE:HE1	8:H:144:VAL:CG2	1.87	0.84
4:D:94:VAL:O	4:D:94:VAL:CG2	2.24	0.84
1:A:18:ILE:HD11	8:H:222:LEU:CD2	2.07	0.84
4:D:99:LEU:HD12	4:D:99:LEU:O	1.78	0.84
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.84
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.84
14:T:117:GLU:HA	14:T:120:MET:HE2	1.58	0.84
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.77	0.84
9:I:54:THR:HA	20:b:13:TRP:HE1	1.42	0.84
2:B:202:LEU:HD12	9:I:86:TYR:CD2	2.13	0.84
6:F:293:SER:HA	6:F:336:LEU:CD1	2.05	0.84
10:P:96:LEU:C	10:P:96:LEU:HD12	2.03	0.84
2:B:170:TYR:CE1	4:D:135:TYR:CZ	2.65	0.84
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.84
13:S:95:LEU:O	13:S:95:LEU:CD1	2.26	0.84
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.92	0.83
7:G:617:ARG:HH12	16:W:128:GLY:C	1.86	0.83
8:H:135:ALA:HB1	8:H:201:THR:HG21	1.60	0.83
17:X:7:LEU:HD12	18:Z:91:LEU:HD22	1.58	0.83
4:D:271:ARG:HD2	8:H:279:ARG:O	1.78	0.83
1:A:41:PHE:HA	16:W:102:GLN:NE2	1.94	0.83
6:F:254:ILE:HA	6:F:262:PHE:CE1	2.13	0.83
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.83
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.14	0.83
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.83
5:E:68:ASN:HD21	23:s:84:ASN:HD21	1.27	0.83
6:F:425:CYS:SG	24:F:502:SF4:FE1	1.70	0.83
23:s:87:LEU:HA	23:s:90:PHE:HD2	1.44	0.83
5:E:68:ASN:HD21	23:s:84:ASN:ND2	1.76	0.82
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.10	0.82
7:G:544:MET:CE	7:G:546:PHE:CZ	2.61	0.82
3:C:223:VAL:CG2	3:C:225:LEU:HD12	2.08	0.82
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.44	0.82
1:A:62:PHE:CE1	8:H:144:VAL:HG23	2.14	0.82
12:R:47:ARG:HB2	21:q:125:VAL:HG11	1.61	0.82
6:F:425:CYS:HG	24:F:502:SF4:FE1	0.52	0.82
3:C:186:ILE:CG1	4:D:113:ILE:HD11	2.08	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.61	0.82
7:G:403:VAL:HG23	7:G:432:ILE:HB	1.61	0.82
8:H:310:PHE:HB3	20:b:33:PRO:HA	1.62	0.82
11:Q:131:LYS:HG2	11:Q:135:ILE:CD1	2.09	0.82
15:V:72:LEU:HD13	15:V:80:VAL:HG11	1.62	0.81
1:A:69:ILE:HD11	8:H:144:VAL:HG13	1.60	0.81
4:D:93:GLY:C	4:D:94:VAL:HG12	2.05	0.81
17:X:18:VAL:HG21	18:Z:74:LEU:HD11	1.60	0.81
2:B:193:GLY:HA2	9:I:154:TYR:CE2	2.16	0.81
7:G:617:ARG:HH12	16:W:129:HIS:N	1.79	0.81
23:s:92:LEU:HB2	23:s:93:PRO:HD2	1.62	0.81
10:P:104:THR:HG21	12:R:46:VAL:HG12	1.60	0.81
4:D:104:GLU:HG3	8:H:130:PHE:HZ	1.02	0.81
18:Z:120:LEU:CD2	18:Z:122:GLY:H	1.94	0.81
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
1:A:21:ALA:O	8:H:60:PRO:HG3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:89:VAL:HB	7:G:94:MET:HG3	1.62	0.81
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.16	0.81
4:D:104:GLU:CG	8:H:130:PHE:CZ	2.52	0.81
14:T:82:ARG:HD2	14:T:125:GLU:HG3	1.61	0.81
17:X:86:TRP:CZ2	19:a:64:LYS:HA	2.16	0.81
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.81
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
7:G:388:ASN:H	7:G:514:ASN:HB3	1.45	0.80
9:I:89:GLU:HG2	21:q:61:TRP:HB3	1.62	0.80
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.63	0.80
7:G:355:LYS:CA	7:G:366:LEU:CD1	2.58	0.80
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.80
1:A:62:PHE:HA	8:H:290:TRP:HH2	1.46	0.80
8:H:256:SER:O	8:H:260:MET:HG2	1.82	0.80
10:P:363:SER:HA	16:W:54:GLN:HE22	1.46	0.80
17:X:18:VAL:HG12	17:X:20:VAL:HG22	1.63	0.80
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.80
1:A:17:LEU:HD22	8:H:222:LEU:HD11	0.81	0.80
6:F:227:PRO:HB2	6:F:228:PRO:HD3	1.62	0.80
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.80
8:H:181:MET:CE	8:H:304:HIS:ND1	2.45	0.80
1:A:41:PHE:CD2	16:W:102:GLN:NE2	2.50	0.79
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.62	0.79
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.22	0.79
6:F:266:GLY:HA3	6:F:271:SER:HA	0.89	0.79
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.98	0.79
7:G:73:GLY:HA2	27:G:803:FES:S1	2.22	0.79
10:P:226:VAL:HG12	10:P:228:LEU:HG	1.63	0.79
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.63	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
1:A:75:LEU:CB	8:H:155:LEU:HD21	2.12	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
7:G:338:VAL:HG13	7:G:546:PHE:HE1	1.47	0.79
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.45	0.79
10:P:51:VAL:HG22	10:P:53:GLY:H	1.48	0.79
10:P:171:ASN:HB3	10:P:327:VAL:CB	2.10	0.79
8:H:142:TYR:OH	8:H:288:LEU:HD22	1.82	0.79
8:H:306:SER:HG	8:H:310:PHE:HE2	1.27	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
7:G:75:CYS:HG	27:G:803:FES:FE1	0.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
3:C:187:LEU:CD2	4:D:113:ILE:CD1	2.61	0.79
8:H:251:LEU:O	8:H:251:LEU:CD1	2.28	0.79
10:P:88:VAL:HG13	10:P:91:ILE:HD11	1.64	0.79
2:B:89:SER:O	8:H:54:LYS:HD3	1.82	0.78
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.78
1:A:2:ASN:HB2	18:Z:143:TYR:CZ	2.19	0.78
7:G:226:CYS:HG	24:G:802:SF4:FE1	1.00	0.78
4:D:160:ASN:HD22	22:r:63:VAL:HB	1.46	0.78
6:F:224:ARG:HD3	11:Q:164:PHE:CE1	2.19	0.78
8:H:35:LYS:HG3	9:I:83:THR:OG1	1.84	0.78
14:T:106:LYS:H	14:T:106:LYS:HD2	1.48	0.78
2:B:121:PHE:HE2	25:B:302:UQ9:H1MB	1.48	0.78
4:D:160:ASN:HD21	22:r:63:VAL:HB	1.49	0.78
10:P:225:ALA:CB	10:P:289:ILE:HB	2.13	0.78
2:B:89:SER:O	8:H:54:LYS:CD	2.32	0.78
3:C:147:ASP:OD1	3:C:148:GLU:OE1	2.00	0.78
6:F:424:ILE:HD11	7:G:73:GLY:O	1.84	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.66	0.78
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.78
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.13	0.78
3:C:170:TRP:CG	3:C:183:LEU:HD21	2.18	0.78
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.78
8:H:65:THR:HB	8:H:124:ASN:HD22	1.49	0.78
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.78
2:B:170:TYR:CD2	9:I:153:ILE:HD13	2.18	0.77
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.77
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.66	0.77
7:G:544:MET:HE3	7:G:546:PHE:HZ	1.39	0.77
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.77
2:B:171:TYR:CD2	4:D:118:ARG:HB3	2.19	0.77
5:E:196:THR:H	5:E:199:ASP:HB2	1.47	0.77
6:F:36:LYS:HB3	6:F:38:GLU:HG2	1.66	0.77
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.77
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.65	0.77
10:P:217:PHE:HB2	10:P:280:ILE:HD13	1.66	0.77
3:C:70:LYS:HD3	15:V:101:GLU:HB2	1.67	0.77
3:C:89:PRO:O	3:C:92:VAL:HG23	1.85	0.77
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.77
1:A:51:PHE:CE1	4:D:103:GLY:HA2	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:188:GLU:HG2	10:P:200:ILE:HD13	1.64	0.77
4:D:104:GLU:CG	8:H:130:PHE:HZ	1.92	0.76
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.50	0.76
17:X:20:VAL:HG23	17:X:25:LEU:HD11	1.67	0.76
3:C:103:THR:HG21	15:V:55:LYS:HE3	1.66	0.76
7:G:355:LYS:HG3	7:G:366:LEU:HD12	1.67	0.76
8:H:91:MET:O	8:H:92:PRO:C	2.26	0.76
2:B:105:MET:HE1	25:B:302:UQ9:H3MA	1.66	0.76
10:P:221:ARG:HD2	10:P:286:ARG:HD2	1.67	0.76
4:D:320:ILE:CG1	9:I:36:TYR:HB2	2.16	0.76
10:P:225:ALA:HB1	10:P:289:ILE:HB	1.68	0.76
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.66	0.76
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.76
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.66	0.76
1:A:62:PHE:CE1	8:H:144:VAL:HG22	2.19	0.76
7:G:632:ILE:HG13	7:G:632:ILE:O	1.84	0.76
9:I:61:LEU:HD21	29:I:301:3PE:C39	2.15	0.76
11:Q:64:LEU:HG	16:W:84:LEU:HD12	1.68	0.76
10:P:266:THR:HG21	10:P:329:PRO:HG3	1.67	0.76
13:S:22:HIS:C	13:S:58:CYS:SG	2.69	0.76
1:A:41:PHE:HA	16:W:102:GLN:HE22	1.49	0.75
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.75
8:H:23:VAL:HG11	19:a:9:LEU:HD21	1.66	0.75
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.75
10:P:301:ILE:HG22	10:P:305:PHE:HE2	1.52	0.75
10:P:359:TYR:O	10:P:360:ARG:HB3	1.86	0.75
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.21	0.75
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.21	0.75
4:D:299:GLN:NE2	9:I:36:TYR:CE2	2.54	0.75
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.75
7:G:335:GLY:HA3	7:G:362:ASP:HB3	1.68	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
7:G:652:ASN:HB3	7:G:655:ARG:NH2	2.01	0.75
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.22	0.75
8:H:135:ALA:CB	8:H:201:THR:CG2	2.49	0.75
14:T:123:GLU:HG2	14:T:130:ILE:HG12	1.65	0.75
17:X:128:VAL:O	17:X:128:VAL:HG23	1.86	0.75
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.05	0.75
2:B:170:TYR:CD2	9:I:153:ILE:HG21	2.22	0.75
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.01	0.75
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:35:LEU:HD13	15:V:48:THR:HG23	1.68	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.75
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.75
7:G:126:LEU:HD13	12:R:89:PRO:HB3	1.67	0.75
8:H:99:ASN:HD21	19:a:40:ARG:CA	1.98	0.75
8:H:19:PHE:CD2	19:a:11:ILE:HG21	2.22	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
10:P:272:LEU:HG	10:P:375:VAL:HG21	1.68	0.75
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.75
5:E:176:LEU:HD12	5:E:184:MET:HE3	1.69	0.75
2:B:89:SER:O	8:H:54:LYS:HE2	1.87	0.74
2:B:68:ARG:HD3	2:B:70:ARG:HG2	1.69	0.74
7:G:127:ASP:HA	12:R:106:TYR:OH	1.86	0.74
4:D:128:THR:H	4:D:131:GLN:HE21	1.35	0.74
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.22	0.74
9:I:180:HIS:CD2	10:P:100:LEU:HD21	2.21	0.74
11:Q:69:GLU:O	11:Q:72:ILE:HG22	1.86	0.74
6:F:184:LYS:HB3	23:s:92:LEU:HD22	1.67	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
17:X:49:GLU:HG3	17:X:50:GLU:HG3	1.70	0.74
10:P:96:LEU:HD12	10:P:97:MET:N	2.01	0.74
1:A:80:GLN:C	20:b:46:ASN:HD21	1.95	0.74
3:C:152:ILE:HD11	3:C:177:PHE:HE2	1.51	0.74
8:H:310:PHE:CD2	20:b:33:PRO:HG3	2.23	0.74
3:C:223:VAL:HG22	3:C:225:LEU:HD12	1.68	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
7:G:382:ARG:HG2	7:G:386:LEU:HD11	1.69	0.74
8:H:5:ASN:ND2	19:a:23:THR:HA	2.03	0.74
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.69	0.74
12:R:31:ILE:HG12	12:R:37:VAL:HB	1.70	0.74
8:H:96:ILE:HG12	18:Z:143:TYR:HH	1.51	0.73
9:I:90:LYS:HB2	21:q:90:LEU:CD2	2.17	0.73
9:I:123:CYS:SG	24:I:302:SF4:FE2	1.79	0.73
10:P:55:VAL:HG21	12:R:43:TYR:CB	2.18	0.73
13:S:42:VAL:HG13	13:S:43:GLU:CD	2.13	0.73
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.70	0.73
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.22	0.73
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.73
8:H:5:ASN:OD1	19:a:23:THR:HA	1.88	0.73
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.69	0.73
6:F:392:MET:CE	6:F:419:ILE:HD12	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:3:LEU:HD13	33:q:201:CDL:H521	1.70	0.73
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.69	0.73
4:D:238:LEU:HB2	9:I:211:TYR:OH	1.89	0.73
3:C:118:VAL:HG12	3:C:120:THR:HG22	1.69	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
17:X:130:LYS:HD2	20:b:59:ASP:CG	2.12	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73
8:H:99:ASN:ND2	19:a:40:ARG:HA	2.03	0.73
1:A:2:ASN:CB	18:Z:143:TYR:CE1	2.65	0.73
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.71	0.73
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.73
6:F:228:PRO:HG2	11:Q:160:TYR:HD2	1.53	0.73
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.24	0.73
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.73
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.73
10:P:134:TRP:HB3	10:P:312:PRO:HG3	1.71	0.73
4:D:93:GLY:O	4:D:94:VAL:HG12	1.89	0.73
4:D:93:GLY:O	4:D:94:VAL:HG13	1.88	0.73
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.70	0.73
8:H:5:ASN:CG	19:a:23:THR:HA	2.13	0.73
6:F:67:GLU:HG3	6:F:71:LYS:HE3	1.70	0.73
7:G:182:CYS:HG	24:G:802:SF4:FE2	0.48	0.73
10:P:73:LEU:HA	10:P:76:MET:HE2	1.71	0.73
18:Z:129:THR:HG23	18:Z:132:GLU:H	1.52	0.73
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.70	0.72
2:B:172:HIS:CD2	2:B:179:ARG:HG2	2.23	0.72
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.54	0.72
8:H:94:PRO:O	19:a:27:HIS:HE1	1.70	0.72
10:P:274:PHE:HE1	10:P:290:PRO:HG3	1.54	0.72
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.71	0.72
1:A:68:GLU:CD	1:A:98:LEU:HG	2.13	0.72
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.72
1:A:62:PHE:HE1	8:H:144:VAL:HG23	1.50	0.72
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.72
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.72
10:P:276:LEU:HD23	10:P:280:ILE:HD12	1.72	0.72
1:A:17:LEU:HD21	8:H:56:PHE:CZ	2.24	0.72
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.69	0.72
8:H:205:SER:HB2	8:H:279:ARG:HH22	1.55	0.72
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.72	0.72
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.20	0.72
8:H:66:THR:HG23	8:H:67:SER:O	1.89	0.72
8:H:172:MET:SD	18:Z:46:GLY:HA2	2.28	0.72
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.20	0.72
2:B:105:MET:CE	25:B:302:UQ9:H3MA	2.18	0.72
10:P:226:VAL:CG1	10:P:228:LEU:HG	2.19	0.72
15:V:28:TYR:OH	15:V:55:LYS:HD3	1.89	0.72
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.70	0.72
8:H:172:MET:HE1	18:Z:46:GLY:HA3	1.71	0.72
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.72
9:I:154:TYR:HA	9:I:169:GLU:OE2	1.90	0.72
10:P:64:PHE:HE1	10:P:209:ARG:O	1.72	0.72
19:a:64:LYS:HE2	19:a:66:LEU:CB	2.19	0.72
2:B:121:PHE:CE2	25:B:302:UQ9:H1MB	2.24	0.72
2:B:170:TYR:CZ	9:I:124:PRO:HB2	2.25	0.72
2:B:170:TYR:OH	9:I:124:PRO:CB	2.38	0.72
10:P:124:ASN:OD1	10:P:125:VAL:HG23	1.89	0.72
10:P:270:ARG:HH21	10:P:327:VAL:C	1.98	0.72
13:S:25:GLN:HG3	13:S:57:GLU:CD	2.15	0.72
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.24	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.71	0.71
8:H:65:THR:HB	8:H:124:ASN:ND2	2.05	0.71
10:P:157:LYS:HB2	10:P:195:PHE:HD1	1.55	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	0.71
5:E:71:GLU:HG3	23:s:94:GLN:HE21	1.54	0.71
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.90	0.71
2:B:105:MET:HE2	25:B:302:UQ9:C3	2.19	0.71
6:F:258:GLY:O	6:F:261:TRP:HB3	1.89	0.71
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.71
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
3:C:187:LEU:HD23	4:D:113:ILE:HD13	1.72	0.71
5:E:185:VAL:HG22	5:E:195:LEU:HD13	1.72	0.71
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.71
8:H:9:LEU:HA	19:a:19:PRO:HB3	1.71	0.71
8:H:260:MET:SD	19:a:16:LEU:C	2.73	0.71
10:P:174:MET:O	10:P:175:LYS:HG2	1.91	0.71
19:a:58:ASN:ND2	19:a:60:TYR:HE1	1.84	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:87:ILE:HG22	16:W:91:MET:HE3	1.73	0.71
2:B:136:THR:HG21	2:B:177:VAL:HG22	1.73	0.71
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
13:S:79:LEU:HA	13:S:82:LEU:HG	1.73	0.71
3:C:120:THR:CG2	15:V:116:ILE:HG21	2.18	0.71
7:G:544:MET:CE	7:G:546:PHE:HZ	2.01	0.71
9:I:49:ASP:C	20:b:10:LYS:NZ	2.49	0.71
11:Q:82:PRO:HD3	11:Q:98:LYS:HG3	1.70	0.71
14:T:104:PHE:HB3	14:T:110:LEU:HD22	1.71	0.71
5:E:240:PRO:HB3	6:F:60:GLY:HA3	1.73	0.70
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.70
7:G:266:ARG:HH12	9:I:131:GLU:HG2	1.54	0.70
9:I:61:LEU:CD1	29:I:301:3PE:H381	2.20	0.70
10:P:165:ILE:HD13	10:P:253:THR:HG22	1.73	0.70
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.70
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.70
4:D:215:GLU:OE2	9:I:93:LEU:HD22	1.90	0.70
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.70
8:H:310:PHE:CB	20:b:33:PRO:HA	2.19	0.70
8:H:316:PRO:HG3	18:Z:57:ARG:HB2	1.73	0.70
1:A:113:TRP:HZ2	8:H:286:MET:HB2	1.56	0.70
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.21	0.70
2:B:95:PHE:CE1	2:B:97:LEU:HG	2.27	0.70
8:H:113:VAL:HG22	8:H:136:VAL:HG23	1.72	0.70
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.70
7:G:617:ARG:NH1	16:W:129:HIS:N	2.39	0.70
7:G:628:GLU:OE1	16:W:122:LEU:HB2	1.92	0.70
10:P:64:PHE:CZ	10:P:242:VAL:HG21	2.26	0.70
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.23	0.70
13:S:42:VAL:HG22	13:S:46:LYS:HE3	1.72	0.70
33:q:201:CDL:H312	33:q:201:CDL:H142	1.72	0.70
1:A:33:LYS:HG2	8:H:61:MET:HE2	0.82	0.70
3:C:120:THR:HG23	3:C:121:ARG:N	2.05	0.70
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.70
18:Z:58:ARG:HG2	20:b:45:ILE:HG12	1.72	0.70
20:b:78:LEU:HD22	20:b:80:TRP:HE1	1.56	0.70
4:D:99:LEU:CD1	4:D:101:LEU:HD13	2.19	0.70
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.70
19:a:7:PRO:O	19:a:11:ILE:HD12	1.92	0.70
21:q:6:VAL:HG21	33:q:201:CDL:HB4	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:1:MET:HB3	19:a:26:ILE:CG2	2.21	0.70
8:H:1:MET:HB3	19:a:26:ILE:HG23	1.73	0.70
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
8:H:85:LEU:HD21	8:H:108:THR:HB	1.74	0.69
4:D:99:LEU:HD13	4:D:101:LEU:CD1	2.20	0.69
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.69
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.57	0.69
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.73	0.69
8:H:310:PHE:HD2	20:b:33:PRO:HG3	1.56	0.69
1:A:2:ASN:HB2	18:Z:143:TYR:HE1	1.49	0.69
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.69
10:P:236:VAL:CG2	10:P:270:ARG:HG2	2.22	0.69
5:E:131:ILE:HD13	5:E:187:ILE:HG12	1.72	0.69
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.69
13:S:62:GLN:HB2	13:S:80:ASN:HB2	1.75	0.69
18:Z:130:LYS:HA	18:Z:133:MET:HE2	1.73	0.69
7:G:338:VAL:CG1	7:G:546:PHE:CE1	2.72	0.69
7:G:617:ARG:NH1	16:W:128:GLY:C	2.50	0.69
15:V:113:LYS:O	15:V:116:ILE:HG13	1.92	0.69
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.28	0.69
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.57	0.69
17:X:59:GLU:HA	17:X:62:LEU:HG	1.73	0.69
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.74	0.69
11:Q:99:MET:HE2	11:Q:126:LEU:HD12	1.73	0.69
14:T:111:ASP:H	14:T:114:ASP:HB2	1.58	0.69
15:V:19:THR:HB	15:V:22:GLU:HG3	1.74	0.69
5:E:185:VAL:HG22	5:E:195:LEU:CD1	2.23	0.69
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.69
8:H:220:PHE:HE2	25:H:400:UQ9:H15	1.57	0.69
3:C:63:TYR:CZ	3:C:67:ILE:HD11	2.28	0.68
14:T:82:ARG:HD2	14:T:125:GLU:CG	2.23	0.68
6:F:410:ASP:OD1	6:F:411:SER:N	2.26	0.68
21:q:137:TRP:CH2	21:q:140:PRO:HD3	2.29	0.68
3:C:223:VAL:HG22	3:C:225:LEU:HD13	1.74	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
7:G:356:ASP:O	7:G:360:LYS:HG3	1.93	0.68
8:H:19:PHE:CD2	19:a:11:ILE:CG2	2.76	0.68
19:a:18:ILE:N	19:a:19:PRO:CD	2.56	0.68
19:a:58:ASN:HB3	19:a:60:TYR:HD1	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:202:TRP:CD2	9:I:76:TYR:HE2	2.12	0.68
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.74	0.68
9:I:89:GLU:OE1	21:q:58:ARG:HG2	1.94	0.68
10:P:91:ILE:HG13	10:P:95:ARG:HH12	1.57	0.68
8:H:42:PRO:HD2	8:H:45:ILE:HG12	1.75	0.68
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.74	0.68
17:X:130:LYS:HD3	20:b:63:MET:HG3	1.75	0.68
2:B:114:MET:HB2	2:B:119:VAL:HG23	1.76	0.68
4:D:202:TRP:CE2	9:I:76:TYR:CE2	2.82	0.68
8:H:283:ASP:OD1	8:H:284:GLN:N	2.26	0.68
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.76	0.68
20:b:31:ILE:HA	20:b:34:MET:HE2	1.76	0.68
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.76	0.68
4:D:94:VAL:HG21	4:D:116:LEU:HB2	1.74	0.68
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.68
10:P:333:PRO:HA	10:P:337:ASP:OD2	1.92	0.68
7:G:652:ASN:HB3	7:G:655:ARG:HH22	1.57	0.68
18:Z:92:GLU:O	18:Z:96:ILE:N	2.26	0.68
2:B:95:PHE:HE1	2:B:97:LEU:HG	1.58	0.68
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.68
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.24	0.68
33:q:201:CDL:H542	22:r:8:ILE:HD11	1.74	0.68
2:B:89:SER:O	8:H:54:LYS:CE	2.42	0.67
2:B:93:MET:CE	2:B:131:MET:HE2	2.24	0.67
2:B:117:PHE:HA	8:H:39:ILE:HG21	1.76	0.67
3:C:87:ILE:CG1	3:C:144:THR:CG2	2.69	0.67
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.67
6:F:300:ILE:HG22	6:F:306:GLY:CA	2.22	0.67
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.29	0.67
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
1:A:105:GLU:HG3	1:A:110:GLY:HA3	1.76	0.67
1:A:113:TRP:CZ2	8:H:286:MET:HB2	2.28	0.67
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.24	0.67
17:X:64:ASN:HD22	18:Z:81:ARG:NH1	1.92	0.67
17:X:134:ASP:OD1	17:X:135:ARG:N	2.27	0.67
21:q:39:VAL:HG21	21:q:89:TRP:CH2	2.30	0.67
1:A:113:TRP:HZ2	8:H:286:MET:CB	2.07	0.67
2:B:105:MET:HE2	25:B:302:UQ9:C2	2.24	0.67
2:B:170:TYR:OH	9:I:124:PRO:CG	2.42	0.67
3:C:223:VAL:HG21	3:C:225:LEU:CD1	2.17	0.67
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:358:LEU:CD1	7:G:366:LEU:CD2	2.65	0.67
13:S:40:ARG:HA	13:S:43:GLU:OE1	1.95	0.67
5:E:131:ILE:HG23	5:E:170:LEU:HA	1.77	0.67
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.67
7:G:382:ARG:NE	7:G:652:ASN:HD21	1.93	0.67
19:a:32:GLY:HA3	19:a:60:TYR:CD2	2.30	0.67
5:E:178:ALA:HB3	5:E:184:MET:SD	2.34	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.27	0.67
8:H:264:LEU:CD2	19:a:12:MET:HE2	2.24	0.67
10:P:166:HIS:CD2	10:P:191:VAL:HG21	2.29	0.67
15:V:106:GLU:HG3	15:V:107:PRO:HD2	1.75	0.67
8:H:5:ASN:HA	19:a:26:ILE:HD12	1.76	0.67
5:E:129:TYR:HA	5:E:188:ASN:HD21	1.60	0.67
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.67
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.48	0.67
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.67
8:H:222:LEU:HA	8:H:225:MET:HE2	1.76	0.67
17:X:46:CYS:HB2	17:X:135:ARG:CZ	2.25	0.67
1:A:61:THR:O	1:A:62:PHE:C	2.35	0.67
4:D:241:LEU:HB3	18:Z:16:TYR:OH	1.95	0.67
17:X:47:ARG:NH2	18:Z:80:ASP:OD1	2.27	0.67
18:Z:105:LYS:HD3	18:Z:108:GLU:OE1	1.95	0.67
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
22:r:8:ILE:O	22:r:11:LEU:HB2	1.95	0.66
1:A:51:PHE:CZ	4:D:103:GLY:HA2	2.30	0.66
3:C:186:ILE:HG13	4:D:113:ILE:HG12	1.76	0.66
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.66
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.66
6:F:109:ARG:HE	6:F:239:PRO:HD3	1.61	0.66
6:F:199:ARG:HD3	23:s:80:PHE:CE2	2.30	0.66
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.66
10:P:226:VAL:HG11	10:P:277:VAL:HG11	1.77	0.66
10:P:266:THR:HG21	10:P:329:PRO:CG	2.25	0.66
13:S:44:LEU:HD11	13:S:95:LEU:HD21	1.78	0.66
4:D:220:ALA:HB2	9:I:98:ARG:HH21	1.60	0.66
6:F:117:ALA:HB1	6:F:131:MET:SD	2.35	0.66
7:G:336:ASN:H	7:G:363:SER:HB2	1.60	0.66
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.66
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.66
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.66
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:266:THR:HG21	10:P:329:PRO:HB3	1.76	0.66
19:a:3:PHE:CE1	33:q:201:CDL:H141	2.31	0.66
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.78	0.66
14:T:93:ILE:HG13	14:T:110:LEU:HG	1.78	0.66
2:B:82:ILE:HA	8:H:57:MET:HE1	1.78	0.66
4:D:93:GLY:C	4:D:94:VAL:CG1	2.63	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
10:P:209:ARG:HA	10:P:352:VAL:HG12	1.78	0.66
22:r:6:ARG:O	22:r:9:GLN:HG2	1.96	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
5:E:197:PRO:HA	5:E:200:ILE:HD12	1.77	0.66
6:F:300:ILE:CG2	6:F:307:VAL:N	2.59	0.66
8:H:96:ILE:HG23	18:Z:143:TYR:CE1	2.30	0.66
4:D:160:ASN:HD21	22:r:63:VAL:CG2	2.08	0.66
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.77	0.66
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.66
2:B:125:PRO:HG3	2:B:148:VAL:HG13	1.77	0.66
1:A:106:TRP:CD1	8:H:291:LYS:HD3	2.31	0.66
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.66
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
8:H:205:SER:HB2	8:H:279:ARG:NH2	2.11	0.66
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.66
5:E:192:TYR:HB3	5:E:195:LEU:HD21	1.78	0.66
7:G:126:LEU:CD1	12:R:89:PRO:HB3	2.26	0.66
8:H:52:ALA:HB2	25:H:400:UQ9:H22	1.78	0.66
8:H:179:TRP:CH2	29:I:301:3PE:H3A2	2.31	0.66
1:A:27:MET:HE3	8:H:59:GLU:HG2	1.78	0.65
5:E:151:LEU:CD1	5:E:200:ILE:HG21	2.26	0.65
7:G:651:PRO:HB2	13:S:57:GLU:O	1.96	0.65
7:G:652:ASN:CB	7:G:655:ARG:NH2	2.59	0.65
9:I:61:LEU:HG	29:I:301:3PE:H372	1.77	0.65
10:P:176:SER:H	10:P:182:ARG:HG2	1.60	0.65
14:T:123:GLU:CD	14:T:130:ILE:H	2.03	0.65
8:H:200:LEU:HD13	8:H:282:TYR:HD1	1.61	0.65
9:I:90:LYS:HD3	21:q:91:HIS:CE1	2.31	0.65
10:P:187:GLY:HA2	10:P:190:GLU:HG2	1.78	0.65
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.77	0.65
2:B:170:TYR:OH	9:I:124:PRO:HB2	1.95	0.65
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.30	0.65
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:55:SER:HB3	19:a:61:TYR:CD2	2.32	0.65
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.65
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.73	0.65
14:T:105:MET:HE2	14:T:139:MET:HG2	1.79	0.65
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.78	0.65
6:F:300:ILE:HG21	6:F:307:VAL:N	2.11	0.65
17:X:18:VAL:HA	17:X:68:LEU:HD21	1.76	0.65
17:X:24:VAL:HG12	17:X:86:TRP:CD1	2.31	0.65
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.78	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
1:A:73:LEU:N	1:A:74:PRO:HD2	2.11	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.65
7:G:614:GLY:O	16:W:129:HIS:HE1	1.80	0.65
8:H:43:TYR:CE2	21:q:27:PHE:HZ	2.15	0.65
10:P:64:PHE:CZ	10:P:242:VAL:CG2	2.79	0.65
3:C:187:LEU:CD2	4:D:113:ILE:HD13	2.27	0.65
4:D:101:LEU:CD1	4:D:106:VAL:HA	2.26	0.65
4:D:386:THR:CG2	9:I:118:LEU:HD13	2.27	0.65
17:X:133:THR:HG22	17:X:135:ARG:H	1.62	0.65
3:C:152:ILE:HD12	3:C:153:ASP:O	1.97	0.65
4:D:353:PRO:HA	18:Z:10:MET:HE1	1.77	0.65
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.27	0.65
9:I:113:CYS:SG	24:I:303:SF4:FE3	1.80	0.65
14:T:87:LEU:HD13	14:T:98:LEU:HD11	1.78	0.65
6:F:196:PHE:HE1	23:s:91:ARG:HD3	1.62	0.64
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.64
9:I:50:MET:N	20:b:10:LYS:HZ1	1.95	0.64
9:I:89:GLU:HG2	21:q:61:TRP:CB	2.26	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
8:H:16:ALA:HB2	19:a:15:CYS:HB2	1.77	0.64
21:q:67:GLU:HG2	21:q:72:ASN:HA	1.78	0.64
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.27	0.64
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.64
5:E:226:PRO:HB2	5:E:229:GLY:O	1.98	0.64
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.64
2:B:146:ARG:O	2:B:147:LYS:C	2.39	0.64
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.80	0.64
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.64
1:A:104:TYR:CZ	1:A:108:GLN:HG3	2.32	0.64
5:E:176:LEU:HB2	5:E:184:MET:HE1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.64
10:P:114:ASP:HA	10:P:117:ARG:HB2	1.80	0.64
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.79	0.64
3:C:63:TYR:CE2	3:C:67:ILE:HD11	2.32	0.64
5:E:180:VAL:HG21	5:E:224:CYS:HA	1.78	0.64
6:F:300:ILE:HD11	6:F:356:VAL:HG21	1.78	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.33	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.64
17:X:86:TRP:HZ2	19:a:64:LYS:HB2	1.63	0.64
6:F:224:ARG:NH1	11:Q:164:PHE:CD1	2.66	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
8:H:42:PRO:HD2	8:H:45:ILE:CG1	2.28	0.64
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.80	0.64
17:X:7:LEU:HD22	18:Z:87:LEU:CD1	2.27	0.64
3:C:184:ARG:NH2	4:D:110:ASP:OD2	2.30	0.64
4:D:79:ASN:HB2	4:D:100:GLU:HB3	1.80	0.64
6:F:235:VAL:HG23	6:F:240:THR:HG21	1.80	0.64
7:G:176:CYS:SG	24:G:802:SF4:FE4	1.78	0.64
3:C:124:ARG:HD2	3:C:148:GLU:OE2	1.98	0.64
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.13	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.64
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.78	0.64
10:P:171:ASN:CB	10:P:327:VAL:HB	2.16	0.64
11:Q:75:ARG:HH22	11:Q:104:ARG:HG3	1.62	0.64
14:T:106:LYS:HD2	14:T:106:LYS:N	2.13	0.64
1:A:39:CYS:CB	4:D:85:GLY:HA3	2.26	0.63
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.63
5:E:68:ASN:HD21	23:s:84:ASN:CG	2.06	0.63
7:G:572:HIS:HB2	7:G:699:SER:OG	1.98	0.63
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.63	0.63
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.63
17:X:86:TRP:CZ2	19:a:64:LYS:CA	2.81	0.63
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.34	0.63
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.33	0.63
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.63
15:V:8:THR:HG23	15:V:8:THR:O	1.97	0.63
22:r:6:ARG:HA	22:r:9:GLN:HG2	1.80	0.63
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.80	0.63
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.63
7:G:571:HIS:CD2	7:G:572:HIS:HD2	2.11	0.63
10:P:266:THR:HG21	10:P:329:PRO:CB	2.29	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.81	0.63
7:G:401:LEU:HD21	7:G:432:ILE:CD1	2.28	0.63
8:H:5:ASN:CA	19:a:26:ILE:HD12	2.28	0.63
10:P:252:ALA:HB2	10:P:338:LEU:HD21	1.81	0.63
12:R:36:GLN:NE2	21:q:127:TYR:HB3	2.13	0.63
22:r:68:ILE:HG13	22:r:68:ILE:O	1.97	0.63
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.39	0.63
6:F:35:LEU:HD23	6:F:40:ARG:HG2	1.81	0.63
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.63
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.80	0.63
13:S:44:LEU:HD11	13:S:95:LEU:CD2	2.28	0.63
3:C:103:THR:HG21	15:V:55:LYS:CE	2.29	0.63
3:C:186:ILE:CG1	4:D:113:ILE:CG1	2.75	0.63
6:F:174:ARG:HG3	23:s:87:LEU:HD11	1.80	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.63
9:I:171:PRO:HB3	21:q:93:MET:CE	2.04	0.63
10:P:207:PHE:CE2	10:P:241:TYR:HD1	2.17	0.63
13:S:20:ARG:HG2	13:S:66:TRP:HB2	1.81	0.63
20:b:65:ASP:O	20:b:66:VAL:C	2.41	0.63
1:A:41:PHE:HD2	16:W:102:GLN:NE2	1.95	0.63
2:B:136:THR:CG2	2:B:177:VAL:HG22	2.28	0.63
2:B:170:TYR:HE2	9:I:153:ILE:HD12	1.63	0.63
14:T:134:ASP:HA	14:T:137:LYS:HZ3	1.63	0.63
22:r:5:THR:HG22	22:r:7:VAL:HG12	1.81	0.63
3:C:186:ILE:HG23	3:C:187:LEU:N	2.14	0.63
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
6:F:388:GLY:HA3	6:F:419:ILE:HD11	1.80	0.63
7:G:388:ASN:HB3	7:G:511:LYS:HE2	1.81	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.63
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.28	0.63
1:A:29:LEU:CD2	8:H:59:GLU:OE2	2.47	0.63
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.28	0.63
2:B:116:ARG:NH2	2:B:117:PHE:CZ	2.66	0.63
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.63
8:H:220:PHE:HE2	25:H:400:UQ9:C15	2.10	0.63
14:T:102:SER:O	14:T:141:PRO:HD3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:31:HIS:HB2	17:X:70:PHE:HZ	1.63	0.63
2:B:193:GLY:HA2	9:I:154:TYR:CD2	2.34	0.62
3:C:189:ASP:OD1	3:C:190:TYR:N	2.32	0.62
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.99	0.62
7:G:136:GLU:HG2	11:Q:85:ASN:HD21	1.64	0.62
3:C:126:GLU:OE2	3:C:143:LYS:HD3	1.99	0.62
3:C:186:ILE:CD1	4:D:113:ILE:HG12	2.29	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.28	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.62
13:S:18:GLU:HB2	13:S:52:PRO:HB2	1.81	0.62
2:B:224:ARG:HG3	10:P:85:ARG:NH1	2.11	0.62
3:C:120:THR:HG21	15:V:116:ILE:CG2	2.22	0.62
6:F:45:LEU:HD11	6:F:129:GLU:OE1	1.99	0.62
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.62
7:G:541:PRO:HB2	7:G:561:PRO:CD	2.28	0.62
2:B:95:PHE:HE1	2:B:97:LEU:CG	2.12	0.62
5:E:183:PRO:HB2	5:E:195:LEU:N	2.14	0.62
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.14	0.62
18:Z:101:VAL:HB	18:Z:102:PRO:HD2	1.81	0.62
3:C:223:VAL:HG23	3:C:225:LEU:CD1	2.26	0.62
4:D:160:ASN:HD21	22:r:63:VAL:CB	2.07	0.62
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.29	0.62
17:X:130:LYS:HG2	20:b:59:ASP:HB2	1.79	0.62
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.26	0.62
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.82	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
10:P:228:LEU:HD21	10:P:277:VAL:HG21	1.81	0.62
12:R:98:GLU:CD	12:R:98:GLU:H	2.07	0.62
22:r:9:GLN:HA	22:r:12:ARG:HG2	1.80	0.62
1:A:58:VAL:HG22	1:A:111:LEU:HD23	1.80	0.62
2:B:199:GLU:HB2	9:I:173:PHE:CE1	2.35	0.62
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	0.62
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.82	0.62
10:P:169:HIS:H	10:P:184:LYS:HE3	1.64	0.62
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.62
16:W:104:THR:O	16:W:108:ARG:HG3	1.99	0.62
1:A:27:MET:HE3	8:H:59:GLU:CG	2.29	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
7:G:652:ASN:C	7:G:652:ASN:OD1	2.42	0.62
15:V:27:LEU:O	15:V:31:THR:HG23	1.99	0.62
33:q:201:CDL:HB32	33:q:201:CDL:HA61	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.82	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
10:P:363:SER:HB3	16:W:51:HIS:CE1	2.35	0.62
11:Q:69:GLU:HA	11:Q:72:ILE:HG22	1.82	0.62
1:A:112:GLU:O	1:A:113:TRP:HB2	1.99	0.62
4:D:145:MET:HA	4:D:148:GLU:HG3	1.80	0.62
7:G:173:MET:HE1	7:G:206:VAL:O	1.99	0.62
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
10:P:97:MET:O	10:P:103:LEU:HD11	2.00	0.62
15:V:9:THR:HG21	15:V:78:GLU:HB2	1.81	0.62
2:B:105:MET:HG2	25:B:302:UQ9:H7A	1.82	0.61
3:C:63:TYR:CE2	3:C:67:ILE:CD1	2.83	0.61
3:C:186:ILE:CG1	4:D:113:ILE:HG12	2.30	0.61
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.61
7:G:306:MET:HG2	7:G:316:TYR:HA	1.82	0.61
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.61
8:H:5:ASN:HD21	19:a:23:THR:HA	1.63	0.61
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.29	0.61
10:P:276:LEU:HD23	10:P:280:ILE:CD1	2.30	0.61
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.61
5:E:71:GLU:OE1	23:s:96:SER:HB3	2.00	0.61
8:H:174:LEU:HD21	18:Z:50:MET:HE3	1.82	0.61
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.35	0.61
1:A:80:GLN:HA	20:b:46:ASN:HD21	1.65	0.61
7:G:388:ASN:H	7:G:514:ASN:HB2	1.65	0.61
8:H:224:PHE:CD2	25:H:400:UQ9:C15	2.75	0.61
9:I:135:ARG:O	9:I:135:ARG:HG2	2.00	0.61
11:Q:62:THR:HB	11:Q:72:ILE:HD11	1.82	0.61
13:S:42:VAL:CG1	13:S:43:GLU:OE2	2.48	0.61
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.61
8:H:310:PHE:HB3	20:b:33:PRO:CA	2.29	0.61
17:X:5:VAL:HG11	18:Z:109:SER:HB3	1.83	0.61
1:A:51:PHE:CE1	8:H:130:PHE:CD1	2.88	0.61
5:E:195:LEU:HD23	5:E:218:ARG:HG3	1.83	0.61
7:G:614:GLY:O	16:W:129:HIS:CE1	2.54	0.61
10:P:235:THR:HG21	10:P:323:HIS:O	2.00	0.61
10:P:321:ARG:O	10:P:325:SER:HB3	2.01	0.61
13:S:22:HIS:O	13:S:58:CYS:SG	2.58	0.61
16:W:58:THR:HG23	16:W:61:GLN:H	1.65	0.61
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:5:ASN:CB	19:a:26:ILE:HD12	2.31	0.61
20:b:63:MET:HB2	20:b:66:VAL:HG12	1.82	0.61
1:A:75:LEU:HB2	8:H:155:LEU:HD21	1.82	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61
4:D:132:ALA:HA	4:D:135:TYR:HD2	1.65	0.61
5:E:142:ARG:HG2	5:E:183:PRO:HD3	1.83	0.61
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.61
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.61
1:A:65:PHE:O	1:A:69:ILE:HG13	2.00	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.61
9:I:54:THR:HA	20:b:13:TRP:NE1	2.11	0.61
3:C:84:GLU:HG2	3:C:141:ARG:HD2	1.83	0.61
5:E:136:THR:HB	27:E:301:FES:S2	2.41	0.61
7:G:473:MET:CE	7:G:514:ASN:HD21	2.12	0.61
10:P:297:VAL:O	10:P:301:ILE:HG12	2.01	0.61
15:V:75:GLY:HA3	15:V:79:GLU:OE1	2.01	0.61
2:B:224:ARG:CG	10:P:85:ARG:HH12	2.09	0.61
4:D:91:ALA:O	4:D:92:HIS:HB2	2.00	0.61
8:H:200:LEU:HD13	8:H:282:TYR:CD1	2.36	0.61
1:A:2:ASN:CB	18:Z:143:TYR:CZ	2.83	0.60
3:C:73:GLN:HG2	15:V:103:LEU:HD21	1.83	0.60
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.60
7:G:117:MET:HE3	7:G:143:SER:CA	2.30	0.60
7:G:421:SER:CB	7:G:427:LEU:HD11	2.30	0.60
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.60
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.60
12:R:47:ARG:HB2	21:q:125:VAL:CG1	2.31	0.60
1:A:41:PHE:CA	16:W:102:GLN:NE2	2.63	0.60
4:D:132:ALA:HA	4:D:135:TYR:CD2	2.36	0.60
12:R:84:GLY:O	12:R:85:ALA:HB3	2.01	0.60
16:W:26:ARG:HB2	16:W:26:ARG:NH1	2.16	0.60
2:B:170:TYR:CD1	4:D:135:TYR:CZ	2.89	0.60
3:C:208:GLU:CG	3:C:221:GLU:HG3	2.32	0.60
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.84	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
8:H:224:PHE:CD2	8:H:228:TYR:HE2	2.14	0.60
1:A:51:PHE:HE1	4:D:80:MET:CE	1.87	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.67	0.60
9:I:106:TYR:OH	12:R:88:HIS:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:209:ARG:O	10:P:210:GLU:HG2	2.00	0.60
6:F:299:LEU:CD1	6:F:300:ILE:HG13	2.30	0.60
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.63	0.60
10:P:238:GLN:HG2	10:P:270:ARG:HG3	1.83	0.60
17:X:124:GLN:HB3	20:b:70:PRO:O	2.01	0.60
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.82	0.60
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.37	0.60
6:F:225:LEU:HD22	7:G:93:ALA:HB3	1.84	0.60
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.65	0.60
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.82	0.60
8:H:200:LEU:CD1	8:H:282:TYR:HA	2.32	0.60
9:I:87:PRO:HG2	9:I:88:PHE:CD2	2.37	0.60
9:I:189:LYS:HG3	9:I:189:LYS:O	2.01	0.60
10:P:228:LEU:HD13	10:P:232:GLY:HA3	1.84	0.60
10:P:320:GLU:O	10:P:324:ILE:HG22	2.00	0.60
19:a:58:ASN:CB	19:a:60:TYR:CE1	2.84	0.60
2:B:121:PHE:HE2	25:B:302:UQ9:C1M	2.14	0.60
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.60
5:E:143:ASP:O	5:E:146:SER:HB3	2.02	0.60
6:F:45:LEU:CD1	6:F:129:GLU:OE1	2.50	0.60
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.67	0.60
17:X:5:VAL:CG1	18:Z:109:SER:HB3	2.32	0.60
1:A:3:LEU:HA	8:H:96:ILE:CD1	2.32	0.60
1:A:55:PHE:HB3	1:A:113:TRP:CD1	2.36	0.60
1:A:80:GLN:CA	20:b:46:ASN:HD21	2.13	0.60
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.32	0.60
6:F:64:LYS:H	6:F:256:ARG:HE	1.49	0.60
6:F:119:GLU:HB3	6:F:124:THR:CG2	2.32	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.60
10:P:236:VAL:HG21	10:P:270:ARG:HG2	1.84	0.60
14:T:92:LYS:HE3	16:W:67:ARG:NH1	2.16	0.60
1:A:29:LEU:HD23	8:H:59:GLU:OE2	2.02	0.60
2:B:99:CYS:HB3	4:D:141:TYR:HB3	1.82	0.60
3:C:195:HIS:HE1	16:W:88:LYS:NZ	1.98	0.60
4:D:104:GLU:CG	8:H:130:PHE:CE1	2.81	0.60
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.60
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.17	0.60
10:P:192:ARG:HH12	10:P:260:GLY:HA2	1.67	0.60
2:B:114:MET:HB2	2:B:119:VAL:CG2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:68:MET:HG3	21:q:71:LYS:HB2	1.83	0.60
2:B:100:CYS:SG	24:B:301:SF4:S2	2.99	0.59
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.02	0.59
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.59
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.84	0.59
5:E:147:ILE:HD11	5:E:195:LEU:HB2	1.84	0.59
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.59
17:X:86:TRP:HZ2	19:a:64:LYS:CB	2.15	0.59
20:b:69:HIS:CD2	20:b:70:PRO:HD2	2.36	0.59
8:H:204:GLU:HA	8:H:208:VAL:O	2.02	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.59
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.59
9:I:105:ARG:NH2	9:I:191:LEU:HD22	2.17	0.59
14:T:80:LYS:HG3	14:T:145:VAL:HG21	1.84	0.59
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.85	0.59
10:P:227:PRO:HB2	10:P:298:TYR:CE1	2.38	0.59
1:A:12:LEU:O	1:A:13:LEU:C	2.44	0.59
5:E:243:GLY:O	6:F:257:ARG:HG3	2.03	0.59
7:G:32:ILE:HG12	7:G:45:PRO:HG3	1.85	0.59
7:G:136:GLU:HG2	11:Q:85:ASN:ND2	2.17	0.59
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.84	0.59
18:Z:75:PHE:HE2	19:a:47:LEU:HD11	1.66	0.59
19:a:2:TRP:CH2	33:q:201:CDL:H522	2.38	0.59
1:A:41:PHE:CB	16:W:102:GLN:HE21	2.16	0.59
3:C:237:PRO:HG2	11:Q:88:GLN:OE1	2.02	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	1.68	0.59
9:I:93:LEU:HD11	9:I:173:PHE:CE2	2.37	0.59
18:Z:58:ARG:HG2	20:b:45:ILE:CG1	2.32	0.59
1:A:41:PHE:HB3	16:W:102:GLN:HE21	1.68	0.59
3:C:186:ILE:HD11	4:D:113:ILE:HG12	1.85	0.59
4:D:388:GLY:HA3	4:D:417:SER:OG	2.03	0.59
10:P:282:GLY:O	10:P:285:HIS:CE1	2.56	0.59
11:Q:161:GLY:HA2	11:Q:164:PHE:CD2	2.38	0.59
1:A:52:SER:O	4:D:103:GLY:CA	2.49	0.59
2:B:144:ALA:O	2:B:145:LEU:C	2.45	0.59
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.59
6:F:261:TRP:HE3	6:F:262:PHE:CD1	2.21	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
8:H:99:ASN:ND2	19:a:40:ARG:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:61:LEU:HG	29:I:301:3PE:C37	2.32	0.59
13:S:42:VAL:CG1	13:S:43:GLU:CD	2.76	0.59
17:X:53:PRO:HD2	18:Z:116:TRP:CG	2.38	0.59
3:C:160:ILE:HG21	4:D:286:TYR:CE1	2.38	0.59
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.55	0.59
4:D:257:GLU:CD	9:I:76:TYR:OH	2.46	0.59
4:D:320:ILE:HG13	9:I:36:TYR:HB2	1.84	0.59
5:E:134:CYS:SG	5:E:175:CYS:HA	2.43	0.59
6:F:224:ARG:HD3	11:Q:164:PHE:CZ	2.37	0.59
6:F:329:LYS:HA	6:F:332:CYS:SG	2.43	0.59
7:G:136:GLU:OE2	7:G:272:ARG:NH1	2.36	0.59
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.59
7:G:401:LEU:HD21	7:G:432:ILE:HD12	1.83	0.59
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.79	0.59
10:P:170:LEU:O	10:P:171:ASN:OD1	2.21	0.59
10:P:236:VAL:HG22	10:P:270:ARG:HG2	1.85	0.59
13:S:14:LEU:HB3	13:S:70:ALA:HB2	1.85	0.59
15:V:14:LEU:CD2	15:V:79:GLU:HG2	2.32	0.59
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.85	0.59
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.59
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.59
12:R:33:HIS:CD2	12:R:34:THR:HG23	2.37	0.59
5:E:184:MET:HG3	5:E:192:TYR:O	2.03	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
10:P:217:PHE:CB	10:P:280:ILE:HD13	2.33	0.58
10:P:300:TRP:HE3	10:P:301:ILE:HD13	1.67	0.58
15:V:38:PHE:CE1	15:V:95:LEU:HB2	2.37	0.58
2:B:105:MET:CE	25:B:302:UQ9:C3M	2.80	0.58
2:B:170:TYR:HD2	9:I:153:ILE:HG21	1.65	0.58
4:D:95:LEU:HD13	4:D:458:PHE:CE1	2.38	0.58
5:E:68:ASN:ND2	23:s:84:ASN:ND2	2.41	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
9:I:38:TYR:CD2	9:I:41:LYS:HD3	2.38	0.58
9:I:90:LYS:H	21:q:90:LEU:HD21	1.68	0.58
2:B:99:CYS:C	2:B:101:ALA:N	2.59	0.58
5:E:221:ARG:O	5:E:225:GLU:HB3	2.03	0.58
6:F:133:HIS:O	6:F:134:ASP:C	2.46	0.58
6:F:379:CYS:SG	24:F:502:SF4:S1	3.02	0.58
7:G:372:PHE:H	7:G:532:PRO:HB2	1.67	0.58
8:H:12:PRO:HB2	19:a:19:PRO:HG3	1.85	0.58
10:P:302:GLY:HA2	10:P:305:PHE:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TRP:CD1	8:H:291:LYS:CD	2.87	0.58
6:F:231:ALA:O	6:F:239:PRO:HA	2.04	0.58
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.86	0.58
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.17	0.58
14:T:90:TYR:CE2	14:T:93:ILE:HG12	2.38	0.58
17:X:15:VAL:HG21	17:X:61:LYS:HG2	1.84	0.58
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.58
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
5:E:188:ASN:O	5:E:189:ASP:HB3	2.03	0.58
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.85	0.58
8:H:174:LEU:HD21	18:Z:50:MET:CE	2.33	0.58
8:H:224:PHE:CE2	25:H:400:UQ9:C14	2.86	0.58
12:R:47:ARG:HG3	12:R:48:PHE:CD2	2.38	0.58
13:S:42:VAL:HG13	13:S:43:GLU:OE2	2.03	0.58
21:q:88:ARG:HG2	21:q:94:THR:OG1	2.03	0.58
6:F:184:LYS:HB3	23:s:92:LEU:CD2	2.33	0.58
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.85	0.58
7:G:386:LEU:O	7:G:387:LEU:C	2.46	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
10:P:209:ARG:CA	10:P:352:VAL:HG12	2.34	0.58
6:F:174:ARG:HB2	23:s:87:LEU:HD11	1.85	0.58
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.68	0.58
19:a:50:ARG:O	19:a:54:ILE:HG13	2.03	0.58
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.58
10:P:223:PHE:CZ	10:P:227:PRO:HG3	2.39	0.58
14:T:104:PHE:HE2	14:T:144:ILE:HD11	1.69	0.58
15:V:6:LYS:CG	15:V:16:VAL:HG23	2.34	0.58
4:D:95:LEU:HD22	4:D:458:PHE:HZ	1.69	0.58
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.58
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.58
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.58
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.04	0.58
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.67	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.86	0.58
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.58
8:H:142:TYR:CE1	8:H:289:LEU:HD12	2.39	0.58
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.57
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:142:TYR:CG	8:H:289:LEU:HD12	2.38	0.57
9:I:50:MET:N	20:b:10:LYS:NZ	2.52	0.57
9:I:180:HIS:CD2	10:P:100:LEU:CD2	2.87	0.57
17:X:9:THR:HB	17:X:12:GLU:HG3	1.86	0.57
19:a:18:ILE:N	19:a:19:PRO:HD3	2.19	0.57
23:s:79:THR:O	23:s:83:LEU:HG	2.03	0.57
5:E:131:ILE:CD1	5:E:185:VAL:HB	2.25	0.57
5:E:183:PRO:HB2	5:E:195:LEU:H	1.68	0.57
5:E:189:ASP:OD1	6:F:163:TYR:HB3	2.04	0.57
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.86	0.57
7:G:275:PRO:HB3	7:G:286:ILE:HG23	1.86	0.57
7:G:289:LYS:NZ	7:G:697:THR:OG1	2.36	0.57
9:I:163:PRO:O	12:R:89:PRO:HD3	2.04	0.57
10:P:91:ILE:HD12	10:P:105:PHE:CD2	2.39	0.57
15:V:114:TRP:CD2	15:V:114:TRP:O	2.56	0.57
17:X:15:VAL:CG2	17:X:61:LYS:HG2	2.35	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
6:F:213:ILE:HG23	6:F:235:VAL:CG2	2.31	0.57
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.16	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:130:ILE:HA	9:I:140:ARG:HH11	1.68	0.57
7:G:661:GLU:O	7:G:661:GLU:CG	2.46	0.57
8:H:30:TYR:HB3	9:I:77:LEU:HA	1.86	0.57
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.35	0.57
8:H:85:LEU:CD2	8:H:108:THR:HB	2.34	0.57
9:I:67:ILE:O	9:I:68:ARG:C	2.47	0.57
17:X:24:VAL:HG12	17:X:86:TRP:CG	2.39	0.57
1:A:15:LEU:HD23	8:H:76:THR:HG21	1.86	0.57
1:A:92:PHE:O	1:A:93:ILE:C	2.46	0.57
2:B:136:THR:HG21	4:D:118:ARG:HG2	1.87	0.57
10:P:293:LEU:CB	10:P:298:TYR:HE2	2.04	0.57
15:V:50:GLN:HE22	22:r:93:LYS:HA	1.69	0.57
2:B:127:GLN:HE22	8:H:212:ASN:HB3	1.67	0.57
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.84	0.57
10:P:271:TYR:HA	10:P:375:VAL:HG22	1.86	0.57
15:V:111:GLN:HG3	15:V:111:GLN:O	2.04	0.57
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.57
4:D:381:HIS:HE1	9:I:161:ALA:O	1.88	0.57
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.87	0.57
7:G:330:LEU:HA	7:G:544:MET:HE1	1.86	0.57
9:I:36:TYR:HD2	22:r:104:TRP:HB2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:7:LEU:HD22	18:Z:87:LEU:HD11	1.85	0.57
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.87	0.57
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.57
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.57
11:Q:163:ASN:OD1	11:Q:164:PHE:CD1	2.58	0.57
15:V:81:ILE:O	15:V:82:LEU:C	2.47	0.57
1:A:1:MET:O	1:A:4:TYR:N	2.38	0.57
4:D:91:ALA:C	4:D:93:GLY:H	2.09	0.57
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.70	0.57
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.68	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
10:P:249:ILE:O	10:P:253:THR:HG23	2.05	0.57
11:Q:64:LEU:HD12	16:W:85:LEU:HD21	1.86	0.57
2:B:124:SER:O	2:B:125:PRO:C	2.43	0.57
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.57
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.40	0.57
8:H:12:PRO:O	19:a:15:CYS:HB3	2.05	0.57
13:S:44:LEU:HD12	13:S:48:HIS:CD2	2.40	0.57
18:Z:125:TYR:HA	18:Z:128:ARG:HD3	1.87	0.57
23:s:92:LEU:HD12	23:s:93:PRO:O	2.05	0.57
2:B:110:PRO:HB3	8:H:33:LEU:O	2.04	0.56
4:D:91:ALA:C	4:D:93:GLY:N	2.58	0.56
4:D:260:GLU:HG2	9:I:68:ARG:HE	1.69	0.56
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.56
7:G:652:ASN:OD1	7:G:652:ASN:O	2.23	0.56
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.56
8:H:186:PHE:HB2	29:I:301:3PE:H2I3	1.87	0.56
4:D:279:THR:HG23	15:V:13:GLY:CA	2.35	0.56
6:F:45:LEU:CD1	6:F:129:GLU:CD	2.77	0.56
7:G:355:LYS:CB	7:G:366:LEU:CD1	2.82	0.56
8:H:224:PHE:O	8:H:225:MET:C	2.47	0.56
8:H:260:MET:SD	19:a:16:LEU:O	2.63	0.56
15:V:45:ARG:O	15:V:49:GLU:HB2	2.04	0.56
1:A:110:GLY:O	1:A:111:LEU:C	2.48	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
3:C:79:CYS:SG	22:r:64:VAL:HG23	2.46	0.56
3:C:210:ARG:NH2	10:P:75:ARG:HD3	2.21	0.56
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.84	0.56
8:H:23:VAL:HG11	19:a:9:LEU:CD2	2.34	0.56
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.56
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.88	0.56
10:P:223:PHE:CE2	10:P:227:PRO:HG3	2.40	0.56
10:P:335:LEU:O	10:P:339:GLY:N	2.39	0.56
12:R:69:VAL:CG1	12:R:112:LYS:HB2	2.35	0.56
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.40	0.56
17:X:20:VAL:HG23	17:X:25:LEU:HD12	1.83	0.56
19:a:37:ARG:HH11	19:a:59:ARG:HD2	1.70	0.56
21:q:68:MET:O	21:q:71:LYS:HB2	2.05	0.56
1:A:41:PHE:CB	16:W:102:GLN:NE2	2.68	0.56
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.05	0.56
4:D:202:TRP:CE2	9:I:76:TYR:HE2	2.22	0.56
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.56
7:G:330:LEU:HD13	7:G:546:PHE:CZ	2.39	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
8:H:93:HIS:CE1	19:a:24:ALA:HB1	2.39	0.56
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.56
10:P:192:ARG:HE	10:P:200:ILE:HD12	1.69	0.56
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.71	0.56
1:A:102:LEU:HD22	8:H:294:LEU:HD23	1.86	0.56
2:B:114:MET:HE1	2:B:121:PHE:CZ	2.41	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56
8:H:43:TYR:CE2	21:q:27:PHE:CZ	2.92	0.56
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.56
20:b:69:HIS:HB3	20:b:72:ASP:OD1	2.06	0.56
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.87	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.41	0.56
9:I:153:ILE:O	9:I:154:TYR:C	2.48	0.56
10:P:54:VAL:O	10:P:54:VAL:HG23	2.05	0.56
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.48	0.56
12:R:35:GLY:O	12:R:36:GLN:HB3	2.05	0.56
13:S:42:VAL:O	13:S:46:LYS:HG3	2.04	0.56
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.56
21:q:60:ARG:HH12	21:q:95:ASP:CA	2.15	0.56
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.56
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.83	0.56
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.41	0.56
10:P:169:HIS:ND1	30:P:401:NDP:H5N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:58:ASN:HB3	19:a:60:TYR:CE1	2.39	0.56
22:r:64:VAL:HB	22:r:65:PRO:HD2	1.87	0.56
23:s:76:ASN:O	23:s:79:THR:HG22	2.05	0.56
1:A:26:GLN:O	2:B:154:GLU:HG2	2.05	0.56
3:C:67:ILE:HA	15:V:43:ALA:HB3	1.87	0.56
6:F:228:PRO:CG	11:Q:160:TYR:HD2	2.19	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.71	0.56
2:B:81:LEU:HD22	26:B:303:PC1:H352	1.87	0.56
5:E:91:TRP:CE3	5:E:125:PRO:HB3	2.41	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56
8:H:137:ALA:HB3	8:H:282:TYR:OH	2.06	0.56
10:P:258:ALA:O	10:P:261:LYS:HB2	2.05	0.56
12:R:38:TYR:HE1	12:R:44:ARG:HE	1.53	0.56
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.21	0.56
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.31	0.56
2:B:170:TYR:CD1	4:D:135:TYR:CE1	2.94	0.56
2:B:170:TYR:HE1	4:D:135:TYR:CZ	2.23	0.56
26:B:303:PC1:H131	8:H:39:ILE:HD11	1.87	0.56
3:C:104:ASN:O	22:r:97:PRO:HD3	2.06	0.56
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.41	0.56
7:G:375:GLU:O	7:G:675:VAL:HG21	2.06	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.56
12:R:33:HIS:HD2	12:R:34:THR:HG23	1.70	0.56
20:b:11:ASN:OD1	20:b:12:ALA:N	2.39	0.56
4:D:228:ARG:HH22	9:I:160:GLU:CD	2.14	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	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
9:I:180:HIS:NE2	10:P:100:LEU:HD21	2.21	0.55
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.87	0.55
13:S:55:ILE:O	13:S:55:ILE:HG13	2.05	0.55
18:Z:89:GLU:O	18:Z:93:GLU:HG2	2.06	0.55
3:C:160:ILE:HD13	4:D:285:ASN:ND2	2.16	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.87	0.55
7:G:400:VAL:HG22	7:G:473:MET:HG2	1.87	0.55
8:H:30:TYR:CE1	19:a:1:MET:O	2.59	0.55
17:X:20:VAL:CG2	17:X:25:LEU:HD11	2.33	0.55
1:A:69:ILE:HG22	1:A:73:LEU:HD21	1.88	0.55
1:A:80:GLN:HA	20:b:46:ASN:ND2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ASP:O	2:B:116:ARG:C	2.45	0.55
2:B:122:ARG:NH2	25:H:400:UQ9:H1MA	2.21	0.55
4:D:88:HIS:ND1	4:D:90:ALA:HB3	2.21	0.55
6:F:42:PHE:HD2	6:F:275:LEU:HD11	1.70	0.55
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.55
15:V:33:ASP:O	15:V:36:LYS:N	2.34	0.55
17:X:86:TRP:CZ2	19:a:64:LYS:CB	2.88	0.55
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.55
7:G:545:LEU:HD21	7:G:547:LEU:HD21	1.88	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55
9:I:90:LYS:HE2	21:q:79:GLY:O	2.06	0.55
17:X:133:THR:HG21	17:X:135:ARG:CZ	2.35	0.55
18:Z:97:ILE:HG13	18:Z:98:MET:H	1.71	0.55
20:b:69:HIS:CG	20:b:70:PRO:HD2	2.41	0.55
1:A:68:GLU:HG3	1:A:69:ILE:N	2.21	0.55
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.67	0.55
7:G:330:LEU:HD13	7:G:546:PHE:HZ	1.71	0.55
8:H:94:PRO:O	19:a:27:HIS:CE1	2.57	0.55
8:H:273:ILE:HD11	29:I:301:3PE:H2A1	1.88	0.55
7:G:382:ARG:CZ	7:G:652:ASN:HD21	2.19	0.55
10:P:91:ILE:HD12	10:P:105:PHE:HD2	1.70	0.55
10:P:96:LEU:C	10:P:96:LEU:CD1	2.72	0.55
11:Q:126:LEU:HD13	11:Q:137:PHE:CE2	2.40	0.55
15:V:22:GLU:O	15:V:23:ARG:C	2.50	0.55
4:D:202:TRP:CE2	9:I:76:TYR:CD2	2.95	0.55
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.89	0.55
5:E:225:GLU:O	5:E:226:PRO:C	2.48	0.55
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.55
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.18	0.55
11:Q:81:VAL:O	11:Q:81:VAL:HG13	2.06	0.55
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.32	0.55
6:F:254:ILE:HG23	6:F:259:GLY:HA2	1.89	0.55
6:F:339:PHE:O	6:F:343:VAL:HG23	2.07	0.55
9:I:63:TRP:NE1	29:I:301:3PE:H292	2.22	0.55
9:I:90:LYS:HD3	21:q:91:HIS:HE1	1.72	0.55
13:S:25:GLN:HG3	13:S:57:GLU:OE1	2.05	0.55
3:C:219:VAL:HG11	16:W:113:THR:CG2	2.37	0.55
6:F:129:GLU:OE2	6:F:287:THR:CB	2.53	0.55
9:I:49:ASP:HA	20:b:10:LYS:NZ	2.21	0.55
10:P:232:GLY:HA2	10:P:273:LEU:HD23	1.88	0.55
17:X:64:ASN:OD1	17:X:64:ASN:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:86:TRP:CH2	19:a:64:LYS:HA	2.41	0.55
19:a:40:ARG:HG2	19:a:41:VAL:HG13	1.87	0.55
20:b:45:ILE:HA	20:b:80:TRP:HH2	1.72	0.55
1:A:94:LEU:O	1:A:97:ILE:HG12	2.07	0.55
1:A:105:GLU:HG2	1:A:111:LEU:HG	1.87	0.55
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
5:E:151:LEU:CD1	5:E:200:ILE:HD13	2.37	0.55
5:E:165:ASP:C	5:E:167:LEU:H	2.13	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
7:G:380:ASP:O	13:S:55:ILE:HG12	2.07	0.55
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.55
10:P:272:LEU:HG	10:P:375:VAL:HG11	1.89	0.55
12:R:69:VAL:HG12	12:R:112:LYS:N	2.21	0.55
13:S:44:LEU:HD22	13:S:91:MET:HG2	1.89	0.55
1:A:111:LEU:HB2	8:H:291:LYS:NZ	2.22	0.54
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.54
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	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:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.54
9:I:56:ASN:O	9:I:60:ILE:HG13	2.06	0.54
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.89	0.54
8:H:93:HIS:CE1	19:a:28:LYS:NZ	2.75	0.54
10:P:296:PHE:CE1	10:P:297:VAL:HG23	2.42	0.54
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.54
6:F:35:LEU:HB2	6:F:291:GLU:HB2	1.89	0.54
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.54
8:H:99:ASN:OD1	19:a:40:ARG:HB2	2.07	0.54
10:P:206:ILE:HG13	30:P:401:NDP:H42N	1.89	0.54
10:P:304:LEU:H	10:P:304:LEU:HD12	1.71	0.54
16:W:27:ASP:HB2	16:W:30:GLU:HG3	1.89	0.54
18:Z:75:PHE:CE2	19:a:47:LEU:HD11	2.42	0.54
2:B:114:MET:SD	2:B:121:PHE:CE1	3.01	0.54
4:D:145:MET:O	4:D:148:GLU:N	2.41	0.54
7:G:388:ASN:N	7:G:514:ASN:HB2	2.22	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
14:T:90:TYR:HD2	14:T:93:ILE:HB	1.73	0.54
16:W:69:MET:C	16:W:71:MET:N	2.62	0.54
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.43	0.54
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.10	0.54
7:G:36:VAL:O	7:G:39:GLN:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
7:G:629:ILE:CD1	16:W:122:LEU:HD21	2.37	0.54
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.54
9:I:72:MET:O	9:I:75:SER:OG	2.23	0.54
13:S:26:ARG:HA	13:S:34:ARG:NH1	2.23	0.54
16:W:42:TRP:CE2	16:W:93:LEU:HG	2.41	0.54
2:B:99:CYS:HB3	4:D:141:TYR:CB	2.38	0.54
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.54
2:B:193:GLY:CA	9:I:154:TYR:CE2	2.90	0.54
4:D:257:GLU:HG2	9:I:72:MET:HE2	1.88	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.37	0.54
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.54
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.54
8:H:182:ALA:HB1	29:I:301:3PE:H2I1	1.88	0.54
2:B:117:PHE:HA	8:H:39:ILE:CG2	2.37	0.54
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.90	0.54
3:C:70:LYS:HE3	3:C:71:TYR:CZ	2.43	0.54
3:C:120:THR:CG2	3:C:121:ARG:N	2.68	0.54
5:E:87:ARG:HD2	23:s:77:THR:HB	1.89	0.54
5:E:130:HIS:NE2	5:E:132:GLN:HG2	2.21	0.54
6:F:80:MET:HE2	6:F:95:THR:HG21	1.90	0.54
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.54
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.54
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.54
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.54
8:H:249:ILE:CG2	17:X:99:HIS:HE1	2.14	0.54
9:I:49:ASP:C	20:b:10:LYS:HZ1	2.15	0.54
11:Q:161:GLY:HA2	11:Q:164:PHE:HD2	1.72	0.54
12:R:44:ARG:HB3	12:R:47:ARG:NH1	2.22	0.54
17:X:9:THR:HG22	17:X:11:GLU:H	1.72	0.54
17:X:41:LYS:CB	17:X:131:VAL:HG11	2.38	0.54
5:E:221:ARG:NH1	6:F:285:PRO:HG2	2.23	0.54
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.90	0.54
6:F:167:SER:CB	23:s:75:TYR:CE2	2.91	0.54
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.54
8:H:63:PRO:HB2	8:H:66:THR:CB	2.12	0.54
10:P:76:MET:HE3	10:P:78:SER:OG	2.08	0.54
10:P:227:PRO:O	10:P:298:TYR:CZ	2.61	0.54
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.54
15:V:35:LEU:CD1	15:V:48:THR:HG23	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASN:HB3	18:Z:143:TYR:OH	2.08	0.54
4:D:220:ALA:CB	9:I:98:ARG:HH21	2.21	0.54
4:D:386:THR:HG23	9:I:118:LEU:HD13	1.89	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
8:H:200:LEU:HG	8:H:285:LEU:HD13	1.89	0.54
13:S:51:LEU:O	13:S:53:ILE:HG13	2.07	0.54
17:X:108:ASP:O	17:X:112:LEU:N	2.41	0.54
1:A:1:MET:O	1:A:2:ASN:C	2.48	0.54
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.54
2:B:116:ARG:O	8:H:39:ILE:HG22	2.08	0.54
4:D:128:THR:H	4:D:131:GLN:NE2	2.02	0.54
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.54
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.54
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.40	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.90	0.54
17:X:133:THR:HG21	17:X:135:ARG:NH1	2.23	0.54
33:q:201:CDL:H191	33:q:201:CDL:H332	1.89	0.54
1:A:65:PHE:O	1:A:68:GLU:HG2	2.08	0.53
2:B:114:MET:HE1	2:B:121:PHE:CE1	2.43	0.53
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.90	0.53
6:F:382:CYS:SG	24:F:502:SF4:S4	3.06	0.53
7:G:360:LYS:HD3	7:G:632:ILE:HB	1.89	0.53
8:H:179:TRP:CH2	29:I:301:3PE:H371	2.42	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
8:H:227:GLU:O	8:H:231:ILE:HG13	2.07	0.53
10:P:122:HIS:CD2	12:R:45:ARG:HB2	2.43	0.53
14:T:86:VAL:HG11	14:T:122:MET:SD	2.48	0.53
17:X:49:GLU:CD	20:b:58:ARG:HH21	2.16	0.53
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.53
6:F:119:GLU:HG3	6:F:127:ASP:OD2	2.07	0.53
6:F:228:PRO:HG2	11:Q:160:TYR:CD2	2.41	0.53
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.53
8:H:63:PRO:O	8:H:66:THR:HG22	2.07	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.38	0.53
10:P:302:GLY:O	10:P:303:LYS:C	2.50	0.53
11:Q:53:ILE:HG12	16:W:26:ARG:O	2.08	0.53
16:W:120:ASP:HB3	16:W:123:SER:OG	2.08	0.53
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.53
7:G:557:ARG:HD3	21:q:144:TYR:CD2	2.43	0.53
8:H:172:MET:HB3	18:Z:49:ARG:HD2	1.89	0.53
17:X:7:LEU:CD2	18:Z:87:LEU:CD1	2.87	0.53
19:a:6:LEU:O	19:a:7:PRO:C	2.44	0.53
20:b:74:LEU:H	20:b:74:LEU:HD12	1.72	0.53
2:B:138:THR:HG21	4:D:116:LEU:HA	1.91	0.53
6:F:362:ASP:O	6:F:363:ILE:C	2.51	0.53
7:G:35:PHE:HB2	7:G:101:ASN:HA	1.90	0.53
8:H:96:ILE:HG23	18:Z:143:TYR:CE2	2.43	0.53
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
12:R:40:GLU:HA	12:R:45:ARG:HH11	1.72	0.53
14:T:79:ILE:HD13	14:T:148:ILE:HG22	1.91	0.53
14:T:80:LYS:O	14:T:84:LEU:HG	2.08	0.53
15:V:44:TYR:CE2	15:V:94:MET:HG3	2.44	0.53
1:A:19:LEU:O	1:A:20:VAL:C	2.48	0.53
1:A:61:THR:O	1:A:64:LEU:N	2.41	0.53
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.91	0.53
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.38	0.53
6:F:388:GLY:CA	6:F:419:ILE:HD11	2.38	0.53
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.09	0.53
7:G:173:MET:SD	7:G:206:VAL:O	2.66	0.53
8:H:133:LEU:O	8:H:136:VAL:HG12	2.08	0.53
10:P:229:VAL:HG22	10:P:298:TYR:CD2	2.44	0.53
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.53
13:S:22:HIS:HB3	13:S:58:CYS:SG	2.48	0.53
20:b:27:GLY:O	20:b:28:LEU:C	2.51	0.53
3:C:125:PHE:HZ	3:C:198:ARG:HE	1.56	0.53
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.53
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.74	0.53
5:E:131:ILE:HD11	5:E:185:VAL:CB	2.24	0.53
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.53
11:Q:61:ILE:O	11:Q:65:THR:HG23	2.09	0.53
17:X:137:LEU:HG	17:X:138:PRO:HD2	1.90	0.53
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.72	0.53
4:D:257:GLU:HG2	9:I:72:MET:CE	2.38	0.53
6:F:126:LYS:HG3	6:F:275:LEU:CB	2.39	0.53
6:F:167:SER:HB3	23:s:75:TYR:CE2	2.43	0.53
6:F:196:PHE:CE1	23:s:91:ARG:HD3	2.44	0.53
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.53
16:W:93:LEU:HD22	16:W:97:ILE:HG13	1.89	0.53
17:X:17:GLU:HA	17:X:64:ASN:HD21	1.74	0.53
18:Z:24:ASN:O	18:Z:25:LEU:C	2.52	0.53
18:Z:128:ARG:HE	18:Z:132:GLU:CD	2.16	0.53
19:a:17:VAL:O	19:a:17:VAL:HG22	2.08	0.53
21:q:21:ARG:O	21:q:25:ARG:HG3	2.09	0.53
4:D:95:LEU:HD12	4:D:96:ARG:H	1.74	0.53
5:E:143:ASP:HB3	5:E:146:SER:HB2	1.91	0.53
5:E:244:VAL:HG11	6:F:64:LYS:NZ	2.23	0.53
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.53
11:Q:79:ILE:H	11:Q:79:ILE:HD12	1.73	0.53
12:R:44:ARG:O	12:R:47:ARG:HG2	2.09	0.53
21:q:69:ASN:CG	21:q:70:GLY:H	2.15	0.53
22:r:6:ARG:HA	22:r:9:GLN:CD	2.34	0.53
5:E:162:THR:HG22	5:E:166:LYS:HA	1.91	0.53
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.24	0.53
6:F:166:ALA:HB1	23:s:80:PHE:CE1	2.44	0.53
10:P:143:ASP:O	10:P:148:ILE:HG12	2.09	0.53
10:P:203:PRO:HG2	30:P:401:NDP:C5N	2.39	0.53
10:P:366:ILE:O	10:P:369:THR:HG22	2.08	0.53
21:q:10:GLY:HA2	33:q:201:CDL:H111	1.91	0.53
1:A:49:LEU:HD23	1:A:49:LEU:H	1.72	0.53
2:B:194:CYS:O	24:B:301:SF4:S2	2.67	0.53
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.74	0.53
9:I:143:THR:HA	12:R:34:THR:HG21	1.89	0.53
13:S:16:LEU:HD21	13:S:19:ILE:HD11	1.89	0.53
13:S:90:ALA:O	13:S:94:VAL:HG23	2.09	0.53
17:X:41:LYS:HB2	17:X:131:VAL:HG11	1.91	0.53
20:b:19:LEU:HB3	20:b:23:PHE:CE2	2.44	0.53
7:G:67:GLU:HB3	11:Q:156:LYS:HD2	1.91	0.52
7:G:243:TRP:NE1	9:I:121:ALA:HB2	2.23	0.52
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.52
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.52
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.52
10:P:130:ILE:HD13	10:P:148:ILE:HG21	1.90	0.52
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.52
17:X:18:VAL:HA	17:X:68:LEU:CD2	2.39	0.52
5:E:179:CYS:HA	27:E:301:FES:S1	2.49	0.52
6:F:226:LYS:O	6:F:227:PRO:C	2.47	0.52
6:F:299:LEU:HD12	6:F:300:ILE:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:179:TRP:CD1	18:Z:43:LEU:HD12	2.45	0.52
10:P:236:VAL:HG23	10:P:271:TYR:C	2.35	0.52
13:S:44:LEU:HD12	13:S:48:HIS:HD2	1.73	0.52
17:X:13:LEU:O	17:X:15:VAL:HG23	2.08	0.52
19:a:58:ASN:CB	19:a:60:TYR:CD1	2.89	0.52
1:A:53:MET:HE3	1:A:55:PHE:CE1	2.45	0.52
1:A:75:LEU:O	1:A:79:ILE:HG12	2.09	0.52
3:C:136:PHE:CE1	22:r:96:THR:HB	2.44	0.52
5:E:162:THR:CG2	5:E:166:LYS:HA	2.39	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.52
9:I:48:VAL:HG21	20:b:11:ASN:CB	2.29	0.52
14:T:102:SER:HB2	14:T:107:ASP:HB2	1.91	0.52
15:V:67:LYS:O	15:V:68:LEU:C	2.52	0.52
22:r:6:ARG:C	22:r:9:GLN:HG2	2.34	0.52
23:s:89:LYS:HG3	23:s:90:PHE:N	2.24	0.52
1:A:15:LEU:O	1:A:16:THR:C	2.51	0.52
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.52
10:P:227:PRO:HB2	10:P:298:TYR:OH	2.08	0.52
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.75	0.52
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.91	0.52
7:G:402:LEU:O	7:G:431:LEU:HA	2.09	0.52
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.52
8:H:51:ASP:OD1	8:H:51:ASP:C	2.52	0.52
10:P:293:LEU:HB2	10:P:298:TYR:OH	2.09	0.52
12:R:33:HIS:HB3	12:R:59:PHE:CD1	2.44	0.52
21:q:6:VAL:HG23	33:q:201:CDL:OA9	2.09	0.52
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.92	0.52
4:D:260:GLU:OE1	9:I:72:MET:SD	2.68	0.52
5:E:229:GLY:O	5:E:231:THR:HG23	2.10	0.52
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.75	0.52
9:I:105:ARG:NH2	12:R:56:ASN:ND2	2.58	0.52
10:P:48:ARG:NH2	10:P:98:GLY:O	2.42	0.52
11:Q:111:LEU:HD12	12:R:47:ARG:HH21	1.75	0.52
4:D:198:THR:OG1	4:D:261:MET:HE1	2.10	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:279:TYR:CD1	10:P:372:ALA:HB2	2.45	0.52
10:P:335:LEU:HB3	10:P:340:VAL:HB	1.92	0.52
13:S:18:GLU:CB	13:S:52:PRO:HB2	2.40	0.52
16:W:31:ALA:O	16:W:34:ARG:N	2.40	0.52
21:q:43:LYS:O	21:q:44:TYR:HB2	2.10	0.52
1:A:73:LEU:N	1:A:74:PRO:CD	2.73	0.52
4:D:271:ARG:CD	8:H:279:ARG:O	2.56	0.52
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.92	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
8:H:260:MET:HE1	19:a:16:LEU:CA	2.39	0.52
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.52
18:Z:50:MET:SD	18:Z:54:ASN:ND2	2.82	0.52
4:D:170:ILE:HG21	4:D:232:VAL:HG21	1.90	0.52
6:F:167:SER:OG	23:s:75:TYR:CE2	2.63	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
21:q:3:LEU:HD13	33:q:201:CDL:C52	2.39	0.52
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.52
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.45	0.52
6:F:225:LEU:CD2	7:G:93:ALA:HB3	2.40	0.52
7:G:35:PHE:CE1	7:G:40:SER:HB2	2.45	0.52
15:V:31:THR:HG22	15:V:88:LEU:HB2	1.92	0.52
16:W:130:ASP:O	16:W:130:ASP:OD1	2.26	0.52
3:C:186:ILE:CG2	3:C:187:LEU:N	2.73	0.51
4:D:101:LEU:HD12	4:D:106:VAL:HA	1.91	0.51
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.51
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.51
7:G:130:ILE:HA	9:I:140:ARG:NH1	2.23	0.51
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.91	0.51
12:R:98:GLU:HA	12:R:113:GLN:CD	2.34	0.51
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.75	0.51
22:r:6:ARG:HA	22:r:9:GLN:CG	2.39	0.51
2:B:92:PRO:HG2	2:B:121:PHE:CD1	2.46	0.51
2:B:95:PHE:HE1	2:B:97:LEU:CD1	2.23	0.51
3:C:190:TYR:HB3	16:W:101:LYS:HG2	1.92	0.51
5:E:59:TYR:O	5:E:62:ILE:HB	2.09	0.51
6:F:234:GLY:HA3	6:F:238:CYS:O	2.10	0.51
6:F:391:TRP:HH2	7:G:118:GLU:OE2	1.92	0.51
7:G:253:VAL:HG12	7:G:253:VAL:O	2.10	0.51
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:524:ALA:HB2	7:G:597:VAL:HG22	1.91	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.53	0.51
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.51
10:P:59:PHE:CD1	10:P:83:PRO:HG2	2.44	0.51
14:T:104:PHE:CB	14:T:110:LEU:HD22	2.39	0.51
1:A:73:LEU:O	1:A:76:PRO:HD2	2.10	0.51
3:C:92:VAL:O	3:C:96:LEU:HD13	2.11	0.51
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.25	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51
5:E:143:ASP:HB3	5:E:146:SER:CB	2.40	0.51
6:F:109:ARG:NE	6:F:239:PRO:HD3	2.25	0.51
7:G:231:LEU:HD12	7:G:231:LEU:O	2.10	0.51
8:H:280:PHE:HD2	8:H:284:GLN:CG	2.23	0.51
10:P:316:LYS:O	10:P:320:GLU:HG3	2.10	0.51
11:Q:131:LYS:HG2	11:Q:135:ILE:HD11	1.89	0.51
11:Q:135:ILE:HD11	11:Q:147:VAL:HG21	1.92	0.51
16:W:110:PHE:O	16:W:111:HIS:C	2.53	0.51
17:X:130:LYS:HG3	20:b:59:ASP:HA	1.92	0.51
18:Z:87:LEU:O	18:Z:91:LEU:HB2	2.10	0.51
2:B:164:CYS:HA	2:B:168:GLY:O	2.11	0.51
2:B:202:LEU:CD1	9:I:86:TYR:CE2	2.90	0.51
3:C:149:LEU:O	16:W:23:ILE:HD11	2.10	0.51
3:C:160:ILE:HB	4:D:286:TYR:CE1	2.45	0.51
3:C:170:TRP:CD1	3:C:183:LEU:HD21	2.44	0.51
3:C:209:LEU:HD21	16:W:108:ARG:NH1	2.25	0.51
5:E:140:MET:HE1	6:F:366:ALA:HA	1.92	0.51
5:E:198:LYS:O	5:E:201:GLU:HB3	2.10	0.51
6:F:119:GLU:CD	28:F:501:FMN:HN3	2.18	0.51
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.51
7:G:611:THR:HG21	11:Q:105:GLU:N	2.25	0.51
7:G:617:ARG:NH1	16:W:129:HIS:HA	2.24	0.51
9:I:49:ASP:C	20:b:10:LYS:HZ3	2.19	0.51
10:P:91:ILE:HG13	10:P:95:ARG:NH1	2.23	0.51
10:P:137:ARG:HG3	10:P:138:ASN:OD1	2.10	0.51
14:T:110:LEU:HD21	14:T:118:ILE:HD12	1.91	0.51
6:F:382:CYS:HA	7:G:74:ASN:O	2.11	0.51
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.51
7:G:304:GLU:HG3	7:G:615:LEU:HD12	1.93	0.51
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.92	0.51
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.51
15:V:42:ALA:O	15:V:43:ALA:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:97:TRP:O	15:V:98:LYS:C	2.52	0.51
17:X:48:TRP:CE2	20:b:55:VAL:HG22	2.45	0.51
18:Z:97:ILE:HG13	18:Z:98:MET:N	2.25	0.51
2:B:87:ARG:HH11	26:B:303:PC1:P	2.34	0.51
3:C:63:TYR:OH	3:C:102:HIS:HE1	1.93	0.51
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.51
5:E:233:LEU:HD23	6:F:43:THR:O	2.10	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.46	0.51
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.92	0.51
7:G:670:GLU:HB2	13:S:42:VAL:CG2	2.40	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:303:TRP:CE3	20:b:29:ALA:CB	2.86	0.51
10:P:270:ARG:HB3	10:P:375:VAL:O	2.11	0.51
12:R:69:VAL:HG11	12:R:112:LYS:HB2	1.92	0.51
14:T:104:PHE:CG	14:T:110:LEU:HD22	2.46	0.51
16:W:95:GLU:HB3	16:W:101:LYS:HG3	1.93	0.51
17:X:129:THR:HB	20:b:68:SER:O	2.11	0.51
4:D:88:HIS:HE1	8:H:205:SER:O	1.94	0.51
4:D:299:GLN:NE2	9:I:36:TYR:CZ	2.78	0.51
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.51
8:H:20:LEU:HD22	8:H:228:TYR:HD1	1.75	0.51
8:H:201:THR:C	8:H:203:GLY:H	2.18	0.51
8:H:312:ALA:HB2	20:b:38:TYR:O	2.10	0.51
10:P:157:LYS:HD3	10:P:195:PHE:CE1	2.46	0.51
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.51
13:S:24:CYS:HB2	13:S:30:SER:HB3	1.93	0.51
17:X:52:ASP:OD1	17:X:53:PRO:HD2	2.11	0.51
4:D:145:MET:O	4:D:146:CYS:C	2.54	0.51
5:E:178:ALA:HB2	5:E:191:TYR:CE2	2.45	0.51
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.51
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.51
10:P:294:PRO:O	10:P:298:TYR:HD2	1.94	0.51
11:Q:85:ASN:O	11:Q:86:ASN:C	2.52	0.51
16:W:67:ARG:O	16:W:71:MET:HB2	2.11	0.51
1:A:25:PRO:HG2	8:H:60:PRO:HD3	1.93	0.51
2:B:127:GLN:NE2	8:H:212:ASN:HB3	2.26	0.51
5:E:39:VAL:HG11	7:G:163:LYS:HE3	1.93	0.51
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.51
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:8:PRO:HD2	18:Z:84:LEU:HD11	1.91	0.51
1:A:68:GLU:O	1:A:69:ILE:C	2.53	0.51
25:B:302:UQ9:H13	25:H:400:UQ9:C3	2.41	0.51
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.40	0.51
5:E:178:ALA:HB2	5:E:191:TYR:HE2	1.76	0.51
5:E:200:ILE:HG22	5:E:204:ILE:HG13	1.92	0.51
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.51
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.51
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.51
10:P:206:ILE:H	30:P:401:NDP:H71N	1.58	0.51
13:S:19:ILE:O	13:S:53:ILE:HA	2.11	0.51
17:X:32:TYR:HE1	17:X:67:ALA:HA	1.76	0.51
3:C:70:LYS:O	15:V:103:LEU:HD12	2.11	0.50
3:C:230:ARG:NH1	9:I:128:ILE:O	2.43	0.50
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.50
4:D:235:ASP:OD2	18:Z:8:GLN:HG3	2.11	0.50
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.77	0.50
6:F:235:VAL:HG12	6:F:236:PHE:CD2	2.47	0.50
6:F:294:VAL:HG12	6:F:337:MET:HB2	1.92	0.50
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
8:H:12:PRO:HB3	19:a:18:ILE:HB	1.93	0.50
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.50
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.25	0.50
22:r:7:VAL:O	22:r:11:LEU:HG	2.10	0.50
1:A:38:GLU:HG2	4:D:83:ASN:OD1	2.11	0.50
2:B:84:TRP:HA	2:B:87:ARG:HG2	1.93	0.50
2:B:99:CYS:C	2:B:101:ALA:H	2.19	0.50
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.50
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.99	0.50
10:P:165:ILE:HG21	10:P:249:ILE:HG23	1.93	0.50
10:P:307:LEU:O	10:P:308:SER:C	2.55	0.50
13:S:23:LEU:HD12	13:S:23:LEU:O	2.11	0.50
14:T:79:ILE:HG23	14:T:126:PHE:CE1	2.47	0.50
16:W:130:ASP:O	16:W:131:PRO:C	2.52	0.50
17:X:7:LEU:HD13	18:Z:87:LEU:HD12	1.93	0.50
18:Z:86:ILE:HG21	18:Z:124:MET:O	2.11	0.50
18:Z:134:SER:O	18:Z:137:ASN:N	2.44	0.50
20:b:41:TYR:CD1	20:b:84:LEU:HD11	2.46	0.50
2:B:117:PHE:HZ	9:I:86:TYR:HB3	1.77	0.50
4:D:141:TYR:O	4:D:144:MET:SD	2.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:376:GLU:HG2	7:G:121:LEU:CD1	2.41	0.50
4:D:376:GLU:HG2	7:G:121:LEU:HD12	1.92	0.50
6:F:300:ILE:CG2	6:F:305:GLY:O	2.44	0.50
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.50
7:G:391:ILE:HG22	7:G:417:ARG:HE	1.75	0.50
10:P:209:ARG:HG2	10:P:352:VAL:HG12	1.93	0.50
13:S:63:PRO:HB2	13:S:79:LEU:HD12	1.93	0.50
14:T:92:LYS:NZ	14:T:92:LYS:HB3	2.27	0.50
15:V:77:VAL:C	15:V:79:GLU:N	2.66	0.50
1:A:42:ASP:OD1	1:A:42:ASP:N	2.45	0.50
2:B:126:ARG:HD3	2:B:151:GLN:O	2.12	0.50
5:E:165:ASP:C	5:E:167:LEU:N	2.64	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.46	0.50
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.08	0.50
8:H:69:SER:C	8:H:71:PHE:N	2.68	0.50
10:P:153:ALA:HB2	10:P:164:PHE:CE2	2.46	0.50
18:Z:119:PRO:HA	18:Z:123:GLU:OE2	2.12	0.50
1:A:49:LEU:HD11	4:D:80:MET:HA	1.93	0.50
3:C:160:ILE:HG21	4:D:286:TYR:HE1	1.77	0.50
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.50
4:D:289:SER:N	4:D:293:LEU:HG	2.26	0.50
8:H:67:SER:HB3	8:H:122:ALA:HA	1.93	0.50
8:H:221:ALA:C	8:H:223:PHE:N	2.68	0.50
11:Q:53:ILE:HG23	16:W:20:VAL:HG23	1.94	0.50
11:Q:112:MET:SD	21:q:126:PRO:HB3	2.51	0.50
2:B:99:CYS:O	2:B:101:ALA:N	2.44	0.50
2:B:170:TYR:OH	9:I:124:PRO:HG3	2.10	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
5:E:176:LEU:HB2	5:E:184:MET:CE	2.41	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
8:H:201:THR:C	8:H:203:GLY:N	2.70	0.50
9:I:105:ARG:NH2	12:R:56:ASN:HD21	2.10	0.50
9:I:111:GLU:OE2	9:I:187:LYS:HE3	2.11	0.50
9:I:200:GLU:HG2	21:q:88:ARG:HB2	1.93	0.50
14:T:130:ILE:HG23	14:T:134:ASP:OD2	2.12	0.50
20:b:67:PRO:HB3	20:b:74:LEU:HB2	1.93	0.50
22:r:6:ARG:O	22:r:9:GLN:CG	2.60	0.50
2:B:100:CYS:HG	24:B:301:SF4:FE4	1.18	0.50
2:B:220:ILE:HD13	10:P:87:ASP:HB2	1.92	0.50
3:C:223:VAL:HG23	3:C:225:LEU:HD12	1.88	0.50
6:F:226:LYS:HD2	6:F:229:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.50
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.50
8:H:23:VAL:HG21	19:a:9:LEU:HD23	1.94	0.50
8:H:155:LEU:O	8:H:315:PRO:HG3	2.12	0.50
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.50
9:I:203:ALA:HB2	21:q:88:ARG:HH11	1.76	0.50
10:P:45:LYS:O	10:P:50:SER:HB3	2.11	0.50
10:P:154:GLN:O	10:P:158:GLU:HG3	2.10	0.50
10:P:223:PHE:CG	10:P:223:PHE:O	2.65	0.50
15:V:8:THR:O	15:V:8:THR:CG2	2.59	0.50
21:q:66:THR:HG23	21:q:74:PHE:CD1	2.47	0.50
3:C:160:ILE:CG2	4:D:286:TYR:CE1	2.95	0.50
4:D:131:GLN:HB2	9:I:124:PRO:HB3	1.94	0.50
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.12	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.50
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.50
8:H:142:TYR:CA	8:H:289:LEU:CD1	2.75	0.50
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.50
10:P:68:TYR:CD2	10:P:242:VAL:HG11	2.46	0.50
10:P:215:ASN:O	10:P:216:HIS:C	2.54	0.50
14:T:120:MET:HE1	16:W:43:TYR:CG	2.47	0.50
16:W:107:MET:HE3	16:W:112:GLU:OE2	2.11	0.50
17:X:76:SER:OG	17:X:77:HIS:N	2.45	0.50
21:q:3:LEU:CD1	33:q:201:CDL:H521	2.40	0.50
23:s:87:LEU:O	23:s:91:ARG:HG3	2.12	0.50
4:D:460:GLU:O	4:D:463:ARG:HG2	2.11	0.50
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.50
5:E:214:LYS:HG3	5:E:214:LYS:O	2.11	0.50
6:F:185:ASN:HA	6:F:189:SER:O	2.11	0.50
7:G:181:ARG:HA	7:G:184:ARG:HH21	1.77	0.50
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.94	0.50
7:G:648:GLU:O	13:S:22:HIS:HE1	1.95	0.50
8:H:200:LEU:HD13	8:H:282:TYR:HA	1.92	0.50
9:I:78:PHE:CD1	22:r:8:ILE:HG23	2.47	0.50
10:P:132:ARG:HD2	10:P:134:TRP:CZ2	2.47	0.50
10:P:163:ARG:HH22	10:P:256:PRO:HA	1.76	0.50
10:P:227:PRO:HB3	10:P:291:TYR:CE1	2.47	0.50
14:T:115:GLN:O	14:T:119:ILE:HG12	2.12	0.50
14:T:144:ILE:O	14:T:148:ILE:HG12	2.12	0.50
15:V:9:THR:HG21	15:V:78:GLU:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:93:LEU:O	16:W:94:GLN:C	2.55	0.50
17:X:45:LEU:HG	17:X:131:VAL:HG23	1.93	0.50
17:X:64:ASN:HD22	18:Z:81:ARG:HH12	1.58	0.50
17:X:128:VAL:O	17:X:128:VAL:CG2	2.58	0.50
18:Z:10:MET:HG3	18:Z:11:PRO:HD2	1.93	0.50
2:B:164:CYS:SG	24:B:301:SF4:S4	3.10	0.49
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.49
6:F:335:VAL:HG12	6:F:336:LEU:O	2.11	0.49
7:G:70:SER:O	7:G:184:ARG:NH1	2.45	0.49
7:G:372:PHE:CZ	7:G:385:TYR:HB3	2.47	0.49
7:G:406:ASN:O	7:G:407:PRO:C	2.53	0.49
7:G:557:ARG:CG	7:G:579:MET:HE3	2.38	0.49
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.49
15:V:95:LEU:O	15:V:95:LEU:HD23	2.12	0.49
17:X:49:GLU:CG	17:X:50:GLU:HG3	2.40	0.49
17:X:141:PRO:O	17:X:142:TYR:HB2	2.11	0.49
19:a:43:TYR:CZ	19:a:47:LEU:HD11	2.46	0.49
1:A:104:TYR:CE2	1:A:108:GLN:HG3	2.47	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.94	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	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
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.49
8:H:168:THR:OG1	18:Z:57:ARG:NH1	2.44	0.49
14:T:84:LEU:HD22	14:T:98:LEU:CD2	2.42	0.49
18:Z:92:GLU:O	18:Z:95:ALA:N	2.44	0.49
1:A:17:LEU:CD2	8:H:222:LEU:CD1	2.51	0.49
2:B:156:ARG:O	10:P:89:TYR:HE1	1.95	0.49
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
7:G:473:MET:HE3	7:G:514:ASN:ND2	2.21	0.49
10:P:236:VAL:HG23	10:P:271:TYR:O	2.13	0.49
4:D:371:MET:CE	9:I:163:PRO:HB3	2.42	0.49
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.42	0.49
8:H:260:MET:HE2	19:a:13:GLY:O	2.12	0.49
9:I:37:LYS:HD3	22:r:110:GLN:O	2.12	0.49
17:X:132:LYS:HB3	20:b:59:ASP:HB3	1.93	0.49
22:r:6:ARG:CA	22:r:9:GLN:HG2	2.42	0.49
1:A:103:ALA:O	1:A:107:THR:HG23	2.12	0.49
3:C:186:ILE:CG2	3:C:187:LEU:HG	2.23	0.49
4:D:215:GLU:OE2	9:I:97:PHE:CD1	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:238:LEU:CB	9:I:211:TYR:OH	2.59	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.12	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.91	0.49
7:G:403:VAL:HG13	7:G:403:VAL:O	2.12	0.49
9:I:180:HIS:HD2	10:P:100:LEU:CD2	2.26	0.49
10:P:209:ARG:CG	10:P:352:VAL:HG12	2.43	0.49
10:P:335:LEU:HD12	10:P:342:PRO:HG3	1.94	0.49
13:S:87:VAL:O	13:S:88:THR:C	2.55	0.49
5:E:240:PRO:HB3	6:F:60:GLY:CA	2.41	0.49
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.95	0.49
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.49
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.76	0.49
10:P:150:ARG:HE	10:P:190:GLU:HB3	1.78	0.49
12:R:48:PHE:HD1	12:R:52:GLN:O	1.95	0.49
4:D:299:GLN:NE2	9:I:36:TYR:CD2	2.80	0.49
6:F:42:PHE:HE1	6:F:137:LYS:HG2	1.76	0.49
6:F:109:ARG:NH2	6:F:232:ASP:O	2.41	0.49
6:F:126:LYS:HG3	6:F:275:LEU:HB3	1.94	0.49
7:G:617:ARG:HH22	16:W:128:GLY:N	2.11	0.49
7:G:665:PHE:O	7:G:668:ALA:N	2.45	0.49
10:P:263:PHE:CE1	10:P:333:PRO:HB2	2.48	0.49
17:X:24:VAL:HG23	17:X:25:LEU:HD12	1.95	0.49
33:q:201:CDL:H511	22:r:8:ILE:HD11	1.93	0.49
2:B:68:ARG:HD3	2:B:70:ARG:CG	2.41	0.49
3:C:80:LEU:O	3:C:81:ASP:HB2	2.12	0.49
3:C:96:LEU:HD22	3:C:155:ILE:HG21	1.94	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.49
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.49
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.95	0.49
12:R:88:HIS:O	12:R:89:PRO:C	2.56	0.49
13:S:16:LEU:HD13	13:S:94:VAL:HG12	1.95	0.49
17:X:129:THR:HA	20:b:67:PRO:O	2.13	0.49
25:B:302:UQ9:H10	4:D:200:PHE:CZ	2.48	0.49
3:C:132:LEU:HD11	4:D:300:TRP:CZ2	2.48	0.49
4:D:137:ASP:OD1	4:D:148:GLU:HG2	2.12	0.49
6:F:234:GLY:O	6:F:237:GLY:N	2.45	0.49
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:5:ASN:HD21	19:a:23:THR:CG2	2.25	0.49
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.94	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
9:I:93:LEU:HD11	9:I:173:PHE:HE2	1.77	0.49
10:P:157:LYS:HD3	10:P:195:PHE:CD1	2.48	0.49
14:T:119:ILE:HD12	14:T:138:LEU:CD1	2.40	0.49
2:B:170:TYR:CE1	4:D:135:TYR:CE2	3.01	0.49
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.95	0.49
4:D:79:ASN:O	4:D:80:MET:C	2.55	0.49
9:I:76:TYR:CE1	9:I:79:ARG:CZ	2.96	0.49
11:Q:62:THR:HB	11:Q:72:ILE:CD1	2.43	0.49
16:W:102:GLN:H	16:W:105:HIS:CD2	2.30	0.49
18:Z:143:TYR:O	18:Z:144:THR:C	2.55	0.49
20:b:60:ASP:HB2	20:b:62:ASN:OD1	2.12	0.49
1:A:18:ILE:HD11	8:H:222:LEU:HD23	1.92	0.48
6:F:299:LEU:HD11	6:F:300:ILE:HG13	1.93	0.48
7:G:382:ARG:HG2	7:G:386:LEU:CD1	2.41	0.48
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.95	0.48
8:H:220:PHE:CE2	25:H:400:UQ9:H15	2.44	0.48
10:P:285:HIS:HB3	10:P:361:TRP:CE3	2.47	0.48
2:B:175:TYR:OH	4:D:117:HIS:HE1	1.96	0.48
4:D:139:LEU:HD13	4:D:424:ILE:HG21	1.94	0.48
4:D:386:THR:CG2	9:I:118:LEU:CD1	2.91	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48
8:H:5:ASN:ND2	19:a:23:THR:HG23	2.26	0.48
8:H:5:ASN:CA	19:a:26:ILE:CD1	2.91	0.48
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.48
10:P:157:LYS:CB	10:P:195:PHE:HD1	2.24	0.48
10:P:299:SER:HB3	10:P:316:LYS:HZ2	1.77	0.48
14:T:99:SER:HB2	14:T:102:SER:CB	2.33	0.48
17:X:49:GLU:OE1	20:b:58:ARG:NH2	2.46	0.48
21:q:19:GLY:O	21:q:23:LEU:N	2.41	0.48
21:q:65:THR:HG22	21:q:81:MET:HE1	1.95	0.48
3:C:234:LEU:O	3:C:234:LEU:CG	2.60	0.48
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.48
4:D:299:GLN:CD	9:I:36:TYR:CD2	2.91	0.48
6:F:327:ILE:HG13	6:F:331:VAL:HB	1.95	0.48
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	0.48
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:146:VAL:HG13	10:P:190:GLU:HG3	1.95	0.48
13:S:95:LEU:HD12	13:S:95:LEU:C	2.33	0.48
16:W:46:VAL:HB	16:W:47:PRO:HD3	1.95	0.48
17:X:74:ILE:O	17:X:77:HIS:O	2.31	0.48
20:b:35:ILE:HG12	20:b:35:ILE:O	2.13	0.48
22:r:110:GLN:HG2	22:r:113:LEU:HD22	1.95	0.48
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.48	0.48
2:B:68:ARG:HG2	2:B:69:SER:N	2.29	0.48
5:E:203:ILE:HD11	5:E:218:ARG:HD3	1.93	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
7:G:183:ILE:HD11	7:G:197:THR:HG23	1.95	0.48
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.48
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
8:H:59:GLU:OE2	8:H:61:MET:SD	2.71	0.48
10:P:76:MET:SD	10:P:254:LYS:HE3	2.54	0.48
10:P:223:PHE:CZ	10:P:227:PRO:CG	2.96	0.48
15:V:31:THR:O	15:V:35:LEU:HG	2.12	0.48
17:X:49:GLU:CG	17:X:50:GLU:N	2.76	0.48
17:X:129:THR:HG21	20:b:70:PRO:HD3	1.95	0.48
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.48
4:D:198:THR:HA	8:H:32:GLN:HG2	1.94	0.48
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
7:G:179:CYS:HG	24:G:802:SF4:FE3	1.28	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48
3:C:229:PHE:CD1	9:I:126:GLN:HG3	2.43	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.48
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.48
4:D:412:VAL:HG12	15:V:114:TRP:CZ2	2.49	0.48
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.53	0.48
7:G:170:LYS:O	7:G:231:LEU:HA	2.13	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
8:H:221:ALA:O	8:H:224:PHE:N	2.46	0.48
19:a:2:TRP:HH2	33:q:201:CDL:H522	1.78	0.48
3:C:67:ILE:HD13	3:C:98:PHE:CZ	2.49	0.48
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.48
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.48
5:E:61:ARG:O	5:E:62:ILE:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:228:GLY:H	6:F:284:HIS:CG	2.32	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.48
14:T:120:MET:HE1	16:W:43:TYR:CD2	2.49	0.48
17:X:10:LEU:H	17:X:10:LEU:HD12	1.77	0.48
2:B:91:TRP:CD1	8:H:54:LYS:HE2	2.48	0.48
4:D:104:GLU:CD	8:H:130:PHE:CE1	2.92	0.48
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.49	0.48
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.27	0.48
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.48
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.78	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
8:H:228:TYR:OH	25:H:400:UQ9:H10B	2.14	0.48
10:P:59:PHE:CD2	10:P:152:ILE:HD13	2.49	0.48
10:P:376:ASN:O	10:P:377:TYR:C	2.57	0.48
17:X:49:GLU:O	17:X:51:LYS:HD2	2.13	0.48
1:A:54:LYS:O	1:A:113:TRP:HA	2.13	0.48
2:B:169:GLY:C	2:B:171:TYR:N	2.69	0.48
3:C:219:VAL:HG11	16:W:113:THR:HG21	1.95	0.48
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.48
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.48
4:D:412:VAL:CG1	15:V:114:TRP:CZ2	2.96	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
7:G:338:VAL:HG13	7:G:546:PHE:CE1	2.37	0.48
7:G:475:VAL:HG11	7:G:516:LEU:HD23	1.95	0.48
8:H:68:MET:O	8:H:71:PHE:HB2	2.14	0.48
8:H:212:ASN:O	8:H:215:TYR:HB2	2.14	0.48
10:P:140:ASP:C	10:P:142:GLU:N	2.68	0.48
10:P:169:HIS:HB2	10:P:184:LYS:HE2	1.96	0.48
19:a:17:VAL:HG22	19:a:21:VAL:HG23	1.95	0.48
6:F:67:GLU:O	6:F:71:LYS:HG2	2.13	0.48
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.48
10:P:94:LEU:O	10:P:97:MET:HG2	2.14	0.48
10:P:134:TRP:HB3	10:P:312:PRO:CG	2.41	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
12:R:51:ARG:O	12:R:52:GLN:HG3	2.13	0.48
14:T:110:LEU:CD2	14:T:118:ILE:HD12	2.44	0.48
17:X:57:LEU:HD11	18:Z:84:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:208:GLU:HG2	3:C:221:GLU:HG3	1.96	0.47
3:C:221:GLU:O	3:C:222:PRO:C	2.56	0.47
4:D:104:GLU:CD	8:H:130:PHE:HE1	2.21	0.47
4:D:385:TYR:HB2	9:I:118:LEU:HD11	1.96	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47
6:F:357:MET:HE1	6:F:363:ILE:HD12	1.95	0.47
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.96	0.47
9:I:152:CYS:SG	24:I:302:SF4:S4	3.12	0.47
10:P:54:VAL:O	10:P:78:SER:HB3	2.14	0.47
10:P:74:GLY:HA2	10:P:102:GLN:OE1	2.14	0.47
10:P:113:LYS:C	10:P:115:SER:H	2.21	0.47
18:Z:120:LEU:HD23	18:Z:121:ILE:N	2.29	0.47
19:a:12:MET:O	19:a:12:MET:HG2	2.14	0.47
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.47
5:E:147:ILE:CD1	5:E:195:LEU:HB2	2.43	0.47
9:I:41:LYS:HG2	9:I:41:LYS:O	2.13	0.47
10:P:80:VAL:HB	10:P:103:LEU:HD22	1.95	0.47
11:Q:78:ARG:O	11:Q:80:PHE:HD1	1.96	0.47
14:T:95:PRO:HG2	14:T:97:LYS:HB3	1.95	0.47
2:B:91:TRP:CD1	2:B:91:TRP:N	2.80	0.47
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.48	0.47
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.44	0.47
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.79	0.47
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.47
7:G:544:MET:HA	7:G:565:PHE:O	2.14	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
8:H:15:ILE:HG21	19:a:15:CYS:SG	2.49	0.47
8:H:174:LEU:CD2	18:Z:50:MET:HE3	2.43	0.47
9:I:49:ASP:CA	20:b:10:LYS:NZ	2.78	0.47
10:P:165:ILE:CD1	10:P:253:THR:HG22	2.42	0.47
12:R:67:GLN:HG3	12:R:68:PRO:HD2	1.96	0.47
13:S:35:ASP:O	13:S:38:VAL:HG22	2.15	0.47
13:S:46:LYS:O	13:S:49:PRO:HD3	2.13	0.47
14:T:80:LYS:HB2	14:T:145:VAL:HG11	1.96	0.47
3:C:123:ASN:HB2	15:V:111:GLN:OE1	2.14	0.47
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.47
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.50	0.47
5:E:206:GLU:HB3	5:E:213:PRO:HB3	1.96	0.47
8:H:1:MET:HG3	19:a:30:THR:HG23	1.93	0.47
8:H:249:ILE:CD1	17:X:99:HIS:CE1	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:76:TYR:HE1	9:I:79:ARG:NH2	2.12	0.47
12:R:88:HIS:ND1	12:R:89:PRO:O	2.47	0.47
17:X:20:VAL:HB	17:X:24:VAL:HG21	1.96	0.47
17:X:48:TRP:O	17:X:51:LYS:HE3	2.15	0.47
1:A:37:TYR:CE2	8:H:208:VAL:HG21	2.32	0.47
6:F:313:ASN:OD1	6:F:359:ARG:NH1	2.48	0.47
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.47
7:G:545:LEU:CD2	7:G:547:LEU:HD21	2.44	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
16:W:28:LEU:O	16:W:32:LYS:HG3	2.15	0.47
2:B:140:LYS:O	2:B:143:PRO:HD2	2.15	0.47
3:C:69:PRO:HD2	15:V:99:PRO:O	2.15	0.47
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.47
5:E:45:GLU:CD	5:E:45:GLU:H	2.21	0.47
6:F:128:ARG:HA	6:F:131:MET:HE2	1.96	0.47
6:F:337:MET:HE2	6:F:337:MET:HA	1.96	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
7:G:385:TYR:CE2	7:G:526:LEU:HB2	2.49	0.47
8:H:5:ASN:HA	19:a:26:ILE:CD1	2.41	0.47
8:H:140:ILE:HG13	8:H:141:SER:N	2.29	0.47
1:A:41:PHE:HD2	16:W:102:GLN:CD	2.22	0.47
1:A:47:ALA:HB1	8:H:126:LYS:N	2.30	0.47
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.47
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.47
2:B:135:GLY:HA2	24:B:301:SF4:S3	2.54	0.47
3:C:130:ASN:HD21	3:C:141:ARG:HE	1.62	0.47
4:D:92:HIS:HB2	4:D:458:PHE:HE2	1.79	0.47
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.47
5:E:43:THR:O	5:E:47:ASN:HB3	2.15	0.47
5:E:47:ASN:HB2	5:E:48:PRO:HD2	1.97	0.47
5:E:71:GLU:CG	23:s:94:GLN:HE21	2.26	0.47
6:F:134:ASP:CG	6:F:137:LYS:HB2	2.39	0.47
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
8:H:65:THR:HA	10:P:359:TYR:HB2	1.97	0.47
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.47
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.47
8:H:187:ILE:HD12	29:I:301:3PE:H261	1.95	0.47
8:H:212:ASN:O	8:H:213:VAL:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:87:PRO:HG2	9:I:88:PHE:CE2	2.50	0.47
13:S:24:CYS:N	13:S:58:CYS:HB2	2.30	0.47
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.14	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.47
7:G:137:CYS:N	11:Q:88:GLN:HE21	2.13	0.47
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.47
9:I:106:TYR:O	9:I:107:PRO:C	2.55	0.47
10:P:169:HIS:H	10:P:184:LYS:CE	2.28	0.47
14:T:107:ASP:O	14:T:108:LEU:HB2	2.15	0.47
14:T:116:VAL:O	14:T:120:MET:HG3	2.15	0.47
18:Z:88:ARG:O	18:Z:92:GLU:HG3	2.14	0.47
20:b:78:LEU:HD22	20:b:80:TRP:NE1	2.26	0.47
1:A:102:LEU:CD2	8:H:295:PRO:HG3	2.45	0.47
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.47
5:E:92:LEU:HG	5:E:92:LEU:O	2.15	0.47
6:F:47:GLY:O	6:F:48:ARG:HB2	2.13	0.47
6:F:382:CYS:SG	24:F:502:SF4:S1	3.13	0.47
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.14	0.47
7:G:380:ASP:CB	13:S:41:TYR:OH	2.62	0.47
7:G:517:HIS:H	7:G:599:THR:CG2	2.28	0.47
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	0.47
8:H:226:ALA:O	8:H:227:GLU:C	2.58	0.47
9:I:144:ARG:NE	9:I:146:ASP:OD2	2.46	0.47
10:P:303:LYS:O	10:P:307:LEU:HG	2.15	0.47
12:R:54:GLU:O	21:q:127:TYR:OH	2.24	0.47
14:T:133:ILE:HG13	14:T:137:LYS:NZ	2.30	0.47
15:V:44:TYR:O	15:V:48:THR:HG22	2.15	0.47
16:W:65:LYS:O	16:W:69:MET:HG2	2.14	0.47
20:b:63:MET:HB2	20:b:66:VAL:CG1	2.45	0.47
1:A:17:LEU:CG	8:H:222:LEU:HD11	2.36	0.47
1:A:24:LEU:N	1:A:25:PRO:CD	2.78	0.47
1:A:48:ARG:HG3	1:A:48:ARG:O	2.14	0.47
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.44	0.47
7:G:462:PHE:CD1	7:G:465:VAL:HB	2.50	0.47
13:S:24:CYS:SG	13:S:61:VAL:O	2.72	0.47
14:T:140:CYS:O	14:T:143:GLU:HB2	2.15	0.47
15:V:64:ASP:OD2	15:V:67:LYS:HG2	2.15	0.47
16:W:84:LEU:HD11	16:W:88:LYS:HE3	1.96	0.47
17:X:54:ARG:HD3	18:Z:116:TRP:CZ3	2.50	0.47
21:q:41:GLU:HG3	21:q:47:LYS:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:q:201:CDL:H1	22:r:4:ALA:HA	1.97	0.47
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.50	0.46
3:C:186:ILE:CD1	4:D:113:ILE:CG1	2.94	0.46
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
6:F:364:VAL:HA	6:F:438:LEU:HD11	1.97	0.46
7:G:158:ARG:NH2	7:G:202:ASN:OD1	2.48	0.46
7:G:648:GLU:O	13:S:22:HIS:CE1	2.68	0.46
7:G:651:PRO:HD2	13:S:56:ARG:HB3	1.96	0.46
8:H:260:MET:CE	19:a:16:LEU:CB	2.76	0.46
10:P:40:VAL:O	10:P:42:PRO:HD3	2.15	0.46
10:P:81:ILE:HD11	12:R:46:VAL:HG21	1.97	0.46
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.46
15:V:79:GLU:O	15:V:80:VAL:C	2.58	0.46
17:X:15:VAL:O	17:X:17:GLU:HG3	2.15	0.46
19:a:22:SER:O	19:a:23:THR:C	2.58	0.46
3:C:232:PHE:HE1	7:G:244:GLU:HG3	1.80	0.46
4:D:127:LYS:HE3	4:D:135:TYR:OH	2.15	0.46
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.15	0.46
6:F:240:THR:HG22	6:F:241:THR:N	2.31	0.46
6:F:262:PHE:HA	6:F:265:PHE:HD2	1.81	0.46
7:G:277:MET:HE1	11:Q:153:PRO:HD3	1.96	0.46
7:G:691:ILE:HG12	7:G:695:TYR:CE2	2.50	0.46
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.46
10:P:73:LEU:CD2	10:P:250:VAL:HG22	2.45	0.46
14:T:90:TYR:HE2	14:T:93:ILE:HG12	1.77	0.46
15:V:6:LYS:HG2	15:V:16:VAL:HG23	1.96	0.46
16:W:49:THR:O	16:W:50:VAL:C	2.56	0.46
1:A:87:MET:HE3	1:A:87:MET:HB3	1.84	0.46
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.46
5:E:107:PRO:O	5:E:110:ARG:HB3	2.15	0.46
8:H:16:ALA:CB	19:a:15:CYS:HB3	2.36	0.46
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.46
8:H:68:MET:O	8:H:71:PHE:CB	2.63	0.46
10:P:59:PHE:HA	10:P:83:PRO:HD2	1.96	0.46
10:P:131:GLY:HA3	30:P:401:NDP:O3D	2.15	0.46
16:W:61:GLN:O	16:W:64:ASP:HB2	2.15	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:60:ARG:HD2	21:q:92:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:GLU:HB2	3:C:186:ILE:HG21	1.97	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.97	0.46
6:F:212:LEU:HD12	6:F:212:LEU:O	2.15	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
6:F:300:ILE:HD13	6:F:307:VAL:HG22	1.96	0.46
8:H:219:PRO:O	8:H:223:PHE:HB2	2.15	0.46
9:I:114:ILE:HD13	12:R:106:TYR:CD1	2.51	0.46
10:P:229:VAL:C	10:P:231:LEU:N	2.73	0.46
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.98	0.46
1:A:34:ALA:O	8:H:64:LEU:N	2.35	0.46
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.46
7:G:30:ASN:O	7:G:45:PRO:HD3	2.16	0.46
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.46
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.98	0.46
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.27	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
8:H:52:ALA:HB2	25:H:400:UQ9:H20A	1.97	0.46
9:I:85:ASN:HB3	9:I:89:GLU:HG3	1.97	0.46
10:P:99:ASP:CG	10:P:100:LEU:H	2.24	0.46
10:P:151:ALA:O	10:P:154:GLN:HB3	2.16	0.46
10:P:230:SER:HB3	10:P:234:LYS:HE3	1.98	0.46
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.46
15:V:24:LEU:O	15:V:25:THR:C	2.58	0.46
21:q:17:HIS:ND1	21:q:26:VAL:HG21	2.30	0.46
21:q:42:ASP:CG	21:q:46:ASN:HB2	2.41	0.46
5:E:142:ARG:CB	5:E:182:ALA:HB3	2.45	0.46
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.46
7:G:330:LEU:HD12	7:G:544:MET:HE1	1.98	0.46
7:G:400:VAL:HG22	7:G:473:MET:CG	2.45	0.46
7:G:403:VAL:HG23	7:G:432:ILE:CB	2.38	0.46
7:G:671:LEU:CD2	13:S:45:LYS:HG2	2.44	0.46
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.46
9:I:63:TRP:CD1	9:I:66:LEU:HB2	2.51	0.46
10:P:73:LEU:HD23	10:P:250:VAL:HG22	1.97	0.46
10:P:228:LEU:HD22	10:P:273:LEU:HD21	1.96	0.46
1:A:72:LEU:C	1:A:74:PRO:HD2	2.40	0.46
4:D:420:TYR:CD2	15:V:114:TRP:HH2	2.33	0.46
5:E:131:ILE:N	5:E:169:THR:O	2.48	0.46
6:F:227:PRO:HB2	6:F:228:PRO:CD	2.40	0.46
6:F:383:THR:O	6:F:384:PRO:C	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:35:PHE:O	7:G:101:ASN:HA	2.16	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.50	0.46
10:P:92:MET:C	10:P:94:LEU:N	2.73	0.46
10:P:223:PHE:HZ	10:P:227:PRO:CG	2.28	0.46
11:Q:69:GLU:HA	11:Q:72:ILE:CG2	2.45	0.46
13:S:24:CYS:CA	13:S:58:CYS:HB2	2.46	0.46
16:W:22:PRO:HG3	16:W:26:ARG:NH2	2.30	0.46
5:E:195:LEU:HD23	5:E:218:ARG:CG	2.45	0.46
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.46
7:G:49:VAL:HB	7:G:91:ALA:HA	1.98	0.46
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.46
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.46
8:H:218:GLY:O	8:H:219:PRO:C	2.56	0.46
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.16	0.46
16:W:38:LEU:HG	16:W:70:PHE:HZ	1.80	0.46
1:A:48:ARG:HH11	8:H:124:ASN:HA	1.81	0.46
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.46
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.46
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.46	0.46
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.46
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.46
8:H:93:HIS:CE1	19:a:24:ALA:CB	2.98	0.46
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.46
8:H:206:GLU:C	8:H:207:LEU:HD12	2.41	0.46
10:P:171:ASN:OD1	10:P:171:ASN:O	2.34	0.46
10:P:220:TYR:CD1	10:P:223:PHE:HE1	2.34	0.46
18:Z:108:GLU:O	18:Z:109:SER:C	2.57	0.46
22:r:8:ILE:HA	22:r:11:LEU:HD12	1.98	0.46
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.46
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.45	0.46
7:G:405:THR:O	7:G:407:PRO:HD3	2.16	0.46
14:T:98:LEU:O	14:T:99:SER:C	2.58	0.46
15:V:35:LEU:HD22	15:V:48:THR:HG21	1.98	0.46
15:V:51:ILE:O	15:V:52:THR:C	2.58	0.46
19:a:2:TRP:CZ2	33:q:201:CDL:H522	2.50	0.46
5:E:196:THR:O	5:E:197:PRO:C	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:50:ASP:C	6:F:52:ARG:N	2.73	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.84	0.45
10:P:276:LEU:CD2	10:P:280:ILE:HD11	2.46	0.45
10:P:354:ARG:HD2	10:P:362:LEU:O	2.16	0.45
11:Q:63:THR:O	16:W:85:LEU:HD21	2.16	0.45
14:T:123:GLU:HA	14:T:128:PHE:O	2.16	0.45
16:W:65:LYS:HE3	16:W:69:MET:SD	2.56	0.45
19:a:4:GLU:O	19:a:7:PRO:HD2	2.16	0.45
23:s:94:GLN:OE1	23:s:94:GLN:N	2.49	0.45
1:A:51:PHE:CE1	8:H:130:PHE:CE1	2.97	0.45
1:A:73:LEU:HA	8:H:151:LEU:HD13	1.98	0.45
3:C:118:VAL:HB	3:C:121:ARG:HD2	1.98	0.45
3:C:155:ILE:O	3:C:156:VAL:C	2.58	0.45
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.45
7:G:35:PHE:CE1	7:G:40:SER:CB	2.99	0.45
7:G:176:CYS:SG	24:G:802:SF4:S1	3.14	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.45
7:G:665:PHE:O	7:G:666:GLN:C	2.57	0.45
8:H:99:ASN:ND2	19:a:40:ARG:CA	2.72	0.45
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.45
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.45
10:P:106:LEU:HB2	12:R:50:ASP:OD2	2.16	0.45
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.96	0.45
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.45
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.45
5:E:180:VAL:HG13	5:E:181:ASN:N	2.31	0.45
5:E:241:GLY:HA2	6:F:63:TYR:CE2	2.51	0.45
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.45
6:F:157:TYR:CG	6:F:212:LEU:HD11	2.51	0.45
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.16	0.45
7:G:83:GLU:O	7:G:84:LYS:C	2.59	0.45
8:H:69:SER:O	8:H:70:LEU:C	2.56	0.45
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.80	0.45
10:P:318:LYS:HA	10:P:321:ARG:HG2	1.97	0.45
10:P:370:LYS:HD3	10:P:371:PRO:O	2.16	0.45
13:S:30:SER:O	13:S:31:GLN:C	2.56	0.45
15:V:43:ALA:O	15:V:44:TYR:C	2.60	0.45
1:A:62:PHE:CD1	8:H:144:VAL:HG23	2.43	0.45
1:A:102:LEU:HD23	8:H:295:PRO:HG3	1.97	0.45
2:B:114:MET:O	2:B:119:VAL:HG22	2.16	0.45
2:B:117:PHE:CD2	2:B:202:LEU:HD21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:PHE:CE2	2:B:202:LEU:HD21	2.52	0.45
2:B:125:PRO:O	2:B:126:ARG:C	2.58	0.45
2:B:202:LEU:HD11	9:I:86:TYR:CD2	2.51	0.45
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.45
4:D:266:ARG:HD3	29:I:301:3PE:P	2.57	0.45
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.16	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.98	0.45
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.31	0.45
11:Q:52:LEU:HA	11:Q:52:LEU:HD23	1.73	0.45
11:Q:163:ASN:OD1	11:Q:164:PHE:CG	2.69	0.45
16:W:31:ALA:O	16:W:32:LYS:C	2.58	0.45
1:A:56:PHE:O	1:A:57:LEU:C	2.58	0.45
3:C:126:GLU:O	3:C:128:VAL:HG23	2.17	0.45
6:F:136:HIS:O	6:F:137:LYS:C	2.59	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.31	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:182:CYS:SG	24:G:802:SF4:S1	3.14	0.45
7:G:383:SER:O	7:G:384:ASN:C	2.58	0.45
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.45
8:H:24:GLU:OE1	8:H:228:TYR:HE1	1.99	0.45
8:H:179:TRP:NE1	18:Z:43:LEU:HD12	2.32	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
10:P:188:GLU:HG3	10:P:202:ARG:HH21	1.82	0.45
16:W:69:MET:C	16:W:71:MET:H	2.24	0.45
1:A:37:TYR:CE1	2:B:125:PRO:HD2	2.52	0.45
1:A:73:LEU:O	8:H:160:TYR:OH	2.35	0.45
2:B:156:ARG:HG2	10:P:89:TYR:OH	2.16	0.45
4:D:241:LEU:CB	18:Z:16:TYR:OH	2.63	0.45
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	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
7:G:330:LEU:CA	7:G:544:MET:HE1	2.46	0.45
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.45
16:W:45:GLU:O	16:W:46:VAL:C	2.59	0.45
23:s:92:LEU:HB2	23:s:93:PRO:CD	2.40	0.45
2:B:136:THR:HG21	2:B:177:VAL:CG2	2.44	0.45
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.81	0.45
4:D:81:THR:HA	4:D:100:GLU:HA	1.98	0.45
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
4:D:386:THR:HG23	9:I:118:LEU:CD1	2.47	0.45
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.45
7:G:35:PHE:CD1	7:G:40:SER:HB2	2.51	0.45
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.45
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.98	0.45
7:G:399:VAL:HG21	7:G:462:PHE:CZ	2.52	0.45
10:P:88:VAL:O	10:P:91:ILE:HG12	2.17	0.45
10:P:203:PRO:HG2	30:P:401:NDP:C6N	2.47	0.45
10:P:235:THR:CG2	10:P:323:HIS:O	2.63	0.45
1:A:41:PHE:CG	16:W:102:GLN:NE2	2.85	0.45
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.45
6:F:335:VAL:HG13	6:F:341:ALA:HB1	1.99	0.45
7:G:422:TRP:HZ2	7:G:441:ARG:HB3	1.82	0.45
7:G:629:ILE:HD11	16:W:122:LEU:HD21	1.98	0.45
8:H:213:VAL:O	8:H:214:GLU:HB2	2.15	0.45
8:H:310:PHE:CD1	20:b:32:MET:HB3	2.52	0.45
11:Q:53:ILE:HG22	16:W:20:VAL:O	2.17	0.45
15:V:33:ASP:O	15:V:34:ILE:C	2.59	0.45
15:V:62:GLU:HA	15:V:63:PRO:HD3	1.82	0.45
16:W:36:ARG:O	16:W:40:ARG:HG3	2.16	0.45
17:X:49:GLU:OE2	20:b:58:ARG:NH2	2.49	0.45
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.32	0.45
2:B:174:SER:HB2	4:D:123:LEU:HD21	1.98	0.45
3:C:183:LEU:HD22	16:W:91:MET:HE1	1.99	0.45
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.45
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.45
6:F:410:ASP:O	6:F:413:TRP:HB3	2.17	0.45
7:G:97:MET:SD	7:G:100:TRP:CZ2	3.10	0.45
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.45
9:I:116:CYS:HB2	9:I:118:LEU:H	1.80	0.45
9:I:135:ARG:O	9:I:136:ALA:HB3	2.16	0.45
10:P:192:ARG:NE	10:P:200:ILE:HD12	2.30	0.45
12:R:84:GLY:O	12:R:85:ALA:CB	2.65	0.45
14:T:99:SER:C	14:T:101:ASN:N	2.74	0.45
21:q:6:VAL:HG21	33:q:201:CDL:CB4	2.44	0.45
21:q:37:THR:O	21:q:49:TYR:HA	2.17	0.45
1:A:30:TYR:HD2	1:A:33:LYS:NZ	2.15	0.45
2:B:156:ARG:O	10:P:89:TYR:CE1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:97:LEU:HD23	4:D:111:PRO:HA	1.98	0.45
6:F:196:PHE:HD1	23:s:91:ARG:HE	1.65	0.45
6:F:300:ILE:CG2	6:F:306:GLY:C	2.90	0.45
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.45
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
12:R:44:ARG:HB3	12:R:47:ARG:HH12	1.82	0.45
17:X:27:ALA:HB1	17:X:85:TYR:CD2	2.52	0.45
1:A:53:MET:HE3	1:A:55:PHE:CD1	2.52	0.44
1:A:97:ILE:HG13	1:A:98:LEU:N	2.32	0.44
3:C:148:GLU:OE2	11:Q:140:LYS:NZ	2.30	0.44
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.44
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.44
5:E:243:GLY:O	5:E:244:VAL:C	2.58	0.44
6:F:226:LYS:N	6:F:227:PRO:CD	2.80	0.44
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.44
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44
8:H:5:ASN:HD21	19:a:23:THR:CA	2.30	0.44
8:H:62:ARG:NH2	8:H:68:MET:HE2	2.32	0.44
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.44
8:H:200:LEU:HD11	8:H:282:TYR:HA	1.98	0.44
10:P:97:MET:HE2	10:P:97:MET:HB3	1.83	0.44
14:T:102:SER:HB2	14:T:107:ASP:CB	2.46	0.44
19:a:66:LEU:HD13	19:a:66:LEU:O	2.17	0.44
21:q:68:MET:HE2	21:q:71:LYS:HD3	1.99	0.44
1:A:62:PHE:HE1	8:H:144:VAL:HG22	1.65	0.44
3:C:149:LEU:O	3:C:151:PRO:HD3	2.17	0.44
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.17	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
6:F:253:THR:O	6:F:257:ARG:HB3	2.16	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.58	0.44
7:G:308:ARG:NH1	7:G:578:PRO:O	2.50	0.44
7:G:382:ARG:CZ	7:G:652:ASN:ND2	2.80	0.44
8:H:65:THR:CB	8:H:124:ASN:HD22	2.21	0.44
8:H:224:PHE:C	8:H:226:ALA:N	2.71	0.44
29:I:301:3PE:H3A2	29:I:301:3PE:H371	1.80	0.44
10:P:141:PHE:HD1	10:P:145:PHE:HE2	1.64	0.44
10:P:146:VAL:O	10:P:147:ASN:C	2.60	0.44
10:P:315:THR:O	10:P:319:VAL:HG23	2.16	0.44
15:V:48:THR:HA	15:V:51:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:HE2	8:H:61:MET:HE1	1.98	0.44
2:B:97:LEU:HB2	2:B:134:ALA:O	2.18	0.44
2:B:99:CYS:O	2:B:102:VAL:N	2.45	0.44
2:B:99:CYS:CB	4:D:141:TYR:CB	2.96	0.44
4:D:88:HIS:CE1	8:H:205:SER:O	2.70	0.44
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.44
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.44
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.44
8:H:230:ASN:O	8:H:231:ILE:C	2.57	0.44
9:I:98:ARG:NH1	9:I:155:CYS:O	2.50	0.44
10:P:128:ASN:HD22	10:P:166:HIS:CD2	2.35	0.44
16:W:104:THR:HG22	16:W:108:ARG:HE	1.82	0.44
21:q:48:TYR:OH	21:q:83:PRO:HD2	2.17	0.44
1:A:60:ILE:O	1:A:61:THR:C	2.57	0.44
2:B:170:TYR:CE1	4:D:135:TYR:OH	2.69	0.44
3:C:47:ARG:HD3	4:D:160:ASN:HA	1.99	0.44
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
6:F:261:TRP:HZ3	6:F:262:PHE:CE2	2.35	0.44
6:F:392:MET:HE2	6:F:416:SER:HA	1.93	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.46	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.44
10:P:81:ILE:HG12	12:R:46:VAL:HG11	1.99	0.44
10:P:244:ASP:HB3	10:P:335:LEU:HD13	1.98	0.44
1:A:53:MET:HE2	1:A:56:PHE:N	2.32	0.44
4:D:137:ASP:OD1	4:D:148:GLU:OE2	2.35	0.44
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.44
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.44
4:D:299:GLN:OE1	9:I:36:TYR:CD2	2.71	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44
5:E:73:HIS:CE1	11:Q:166:TRP:CD2	3.05	0.44
5:E:81:VAL:O	5:E:82:LEU:C	2.59	0.44
6:F:36:LYS:CB	6:F:38:GLU:HG2	2.42	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
7:G:304:GLU:CG	7:G:305:PRO:HD2	2.48	0.44
7:G:450:LYS:HG3	7:G:450:LYS:O	2.18	0.44
7:G:629:ILE:HD11	16:W:122:LEU:HD11	2.00	0.44
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.44
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.44
8:H:194:ASN:HB2	8:H:227:GLU:OE2	2.17	0.44
9:I:61:LEU:HD21	29:I:301:3PE:C38	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:168:SER:O	10:P:203:PRO:HD2	2.16	0.44
10:P:276:LEU:CD2	10:P:280:ILE:CD1	2.95	0.44
12:R:46:VAL:O	12:R:47:ARG:C	2.58	0.44
16:W:77:THR:O	16:W:79:PRO:HD3	2.16	0.44
16:W:124:LYS:O	16:W:125:PHE:C	2.58	0.44
17:X:84:GLU:C	17:X:87:THR:HG22	2.42	0.44
1:A:91:ALA:O	1:A:94:LEU:HB3	2.17	0.44
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.98	0.44
5:E:163:THR:HG23	5:E:168:PHE:O	2.17	0.44
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:309:ASN:OD1	7:G:310:GLU:N	2.51	0.44
7:G:617:ARG:HH22	16:W:128:GLY:H	1.64	0.44
8:H:96:ILE:CG1	18:Z:143:TYR:OH	2.44	0.44
10:P:232:GLY:O	10:P:273:LEU:HB3	2.18	0.44
10:P:321:ARG:HA	10:P:325:SER:HB2	2.00	0.44
11:Q:69:GLU:O	11:Q:72:ILE:CG2	2.61	0.44
18:Z:133:MET:O	18:Z:134:SER:C	2.60	0.44
1:A:38:GLU:CD	1:A:43:PRO:HA	2.42	0.44
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.99	0.44
6:F:119:GLU:H	6:F:159:ARG:HD2	1.83	0.44
6:F:299:LEU:C	6:F:299:LEU:CD1	2.91	0.44
7:G:304:GLU:HB3	7:G:316:TYR:HD1	1.83	0.44
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.44
9:I:57:ALA:HB2	20:b:13:TRP:O	2.17	0.44
9:I:152:CYS:SG	24:I:302:SF4:S2	3.16	0.44
10:P:221:ARG:HD2	10:P:286:ARG:CD	2.43	0.44
10:P:227:PRO:HB2	10:P:298:TYR:HE1	1.78	0.44
14:T:140:CYS:O	14:T:141:PRO:C	2.59	0.44
15:V:31:THR:O	15:V:33:ASP:N	2.50	0.44
16:W:98:LYS:HD3	16:W:100:TRP:CZ2	2.53	0.44
17:X:49:GLU:CG	17:X:50:GLU:H	2.30	0.44
23:s:83:LEU:O	23:s:87:LEU:HD13	2.18	0.44
1:A:67:LEU:O	1:A:70:ALA:HB3	2.18	0.44
1:A:93:ILE:O	1:A:97:ILE:HG23	2.18	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
5:E:79:LEU:HB2	5:E:80:PRO:HD3	2.00	0.44
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.44
10:P:283:MET:HG2	10:P:353:LEU:HD12	1.99	0.44
10:P:293:LEU:HB3	10:P:294:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:299:SER:HB3	10:P:316:LYS:NZ	2.33	0.44
13:S:20:ARG:CG	13:S:66:TRP:HB2	2.46	0.44
14:T:147:TYR:O	14:T:148:ILE:C	2.61	0.44
15:V:31:THR:O	15:V:32:LEU:C	2.61	0.44
15:V:50:GLN:NE2	22:r:94:ALA:H	2.15	0.44
17:X:73:GLN:O	17:X:77:HIS:N	2.51	0.44
1:A:21:ALA:O	8:H:60:PRO:CG	2.61	0.44
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.52	0.44
3:C:153:ASP:OD1	3:C:153:ASP:N	2.50	0.44
3:C:229:PHE:CE1	9:I:126:GLN:CG	2.71	0.44
4:D:385:TYR:HD2	9:I:122:ILE:CD1	2.31	0.44
5:E:133:VAL:HG22	5:E:185:VAL:HG12	2.00	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
6:F:410:ASP:OD1	6:F:410:ASP:C	2.58	0.44
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.58	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.47	0.44
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.52	0.44
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.44
11:Q:75:ARG:NH1	11:Q:102:ASP:OD1	2.51	0.44
16:W:31:ALA:C	16:W:33:ARG:N	2.74	0.44
1:A:15:LEU:O	1:A:18:ILE:N	2.51	0.43
1:A:97:ILE:O	1:A:98:LEU:C	2.57	0.43
1:A:108:GLN:O	1:A:109:LYS:C	2.59	0.43
3:C:127:ILE:H	3:C:127:ILE:HD12	1.83	0.43
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
4:D:198:THR:HG21	8:H:275:ALA:HB1	1.99	0.43
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
6:F:311:TRP:CH2	6:F:333:GLU:HB3	2.53	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.43
7:G:173:MET:CE	7:G:206:VAL:O	2.64	0.43
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.43
7:G:662:THR:HB	13:S:25:GLN:NE2	2.33	0.43
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.43	0.43
8:H:35:LYS:HG2	9:I:81:PRO:HG3	1.99	0.43
11:Q:112:MET:HG2	11:Q:114:TRP:CE2	2.52	0.43
21:q:9:ARG:O	21:q:13:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:145:MET:O	4:D:148:GLU:HG3	2.18	0.43
5:E:47:ASN:HB2	5:E:48:PRO:CD	2.47	0.43
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.43
8:H:14:LEU:HD23	8:H:14:LEU:HA	1.86	0.43
8:H:134:ARG:HB3	8:H:282:TYR:CD1	2.53	0.43
8:H:200:LEU:CD1	8:H:285:LEU:HD13	2.48	0.43
9:I:59:ARG:O	9:I:59:ARG:HG2	2.18	0.43
10:P:72:HIS:O	10:P:73:LEU:C	2.61	0.43
10:P:114:ASP:O	10:P:118:LYS:HG2	2.18	0.43
10:P:231:LEU:HB2	10:P:233:PHE:HD1	1.82	0.43
10:P:231:LEU:CD2	10:P:292:PRO:HB3	2.48	0.43
10:P:266:THR:CG2	10:P:329:PRO:HB3	2.47	0.43
14:T:103:HIS:O	14:T:107:ASP:N	2.51	0.43
20:b:37:PRO:O	20:b:40:LYS:NZ	2.51	0.43
2:B:90:LEU:HD22	2:B:130:VAL:HG21	1.99	0.43
2:B:99:CYS:O	2:B:100:CYS:C	2.57	0.43
4:D:95:LEU:HG	4:D:96:ARG:N	2.32	0.43
4:D:140:ASP:CB	4:D:147:ASN:HD21	2.25	0.43
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.42	0.43
5:E:196:THR:O	5:E:199:ASP:N	2.51	0.43
6:F:119:GLU:HB3	6:F:124:THR:HG22	2.00	0.43
7:G:75:CYS:SG	27:G:803:FES:S2	3.16	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.50	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
7:G:359:ASN:C	7:G:361:VAL:O	2.61	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
9:I:61:LEU:CG	29:I:301:3PE:H381	2.48	0.43
10:P:110:ALA:HB1	10:P:148:ILE:CD1	2.48	0.43
10:P:275:HIS:CE1	10:P:373:LYS:HE2	2.53	0.43
10:P:293:LEU:C	10:P:298:TYR:HE2	2.26	0.43
15:V:56:LEU:O	15:V:60:LYS:HG2	2.17	0.43
19:a:57:VAL:HG22	19:a:57:VAL:O	2.18	0.43
21:q:42:ASP:OD1	21:q:46:ASN:HB2	2.18	0.43
2:B:171:TYR:HD2	4:D:118:ARG:HB3	1.78	0.43
4:D:235:ASP:OD2	18:Z:8:GLN:OE1	2.36	0.43
6:F:174:ARG:CG	23:s:87:LEU:HD11	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
13:S:35:ASP:O	13:S:36:PHE:C	2.60	0.43
15:V:31:THR:C	15:V:33:ASP:N	2.73	0.43
16:W:33:ARG:NH2	16:W:37:GLU:OE2	2.50	0.43
17:X:7:LEU:HD22	18:Z:87:LEU:HD12	1.99	0.43
1:A:37:TYR:CE1	2:B:125:PRO:CD	3.02	0.43
2:B:77:LYS:HD3	2:B:77:LYS:HA	1.64	0.43
2:B:146:ARG:NH2	3:C:211:TYR:CE2	2.86	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.34	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
6:F:424:ILE:CA	7:G:76:ARG:NH1	2.82	0.43
7:G:61:PRO:HB3	7:G:146:PHE:CD2	2.53	0.43
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.43
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.18	0.43
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.43
8:H:174:LEU:CD2	18:Z:50:MET:CE	2.97	0.43
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.43
10:P:111:ARG:NH1	10:P:138:ASN:HB3	2.33	0.43
13:S:18:GLU:OE2	13:S:68:ARG:NE	2.50	0.43
19:a:18:ILE:O	19:a:22:SER:HB3	2.18	0.43
22:r:5:THR:CG2	22:r:7:VAL:HG12	2.46	0.43
3:C:219:VAL:HG21	16:W:113:THR:HG21	2.01	0.43
4:D:145:MET:HA	4:D:148:GLU:CG	2.49	0.43
6:F:110:PRO:CB	6:F:152:ARG:HE	2.18	0.43
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.47	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
7:G:517:HIS:H	7:G:599:THR:HG21	1.84	0.43
8:H:7:LEU:HD13	8:H:7:LEU:HA	1.75	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.97	0.43
10:P:187:GLY:O	10:P:188:GLU:C	2.62	0.43
10:P:293:LEU:HD12	10:P:298:TYR:OH	2.19	0.43
11:Q:156:LYS:HE2	11:Q:156:LYS:HB3	1.84	0.43
14:T:105:MET:HE1	14:T:115:GLN:HG3	1.99	0.43
16:W:87:ILE:O	16:W:88:LYS:C	2.61	0.43
17:X:140:ASN:N	17:X:141:PRO:CD	2.81	0.43
1:A:65:PHE:CD2	8:H:294:LEU:HD21	2.53	0.43
2:B:123:ALA:O	2:B:124:SER:C	2.61	0.43
2:B:169:GLY:O	2:B:170:TYR:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.43
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
7:G:355:LYS:CG	7:G:366:LEU:HD12	2.43	0.43
8:H:179:TRP:CZ3	29:I:301:3PE:H371	2.54	0.43
8:H:196:ALA:C	8:H:198:PHE:N	2.76	0.43
8:H:257:THR:O	8:H:260:MET:HB2	2.19	0.43
8:H:280:PHE:HD2	8:H:284:GLN:HG3	1.81	0.43
10:P:304:LEU:HA	10:P:307:LEU:HG	2.00	0.43
13:S:85:ASP:OD1	13:S:86:GLU:N	2.51	0.43
16:W:98:LYS:HD3	16:W:100:TRP:CE2	2.53	0.43
17:X:122:LEU:O	18:Z:66:GLU:OE1	2.37	0.43
17:X:130:LYS:HE2	17:X:130:LYS:HB3	1.79	0.43
4:D:82:LEU:HG	4:D:83:ASN:O	2.19	0.43
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.43
5:E:144:SER:O	5:E:147:ILE:HB	2.19	0.43
6:F:126:LYS:HE2	6:F:274:LYS:HZ3	1.84	0.43
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.43
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.43
7:G:462:PHE:CZ	7:G:466:LEU:HD21	2.54	0.43
7:G:611:THR:CG2	11:Q:104:ARG:C	2.91	0.43
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
7:G:664:TYR:OH	13:S:23:LEU:HD11	2.18	0.43
8:H:260:MET:HG3	19:a:17:VAL:HB	2.00	0.43
8:H:310:PHE:CE1	20:b:32:MET:HB3	2.53	0.43
9:I:71:GLY:O	22:r:15:ALA:HB1	2.19	0.43
9:I:135:ARG:HD2	12:R:61:ILE:CG1	2.49	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:144:VAL:HG23	10:P:145:PHE:CD2	2.54	0.43
11:Q:61:ILE:HG12	11:Q:140:LYS:HG2	2.01	0.43
15:V:39:PRO:O	15:V:40:LYS:C	2.60	0.43
15:V:82:LEU:HG	15:V:86:LYS:HE2	2.00	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:66:THR:HG23	21:q:74:PHE:HD1	1.83	0.43
3:C:117:ASP:OD1	3:C:124:ARG:HB2	2.18	0.43
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.43
4:D:376:GLU:OE1	7:G:150:ARG:O	2.36	0.43
5:E:138:PRO:HG3	6:F:355:ILE:HD13	1.99	0.43
5:E:230:LEU:C	5:E:232:SER:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:184:ARG:O	7:G:185:PHE:C	2.60	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.34	0.43
7:G:283:GLU:O	7:G:283:GLU:CG	2.50	0.43
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.59	0.43
8:H:138:GLN:HG3	8:H:139:THR:N	2.34	0.43
8:H:310:PHE:HB2	20:b:33:PRO:HA	1.99	0.43
15:V:56:LEU:HG	15:V:60:LYS:HE3	2.01	0.43
17:X:131:VAL:HG23	17:X:131:VAL:O	2.19	0.43
2:B:194:CYS:SG	4:D:138:ARG:NE	2.91	0.43
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.01	0.43
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.43
7:G:246:ARG:NH1	11:Q:106:ARG:HE	2.17	0.43
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.43
8:H:8:THR:CB	19:a:22:SER:CB	2.97	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
14:T:104:PHE:O	14:T:110:LEU:HB2	2.19	0.43
15:V:62:GLU:OE2	15:V:64:ASP:HB3	2.19	0.43
18:Z:120:LEU:O	18:Z:121:ILE:C	2.61	0.43
18:Z:134:SER:C	18:Z:136:ALA:N	2.76	0.43
19:a:1:MET:HG3	33:q:201:CDL:OB2	2.18	0.43
20:b:31:ILE:O	20:b:35:ILE:HG22	2.18	0.43
21:q:14:VAL:HG13	21:q:23:LEU:HG	2.01	0.43
1:A:42:ASP:O	1:A:43:PRO:C	2.61	0.42
2:B:81:LEU:CD2	26:B:303:PC1:H352	2.48	0.42
3:C:227:GLN:NE2	9:I:129:THR:HG21	2.34	0.42
5:E:71:GLU:HG3	23:s:94:GLN:NE2	2.27	0.42
6:F:45:LEU:HG	6:F:46:TYR:CE1	2.54	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
6:F:157:TYR:CG	6:F:212:LEU:CD1	3.01	0.42
7:G:165:ILE:CG2	7:G:169:VAL:HB	2.48	0.42
9:I:63:TRP:HZ2	29:I:301:3PE:C2C	2.32	0.42
10:P:226:VAL:HG11	10:P:228:LEU:HG	2.00	0.42
10:P:336:GLU:H	10:P:336:GLU:CD	2.25	0.42
11:Q:57:GLU:HG3	11:Q:58:LYS:O	2.19	0.42
12:R:43:TYR:C	12:R:45:ARG:H	2.26	0.42
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.42
13:S:44:LEU:CD2	13:S:91:MET:HG2	2.48	0.42
16:W:23:ILE:HD12	16:W:80:ARG:O	2.19	0.42
17:X:128:VAL:HG12	20:b:54:PRO:HB2	2.01	0.42
18:Z:128:ARG:HB3	18:Z:132:GLU:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:143:TYR:O	18:Z:144:THR:HB	2.15	0.42
2:B:153:PRO:HG3	8:H:58:LYS:HD2	2.01	0.42
3:C:114:THR:OG1	4:D:421:ARG:NH1	2.52	0.42
6:F:227:PRO:CB	6:F:228:PRO:HD3	2.40	0.42
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.42
7:G:291:ARG:HD2	7:G:292:PHE:CE2	2.54	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.42
9:I:67:ILE:O	9:I:70:LEU:N	2.53	0.42
11:Q:69:GLU:C	11:Q:72:ILE:HG22	2.44	0.42
16:W:69:MET:O	16:W:71:MET:N	2.53	0.42
16:W:104:THR:HG22	16:W:108:ARG:NE	2.34	0.42
18:Z:12:PRO:CD	18:Z:16:TYR:CZ	3.01	0.42
19:a:37:ARG:NH1	19:a:59:ARG:HD2	2.34	0.42
1:A:27:MET:HE1	8:H:60:PRO:O	2.19	0.42
1:A:71:LEU:HB2	1:A:94:LEU:HD21	2.01	0.42
1:A:74:PRO:C	1:A:76:PRO:HD2	2.44	0.42
3:C:208:GLU:HG3	3:C:221:GLU:HG3	2.00	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.42
7:G:224:ASP:OD2	7:G:291:ARG:NH1	2.48	0.42
7:G:651:PRO:O	7:G:654:VAL:HG12	2.19	0.42
10:P:271:TYR:CA	10:P:375:VAL:HG22	2.50	0.42
16:W:53:MET:O	16:W:54:GLN:C	2.62	0.42
3:C:72:VAL:HG22	3:C:87:ILE:HG22	2.01	0.42
3:C:202:PRO:O	3:C:203:LEU:C	2.62	0.42
4:D:128:THR:H	4:D:131:GLN:HG2	1.83	0.42
4:D:202:TRP:NE1	9:I:76:TYR:HD2	2.17	0.42
4:D:375:MET:HE1	7:G:126:LEU:HA	2.00	0.42
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.42
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.42
6:F:174:ARG:CB	23:s:87:LEU:HD11	2.48	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
6:F:363:ILE:HG23	6:F:364:VAL:N	2.33	0.42
6:F:412:LEU:CD2	6:F:435:VAL:HG13	2.48	0.42
7:G:380:ASP:HB2	13:S:41:TYR:OH	2.19	0.42
7:G:388:ASN:N	7:G:514:ASN:CB	2.69	0.42
7:G:480:ALA:O	7:G:481:LEU:C	2.63	0.42
8:H:67:SER:HG	8:H:121:TRP:HZ3	1.67	0.42
9:I:189:LYS:O	9:I:189:LYS:CG	2.65	0.42
11:Q:57:GLU:CD	11:Q:58:LYS:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:126:LEU:CD1	11:Q:137:PHE:CE2	3.03	0.42
13:S:16:LEU:HD11	13:S:19:ILE:HG12	2.01	0.42
18:Z:111:PHE:CD1	18:Z:117:VAL:HG21	2.55	0.42
18:Z:134:SER:O	18:Z:138:PHE:N	2.47	0.42
19:a:18:ILE:H	19:a:19:PRO:HD3	1.85	0.42
20:b:45:ILE:N	20:b:80:TRP:HH2	2.17	0.42
20:b:69:HIS:H	20:b:72:ASP:CG	2.28	0.42
1:A:30:TYR:HD2	1:A:33:LYS:HZ1	1.68	0.42
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.42
3:C:120:THR:CG2	3:C:121:ARG:H	2.32	0.42
5:E:73:HIS:HE1	11:Q:166:TRP:CG	2.38	0.42
5:E:155:LEU:CD1	5:E:204:ILE:HD13	2.50	0.42
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.34	0.42
7:G:65:TYR:HB2	7:G:92:CYS:SG	2.60	0.42
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.37	0.42
7:G:272:ARG:HE	7:G:274:LEU:CD2	2.22	0.42
7:G:670:GLU:HB2	13:S:42:VAL:HG23	2.01	0.42
8:H:5:ASN:OD1	19:a:23:THR:CA	2.61	0.42
10:P:96:LEU:HD12	10:P:97:MET:CA	2.49	0.42
10:P:110:ALA:HB1	10:P:148:ILE:HD12	2.02	0.42
11:Q:98:LYS:NZ	11:Q:127:THR:OG1	2.52	0.42
14:T:107:ASP:C	14:T:108:LEU:HD12	2.45	0.42
16:W:69:MET:O	16:W:70:PHE:C	2.60	0.42
1:A:3:LEU:CA	8:H:96:ILE:HD13	2.45	0.42
1:A:108:GLN:OE1	1:A:108:GLN:HA	2.19	0.42
25:B:302:UQ9:H4MB	25:B:302:UQ9:O3	2.19	0.42
4:D:141:TYR:CE1	4:D:457:VAL:HG13	2.53	0.42
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.42
5:E:184:MET:HE2	5:E:184:MET:HB3	1.74	0.42
6:F:114:VAL:HG21	6:F:235:VAL:HG21	2.01	0.42
6:F:235:VAL:CG2	6:F:240:THR:HG21	2.48	0.42
7:G:117:MET:SD	7:G:143:SER:HB2	2.58	0.42
7:G:355:LYS:HG3	7:G:366:LEU:CD1	2.43	0.42
7:G:480:ALA:O	7:G:483:ARG:HG3	2.20	0.42
7:G:671:LEU:HD12	13:S:42:VAL:HG23	2.02	0.42
8:H:15:ILE:CB	19:a:15:CYS:SG	3.08	0.42
17:X:124:GLN:O	20:b:70:PRO:HB3	2.20	0.42
5:E:78:VAL:HG23	5:E:79:LEU:H	1.84	0.42
5:E:78:VAL:HG21	6:F:218:GLY:O	2.20	0.42
5:E:240:PRO:CB	6:F:60:GLY:HA3	2.46	0.42
6:F:41:ILE:HD13	6:F:250:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:261:TRP:CE3	6:F:262:PHE:CD1	3.05	0.42
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.42
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.42
8:H:17:MET:SD	8:H:229:THR:OG1	2.65	0.42
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.42
13:S:32:GLY:HA2	13:S:35:ASP:CG	2.44	0.42
13:S:79:LEU:HA	13:S:82:LEU:CG	2.46	0.42
15:V:13:GLY:O	15:V:14:LEU:C	2.62	0.42
18:Z:30:LEU:HD12	18:Z:30:LEU:H	1.84	0.42
1:A:80:GLN:C	20:b:46:ASN:ND2	2.71	0.42
1:A:113:TRP:HZ2	8:H:286:MET:HB3	1.82	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.19	0.42
4:D:144:MET:HG2	4:D:223:HIS:H	1.85	0.42
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.82	0.42
4:D:198:THR:OG1	4:D:261:MET:SD	2.78	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:398:ARG:HH21	7:G:155:GLU:HG3	1.83	0.42
7:G:496:MET:O	7:G:500:ILE:HG13	2.20	0.42
7:G:555:ILE:HD13	7:G:560:LEU:HD11	2.01	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.52	0.42
8:H:90:PRO:O	8:H:91:MET:C	2.60	0.42
8:H:93:HIS:CE1	19:a:24:ALA:HA	2.55	0.42
10:P:75:ARG:C	10:P:77:GLY:H	2.28	0.42
10:P:225:ALA:HB3	10:P:291:TYR:CE2	2.55	0.42
10:P:309:PRO:HG2	10:P:310:PHE:CD2	2.54	0.42
11:Q:126:LEU:CD1	11:Q:137:PHE:HE2	2.33	0.42
15:V:11:LEU:H	15:V:11:LEU:HD12	1.85	0.42
17:X:32:TYR:CE1	17:X:67:ALA:HB2	2.55	0.42
17:X:41:LYS:HB3	17:X:131:VAL:HG11	2.02	0.42
1:A:18:ILE:CG1	8:H:222:LEU:CD2	2.97	0.42
1:A:24:LEU:H	1:A:25:PRO:HD3	1.84	0.42
2:B:69:SER:O	2:B:70:ARG:C	2.61	0.42
2:B:95:PHE:HE1	2:B:97:LEU:HD11	1.84	0.42
2:B:126:ARG:HG3	8:H:214:GLU:HA	2.02	0.42
3:C:87:ILE:HG21	3:C:95:THR:HG21	2.02	0.42
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.42
5:E:145:ASP:O	5:E:146:SER:C	2.62	0.42
5:E:226:PRO:CA	6:F:286:CYS:HB3	2.50	0.42
6:F:300:ILE:CG2	6:F:306:GLY:CA	2.95	0.42
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	0.42
8:H:95:LEU:HA	19:a:23:THR:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:138:GLN:OE1	8:H:200:LEU:HD12	2.19	0.42
11:Q:99:MET:HB2	11:Q:128:PHE:HE2	1.84	0.42
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.42
15:V:37:HIS:HB2	15:V:95:LEU:HD11	2.01	0.42
17:X:59:GLU:OE2	17:X:135:ARG:HD3	2.19	0.42
21:q:75:TRP:HA	21:q:75:TRP:CE3	2.55	0.42
1:A:49:LEU:HD23	1:A:49:LEU:N	2.34	0.42
1:A:93:ILE:O	1:A:97:ILE:HG12	2.20	0.42
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.53	0.42
2:B:169:GLY:O	2:B:171:TYR:N	2.53	0.42
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.42
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.42
3:C:53:THR:O	3:C:54:HIS:C	2.60	0.42
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.42
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.42
4:D:233:HIS:CE1	9:I:160:GLU:OE1	2.73	0.42
5:E:73:HIS:ND1	11:Q:166:TRP:CE2	2.88	0.42
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.42
6:F:70:LEU:O	6:F:71:LYS:C	2.63	0.42
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
8:H:59:GLU:OE1	8:H:61:MET:SD	2.78	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
8:H:196:ALA:HA	8:H:199:ASP:HB2	2.00	0.42
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.42
9:I:182:GLU:HA	21:q:124:TYR:HD2	1.85	0.42
10:P:140:ASP:O	10:P:141:PHE:C	2.62	0.42
14:T:85:TYR:CZ	14:T:89:LEU:HD11	2.55	0.42
15:V:47:TYR:O	15:V:50:GLN:HB3	2.20	0.42
15:V:114:TRP:O	15:V:114:TRP:CE3	2.72	0.42
16:W:53:MET:O	16:W:103:ARG:HG2	2.20	0.42
21:q:20:LEU:HD23	21:q:20:LEU:C	2.45	0.42
1:A:46:SER:O	1:A:47:ALA:HB3	2.20	0.41
1:A:75:LEU:N	1:A:76:PRO:CD	2.83	0.41
1:A:99:SER:O	1:A:100:LEU:C	2.63	0.41
3:C:47:ARG:HG2	4:D:160:ASN:HB3	2.02	0.41
5:E:99:LYS:O	5:E:99:LYS:HD3	2.20	0.41
5:E:198:LYS:HA	5:E:201:GLU:HB3	2.02	0.41
6:F:315:LEU:HD22	6:F:363:ILE:HD13	2.02	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:330:LEU:HD12	7:G:544:MET:CE	2.50	0.41
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.41
8:H:1:MET:HE2	19:a:29:PHE:CD2	2.55	0.41
8:H:67:SER:N	8:H:122:ALA:O	2.52	0.41
8:H:273:ILE:CD1	29:I:301:3PE:H2A1	2.50	0.41
12:R:31:ILE:CG2	12:R:35:GLY:HA2	2.50	0.41
12:R:79:CYS:O	12:R:88:HIS:CE1	2.73	0.41
14:T:90:TYR:HD2	14:T:93:ILE:CB	2.32	0.41
14:T:112:SER:O	14:T:116:VAL:HG23	2.20	0.41
15:V:90:LEU:O	15:V:94:MET:N	2.44	0.41
17:X:84:GLU:HA	17:X:87:THR:CG2	2.50	0.41
19:a:34:LYS:O	19:a:35:GLU:C	2.63	0.41
19:a:58:ASN:O	19:a:59:ARG:C	2.60	0.41
1:A:61:THR:OG1	1:A:62:PHE:N	2.52	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.03	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.41
6:F:126:LYS:HG3	6:F:275:LEU:HB2	2.01	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.41
8:H:157:ASN:ND2	8:H:164:THR:OG1	2.49	0.41
9:I:144:ARG:NH2	11:Q:112:MET:O	2.53	0.41
13:S:62:GLN:O	13:S:64:LYS:HG3	2.20	0.41
14:T:90:TYR:OH	14:T:92:LYS:HD3	2.20	0.41
14:T:133:ILE:HG13	14:T:137:LYS:HZ2	1.85	0.41
15:V:81:ILE:O	15:V:84:ALA:N	2.53	0.41
16:W:86:VAL:O	16:W:90:LYS:N	2.41	0.41
18:Z:116:TRP:CZ2	18:Z:119:PRO:HD3	2.55	0.41
19:a:55:SER:HB3	19:a:61:TYR:CE2	2.54	0.41
20:b:74:LEU:HD12	20:b:74:LEU:N	2.35	0.41
1:A:57:LEU:O	1:A:58:VAL:C	2.62	0.41
1:A:61:THR:C	1:A:63:LEU:N	2.75	0.41
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.41
2:B:100:CYS:SG	24:B:301:SF4:S3	3.19	0.41
2:B:114:MET:O	2:B:115:ASP:C	2.62	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
7:G:567:VAL:HG23	7:G:567:VAL:O	2.20	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
8:H:260:MET:SD	19:a:16:LEU:CB	3.08	0.41
14:T:90:TYR:CD2	14:T:93:ILE:HG12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:59:VAL:HG12	16:W:63:ARG:HD2	2.01	0.41
17:X:75:LYS:O	17:X:79:ALA:HB2	2.19	0.41
19:a:52:ARG:HG3	19:a:57:VAL:O	2.19	0.41
20:b:72:ASP:HB3	20:b:74:LEU:CD1	2.50	0.41
20:b:72:ASP:HB3	20:b:74:LEU:HD12	2.02	0.41
21:q:69:ASN:CG	21:q:70:GLY:N	2.78	0.41
21:q:81:MET:HE2	21:q:81:MET:HB3	1.92	0.41
1:A:37:TYR:CE1	2:B:125:PRO:CG	3.04	0.41
2:B:93:MET:HB2	2:B:128:ALA:CB	2.50	0.41
2:B:116:ARG:NH2	9:I:86:TYR:H	2.18	0.41
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.41
4:D:375:MET:CG	7:G:121:LEU:HD22	2.50	0.41
4:D:376:GLU:CD	7:G:150:ARG:O	2.63	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.02	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.20	0.41
8:H:20:LEU:HD12	19:a:12:MET:CE	2.51	0.41
8:H:42:PRO:HD2	8:H:45:ILE:CD1	2.51	0.41
9:I:36:TYR:HB3	22:r:104:TRP:HE3	1.85	0.41
9:I:61:LEU:CD2	29:I:301:3PE:H391	2.34	0.41
9:I:128:ILE:HG22	9:I:130:ILE:HG23	2.01	0.41
29:I:301:3PE:H3H1	18:Z:43:LEU:CD2	2.50	0.41
15:V:20:PRO:HG3	15:V:65:VAL:HG22	2.02	0.41
17:X:52:ASP:OD1	18:Z:116:TRP:HB2	2.20	0.41
18:Z:125:TYR:O	18:Z:128:ARG:HB2	2.20	0.41
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.55	0.41
2:B:122:ARG:HH21	25:H:400:UQ9:H1MA	1.85	0.41
4:D:160:ASN:HD21	22:r:63:VAL:HG21	1.85	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.02	0.41
5:E:190:ASN:HB3	5:E:192:TYR:CE1	2.55	0.41
6:F:44:ASN:O	6:F:45:LEU:C	2.62	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:136:GLU:HA	11:Q:88:GLN:HE21	1.85	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
7:G:308:ARG:HG3	7:G:581:ASP:HA	2.02	0.41
8:H:224:PHE:CG	25:H:400:UQ9:H15B	2.50	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.41
10:P:227:PRO:HB3	10:P:291:TYR:CZ	2.55	0.41
17:X:16:GLU:O	17:X:64:ASN:ND2	2.53	0.41
17:X:31:HIS:CB	17:X:70:PHE:HZ	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:23:ARG:CG	18:Z:25:LEU:HD13	2.51	0.41
21:q:68:MET:HG3	21:q:68:MET:O	2.21	0.41
33:q:201:CDL:C1	22:r:4:ALA:HA	2.51	0.41
2:B:121:PHE:CD1	2:B:121:PHE:N	2.88	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
5:E:233:LEU:H	6:F:37:ASP:CG	2.29	0.41
5:E:244:VAL:HG12	5:E:246:ALA:H	1.85	0.41
6:F:226:LYS:N	6:F:227:PRO:HD2	2.34	0.41
6:F:379:CYS:SG	24:F:502:SF4:S2	3.19	0.41
7:G:49:VAL:HG11	7:G:80:VAL:HG21	2.02	0.41
7:G:82:ILE:HD13	7:G:100:TRP:CZ3	2.55	0.41
7:G:475:VAL:HG22	7:G:514:ASN:OD1	2.20	0.41
8:H:99:ASN:HD21	19:a:40:ARG:C	2.29	0.41
29:I:301:3PE:H222	29:I:301:3PE:H2	1.58	0.41
10:P:227:PRO:HB2	10:P:298:TYR:CZ	2.56	0.41
10:P:237:LYS:HE2	10:P:322:ILE:O	2.20	0.41
11:Q:160:TYR:CE2	11:Q:164:PHE:CZ	3.09	0.41
17:X:21:SER:O	17:X:24:VAL:HG22	2.21	0.41
17:X:69:ASN:O	17:X:70:PHE:C	2.63	0.41
17:X:89:LEU:HD21	17:X:95:GLN:HB3	2.02	0.41
1:A:57:LEU:C	1:A:57:LEU:HD23	2.46	0.41
1:A:80:GLN:O	20:b:46:ASN:OD1	2.38	0.41
3:C:151:PRO:HG2	16:W:23:ILE:HG23	2.03	0.41
6:F:39:ASP:HA	6:F:261:TRP:CZ2	2.56	0.41
6:F:209:GLU:N	28:F:501:FMN:O2'	2.53	0.41
6:F:336:LEU:C	6:F:336:LEU:HD12	2.44	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.20	0.41
7:G:51:GLN:HE22	11:Q:158:LYS:HB2	1.85	0.41
7:G:307:VAL:O	7:G:308:ARG:C	2.63	0.41
8:H:8:THR:O	8:H:9:LEU:CB	2.67	0.41
8:H:314:VAL:HG23	18:Z:58:ARG:HH21	1.85	0.41
10:P:220:TYR:HA	10:P:223:PHE:CE1	2.55	0.41
10:P:262:THR:HG22	10:P:263:PHE:N	2.35	0.41
10:P:301:ILE:HG22	10:P:305:PHE:CE2	2.42	0.41
12:R:40:GLU:HA	12:R:45:ARG:NH1	2.35	0.41
14:T:104:PHE:CE2	14:T:144:ILE:HD11	2.53	0.41
14:T:105:MET:HE3	14:T:139:MET:HE2	2.03	0.41
20:b:32:MET:N	20:b:33:PRO:CD	2.84	0.41
20:b:80:TRP:O	20:b:81:LEU:C	2.64	0.41
21:q:42:ASP:OD1	21:q:42:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:CB	8:H:61:MET:HE2	2.44	0.41
3:C:134:LEU:HD12	3:C:134:LEU:H	1.86	0.41
4:D:119:GLY:O	4:D:123:LEU:HD23	2.21	0.41
4:D:269:ARG:O	4:D:273:VAL:HG23	2.21	0.41
5:E: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:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:109:ARG:HH21	6:F:239:PRO:CD	2.33	0.41
6:F:119:GLU:OE1	6:F:119:GLU:HA	2.21	0.41
6:F:258:GLY:O	6:F:262:PHE:HD1	2.03	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:339:ALA:CB	7:G:537:ILE:CD1	2.96	0.41
7:G:403:VAL:HG13	7:G:476:LEU:CD1	2.50	0.41
7:G:611:THR:HG23	11:Q:104:ARG:O	2.20	0.41
7:G:652:ASN:HA	7:G:655:ARG:CZ	2.50	0.41
8:H:89:LEU:HD12	8:H:89:LEU:HA	1.87	0.41
10:P:128:ASN:HD21	10:P:149:PRO:HB3	1.84	0.41
13:S:63:PRO:HB2	13:S:79:LEU:CD1	2.50	0.41
16:W:87:ILE:CG2	16:W:91:MET:HE3	2.45	0.41
1:A:41:PHE:CD2	16:W:102:GLN:CD	2.99	0.41
1:A:69:ILE:O	1:A:73:LEU:HG	2.20	0.41
1:A:106:TRP:CE3	1:A:107:THR:HG22	2.56	0.41
2:B:115:ASP:OD1	2:B:120:VAL:HG22	2.21	0.41
2:B:170:TYR:CZ	9:I:124:PRO:CB	2.99	0.41
2:B:171:TYR:O	2:B:172:HIS:C	2.64	0.41
3:C:127:ILE:HD11	3:C:175:VAL:HG21	2.02	0.41
3:C:186:ILE:C	4:D:113:ILE:HD11	2.45	0.41
4:D:158:LEU:O	4:D:392:PRO:HG2	2.21	0.41
4:D:259:GLU:C	4:D:261:MET:N	2.75	0.41
5:E:77:ALA:C	5:E:80:PRO:HD2	2.46	0.41
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.96	0.41
6:F:45:LEU:HD13	6:F:129:GLU:OE1	2.20	0.41
6:F:296:LEU:HB2	6:F:337:MET:HE3	2.03	0.41
6:F:306:GLY:O	6:F:307:VAL:C	2.64	0.41
7:G:557:ARG:HD3	21:q:144:TYR:CE2	2.56	0.41
8:H:124:ASN:O	8:H:124:ASN:CG	2.62	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.50	0.41
9:I:107:PRO:O	9:I:108:SER:C	2.63	0.41
10:P:147:ASN:N	10:P:147:ASN:ND2	2.69	0.41
10:P:170:LEU:HG	10:P:171:ASN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:286:ARG:NH1	10:P:358:THR:HG22	2.36	0.41
10:P:293:LEU:CA	10:P:298:TYR:HE2	2.34	0.41
11:Q:71:HIS:NE2	11:Q:120:PRO:HD2	2.36	0.41
11:Q:78:ARG:O	11:Q:80:PHE:CD1	2.74	0.41
11:Q:86:ASN:OD1	11:Q:86:ASN:O	2.39	0.41
13:S:35:ASP:HA	13:S:38:VAL:HG22	2.02	0.41
14:T:122:MET:HG3	14:T:144:ILE:HG21	2.02	0.41
15:V:65:VAL:O	15:V:66:LYS:C	2.60	0.41
17:X:28:ALA:HB3	17:X:71:PHE:HE1	1.86	0.41
18:Z:10:MET:HE2	18:Z:10:MET:HB2	1.59	0.41
19:a:49:GLU:O	19:a:50:ARG:C	2.62	0.41
21:q:43:LYS:C	21:q:45:GLY:H	2.29	0.41
33:q:201:CDL:HB61	33:q:201:CDL:H322	2.03	0.41
22:r:4:ALA:O	22:r:5:THR:C	2.63	0.41
1:A:103:ALA:O	1:A:106:TRP:HB3	2.20	0.41
6:F:262:PHE:HA	6:F:265:PHE:CD2	2.56	0.41
6:F:300:ILE:HD13	6:F:307:VAL:CG2	2.50	0.41
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.03	0.41
6:F:427:LEU:HB2	28:F:501:FMN:C7M	2.51	0.41
7:G:506:VAL:CG2	7:G:510:TRP:HB3	2.51	0.41
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.41
9:I:90:LYS:HB2	21:q:90:LEU:HD23	2.00	0.41
10:P:79:GLN:HE21	10:P:79:GLN:HB3	1.63	0.41
11:Q:130:ALA:O	11:Q:131:LYS:C	2.62	0.41
12:R:32:THR:C	12:R:34:THR:N	2.75	0.41
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.88	0.40
3:C:160:ILE:CB	4:D:286:TYR:CE1	3.04	0.40
4:D:84:PHE:O	4:D:96:ARG:HA	2.21	0.40
4:D:116:LEU:O	4:D:118:ARG:HG3	2.21	0.40
6:F:64:LYS:HE3	6:F:67:GLU:OE1	2.21	0.40
6:F:102:MET:HE2	6:F:149:MET:HB2	2.02	0.40
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.51	0.40
7:G:193:ASP:OD1	7:G:193:ASP:N	2.53	0.40
7:G:356:ASP:OD2	7:G:645:ARG:NE	2.51	0.40
11:Q:85:ASN:C	11:Q:87:MET:N	2.77	0.40
11:Q:132:GLU:H	11:Q:132:GLU:CD	2.27	0.40
11:Q:160:TYR:CE2	11:Q:164:PHE:CE2	3.09	0.40
14:T:126:PHE:CE1	14:T:148:ILE:HG21	2.57	0.40
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.36	0.40
18:Z:101:VAL:HB	18:Z:102:PRO:CD	2.49	0.40
19:a:41:VAL:O	19:a:42:GLN:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:7:VAL:HG13	22:r:8:ILE:N	2.37	0.40
1:A:33:LYS:CG	8:H:61:MET:CE	2.59	0.40
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.20	0.40
2:B:137:LEU:HD11	2:B:142:ALA:HA	2.03	0.40
3:C:213:ASP:CG	10:P:67:ARG:HH21	2.29	0.40
4:D:181:LEU:HD21	4:D:210:MET:CB	2.51	0.40
5:E:65:ILE:O	5:E:66:VAL:C	2.62	0.40
5:E:167:LEU:HA	5:E:167:LEU:HD12	1.79	0.40
5:E:174:GLU:O	5:E:175:CYS:C	2.63	0.40
5:E:179:CYS:SG	6:F:123:GLY:N	2.78	0.40
6:F:199:ARG:HD3	23:s:80:PHE:CD2	2.55	0.40
6:F:208:GLU:OE1	6:F:210:THR:N	2.53	0.40
6:F:226:LYS:HD3	6:F:226:LYS:HA	1.90	0.40
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.86	0.40
8:H:171:HIS:HB3	18:Z:49:ARG:HD3	2.04	0.40
8:H:199:ASP:O	8:H:200:LEU:C	2.64	0.40
8:H:205:SER:CB	8:H:279:ARG:HH22	2.30	0.40
10:P:294:PRO:O	10:P:298:TYR:CD2	2.74	0.40
10:P:357:ARG:NH2	10:P:364:SER:HB3	2.36	0.40
17:X:134:ASP:OD1	17:X:134:ASP:C	2.63	0.40
21:q:42:ASP:OD1	21:q:46:ASN:N	2.45	0.40
33:q:201:CDL:H121	33:q:201:CDL:H151	1.86	0.40
3:C:48:PRO:HD3	4:D:162:GLN:OE1	2.21	0.40
3:C:127:ILE:HD12	3:C:127:ILE:N	2.36	0.40
4:D:142:VAL:CG1	4:D:182:ASN:HA	2.51	0.40
4:D:198:THR:N	4:D:199:PRO:CD	2.83	0.40
4:D:213:PHE:O	4:D:214:TYR:C	2.65	0.40
5:E:63:GLU:O	5:E:64:ALA:C	2.64	0.40
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.40
6:F:413:TRP:CH2	6:F:436:GLN:HG2	2.56	0.40
7:G:136:GLU:CA	11:Q:88:GLN:HE21	2.34	0.40
7:G:161:GLU:OE2	12:R:96:ASP:HB3	2.21	0.40
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.40
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.40
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.40
7:G:546:PHE:N	7:G:546:PHE:CD1	2.89	0.40
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.40
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.40
8:H:145:THR:HG22	8:H:289:LEU:HD11	2.03	0.40
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.43	0.40
8:H:264:LEU:HD23	19:a:12:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:192:ASN:OD1	9:I:193:ASN:N	2.54	0.40
10:P:175:LYS:HB3	10:P:175:LYS:HE2	1.89	0.40
10:P:230:SER:C	10:P:232:GLY:N	2.77	0.40
15:V:114:TRP:CE3	15:V:114:TRP:HA	2.57	0.40
1:A:49:LEU:H	1:A:49:LEU:CD2	2.34	0.40
2:B:84:TRP:CZ3	26:B:303:PC1:H351	2.56	0.40
2:B:145:LEU:O	2:B:146:ARG:C	2.64	0.40
3:C:197:PHE:CZ	4:D:121:GLU:HB2	2.56	0.40
4:D:313:GLN:HE21	4:D:313:GLN:HB2	1.67	0.40
6:F:157:TYR:CD2	6:F:212:LEU:HD13	2.57	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
7:G:136:GLU:C	11:Q:88:GLN:HE21	2.29	0.40
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.55	0.40
7:G:557:ARG:HG3	7:G:579:MET:HB2	2.03	0.40
8:H:23:VAL:O	8:H:23:VAL:CG1	2.69	0.40
9:I:117:LYS:HG2	9:I:130:ILE:HD11	2.04	0.40
10:P:113:LYS:O	10:P:114:ASP:CB	2.68	0.40
13:S:16:LEU:HD21	13:S:19:ILE:CD1	2.50	0.40
14:T:132:ASP:HA	16:W:40:ARG:HH22	1.87	0.40
15:V:9:THR:OG1	15:V:14:LEU:O	2.39	0.40
16:W:58:THR:O	16:W:59:VAL:C	2.62	0.40
17:X:49:GLU:HG3	17:X:50:GLU:N	2.36	0.40
18:Z:10:MET:O	18:Z:11:PRO:C	2.63	0.40
20:b:66:VAL:HG13	20:b:66:VAL:O	2.20	0.40
2:B:89:SER:HB2	2:B:91:TRP:HE1	1.85	0.40
3:C:110:LEU:HD22	3:C:155:ILE:HD11	2.02	0.40
5:E:247:GLY:O	6:F:79:GLU:CD	2.65	0.40
6:F:177:TYR:O	6:F:178:GLU:C	2.64	0.40
6:F:227:PRO:HB3	7:G:95:PRO:HD3	2.02	0.40
6:F:280:GLY:O	6:F:356:VAL:HB	2.21	0.40
6:F:293:SER:N	6:F:337:MET:O	2.51	0.40
6:F:427:LEU:HB2	28:F:501:FMN:HM73	2.03	0.40
7:G:63:PHE:HZ	7:G:139:LEU:HA	1.87	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.09	0.40
7:G:177:ILE:HG12	7:G:228:VAL:CG2	2.51	0.40
7:G:251:ILE:HG22	7:G:252:ASP:N	2.35	0.40
7:G:341:ILE:HD12	7:G:555:ILE:CG1	2.47	0.40
8:H:82:ALA:HA	8:H:85:LEU:HD12	2.02	0.40
8:H:272:TRP:NE1	9:I:70:LEU:O	2.51	0.40
8:H:316:PRO:CG	18:Z:57:ARG:HB3	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:90:LYS:CD	21:q:91:HIS:CE1	3.04	0.40
9:I:197:TRP:O	9:I:201:ILE:N	2.51	0.40
10:P:64:PHE:CE2	10:P:242:VAL:HG22	2.56	0.40
10:P:83:PRO:C	10:P:108:TRP:CD1	3.00	0.40
10:P:141:PHE:CD1	10:P:145:PHE:HE2	2.39	0.40
10:P:311:GLU:HA	10:P:312:PRO:HD2	1.93	0.40
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.40
13:S:44:LEU:CD1	13:S:95:LEU:HD21	2.50	0.40
15:V:38:PHE:CD1	15:V:95:LEU:HD12	2.56	0.40
19:a:43:TYR:O	19:a:47:LEU:HD13	2.22	0.40
20:b:25:VAL:O	20:b:26:TRP:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	111/115 (96%)	100 (90%)	11 (10%)	0	100	100
2	B	155/224 (69%)	142 (92%)	12 (8%)	1 (1%)	21	54
3	C	195/263 (74%)	186 (95%)	9 (5%)	0	100	100
4	D	383/463 (83%)	356 (93%)	27 (7%)	0	100	100
5	E	208/248 (84%)	191 (92%)	17 (8%)	0	100	100
6	F	424/464 (91%)	403 (95%)	21 (5%)	0	100	100
7	G	685/727 (94%)	636 (93%)	49 (7%)	0	100	100
8	H	313/318 (98%)	291 (93%)	21 (7%)	1 (0%)	36	65
9	I	168/212 (79%)	153 (91%)	15 (9%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	123 (88%)	17 (12%)	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	108/145 (74%)	99 (92%)	9 (8%)	0	100	100
22	r	38/113 (34%)	38 (100%)	0	0	100	100
23	s	21/104 (20%)	20 (95%)	1 (5%)	0	100	100
All	All	4136/5036 (82%)	3824 (92%)	309 (8%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
18	Z	18	PRO
2	B	195	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	102/104 (98%)	101 (99%)	1 (1%)	68	75
2	B	133/185 (72%)	131 (98%)	2 (2%)	57	70
3	C	180/227 (79%)	180 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	341/370 (92%)	340 (100%)	1 (0%)	86	83
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	279/280 (100%)	278 (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	67
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	66
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	103/131 (79%)	103 (100%)	0	100	100
22	r	40/96 (42%)	39 (98%)	1 (2%)	42	63
23	s	23/95 (24%)	23 (100%)	0	100	100
All	All	3636/4292 (85%)	3620 (100%)	16 (0%)	81	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
2	B	104	MET
2	B	170	TYR
4	D	232	VAL
5	E	99	LYS
5	E	200	ILE
6	F	137	LYS
7	G	271	MET
8	H	66	THR
10	P	318	LYS
11	Q	125	VAL
11	Q	135	ILE
13	S	48	HIS

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Mol	Chain	Res	Type
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 (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	83	ASN
2	B	172	HIS
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	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	160	ASN
4	D	182	ASN
4	D	234	GLN
4	D	285	ASN
4	D	313	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	68	ASN
5	E	132	GLN
5	E	152	GLN
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
7	G	51	GLN
7	G	66	HIS
7	G	74	ASN
7	G	101	ASN
7	G	140	GLN

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Mol	Chain	Res	Type
7	G	336	ASN
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	32	GLN
8	H	47	GLN
8	H	93	HIS
8	H	97	ASN
8	H	169	GLN
8	H	258	ASN
9	I	180	HIS
10	P	79	GLN
10	P	147	ASN
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	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	8	GLN
18	Z	24	ASN
18	Z	76	GLN

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Mol	Chain	Res	Type
18	Z	90	ASN
19	a	27	HIS
20	b	46	ASN
21	q	59	HIS
21	q	91	HIS
21	q	135	HIS
23	s	76	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	SF4	I	303	9	0,12,12	-	-	-		
30	NDP	P	401	-	49,52,52	1.21	6 (12%)	66,80,80	1.67	12 (18%)
33	CDL	q	201	-	56,56,99	1.21	4 (7%)	62,68,111	1.29	6 (9%)
25	UQ9	B	302	-	21,21,58	0.94	2 (9%)	25,28,73	0.83	0
24	SF4	G	801	7	0,12,12	-	-	-		
25	UQ9	H	400	-	35,35,58	0.79	2 (5%)	42,45,73	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	FES	G	803	7	0,4,4	-	-	-		
29	3PE	I	301	-	50,50,50	0.90	2 (4%)	53,55,55	1.07	4 (7%)
24	SF4	G	802	7	0,12,12	-	-	-		
24	SF4	I	302	9	0,12,12	-	-	-		
24	SF4	F	502	6	0,12,12	-	-	-		
24	SF4	B	301	2	0,12,12	-	-	-		
27	FES	E	301	5	0,4,4	-	-	-		
28	FMN	F	501	-	33,33,33	1.41	5 (15%)	48,50,50	1.20	6 (12%)
32	EHZ	W	201	-	30,34,37	1.81	7 (23%)	40,44,47	1.41	5 (12%)
26	PC1	B	303	-	34,34,53	1.14	2 (5%)	40,42,61	1.15	3 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	FES	E	301	5	-	-	0/1/1/1
24	SF4	I	303	9	-	-	0/6/5/5
30	NDP	P	401	-	-	6/34/77/77	0/5/5/5
33	CDL	q	201	-	-	18/67/67/110	-
25	UQ9	H	400	-	-	7/30/54/81	0/1/1/1
25	UQ9	B	302	-	-	2/13/37/81	0/1/1/1
29	3PE	I	301	-	-	18/54/54/54	-
24	SF4	G	801	7	-	-	0/6/5/5
27	FES	G	803	7	-	-	0/1/1/1
24	SF4	G	802	7	-	-	0/6/5/5
24	SF4	I	302	9	-	-	0/6/5/5
24	SF4	B	301	2	-	-	0/6/5/5
24	SF4	F	502	6	-	-	0/6/5/5
32	EHZ	W	201	-	-	26/42/42/45	-
28	FMN	F	501	-	-	4/18/18/18	0/3/3/3
26	PC1	B	303	-	-	11/38/38/57	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	201	EHZ	C15-N2	5.42	1.45	1.33
32	W	201	EHZ	C12-N1	5.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	501	FMN	C9A-C5A	4.83	1.49	1.41
33	q	201	CDL	OA8-CA7	4.23	1.45	1.33
30	P	401	NDP	C5A-C4A	4.17	1.46	1.39
26	B	303	PC1	O31-C31	4.17	1.45	1.33
33	q	201	CDL	OA6-CA5	4.15	1.46	1.34
33	q	201	CDL	OB8-CB7	4.13	1.45	1.33
33	q	201	CDL	OB6-CB5	4.10	1.45	1.34
29	I	301	3PE	O31-C31	4.09	1.45	1.33
29	I	301	3PE	O21-C21	4.07	1.45	1.34
26	B	303	PC1	O21-C21	4.01	1.45	1.34
30	P	401	NDP	C6N-C5N	3.29	1.39	1.33
28	F	501	FMN	C8-C7	3.13	1.48	1.40
28	F	501	FMN	C4-N3	-2.79	1.33	1.38
32	W	201	EHZ	P1-O7	2.67	1.65	1.54
25	H	400	UQ9	C3-C2	-2.67	1.41	1.48
25	H	400	UQ9	C4-C5	-2.51	1.41	1.48
30	P	401	NDP	C8A-N7A	2.47	1.36	1.31
30	P	401	NDP	C5A-N7A	-2.46	1.34	1.39
32	W	201	EHZ	O4-C15	-2.43	1.18	1.23
32	W	201	EHZ	O3-C12	-2.41	1.18	1.23
30	P	401	NDP	C5A-C6A	2.38	1.47	1.41
28	F	501	FMN	C5A-N5	-2.34	1.35	1.39
25	B	302	UQ9	C3-C2	-2.33	1.42	1.48
32	W	201	EHZ	C9-S1	2.30	1.81	1.76
32	W	201	EHZ	P1-OP3	-2.24	1.46	1.54
25	B	302	UQ9	C4-C5	-2.18	1.42	1.48
28	F	501	FMN	C4A-N5	2.12	1.34	1.30
30	P	401	NDP	C4A-N9A	-2.06	1.33	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	P	401	NDP	C5A-C4A-N3A	-5.99	118.93	126.75
32	W	201	EHZ	C8-C9-S1	4.96	119.76	113.63
30	P	401	NDP	N3A-C4A-N9A	4.71	134.84	127.08
33	q	201	CDL	OA6-CA5-C11	4.23	120.62	111.50
30	P	401	NDP	PN-O3-PA	-4.05	118.94	132.83
33	q	201	CDL	OB6-CB5-C51	3.96	120.03	111.50
26	B	303	PC1	O21-C21-C22	3.78	119.66	111.50
30	P	401	NDP	C2A-N3A-C4A	3.78	120.68	111.75
29	I	301	3PE	O21-C21-C22	3.21	118.43	111.50
30	P	401	NDP	N3A-C2A-N1A	-3.17	123.65	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	q	201	CDL	OA8-CA7-C31	3.16	121.83	111.91
30	P	401	NDP	C4A-C5A-N7A	-3.16	106.77	110.62
29	I	301	3PE	C2-O21-C21	-3.07	110.23	117.79
29	I	301	3PE	O31-C31-C32	2.98	121.25	111.91
30	P	401	NDP	C4A-N9A-C8A	2.90	108.87	105.73
26	B	303	PC1	O31-C31-C32	2.78	120.64	111.91
33	q	201	CDL	OB8-CB7-C71	2.73	120.47	111.91
30	P	401	NDP	C5A-N7A-C8A	2.71	107.36	103.51
26	B	303	PC1	C2-O21-C21	-2.69	111.17	117.79
33	q	201	CDL	CA4-OA6-CA5	-2.56	111.49	117.79
28	F	501	FMN	C4A-C10-N1	-2.53	118.86	124.73
28	F	501	FMN	O4-C4-C4A	-2.50	119.95	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
30	P	401	NDP	C2B-C1B-N9A	-2.34	109.59	113.53
28	F	501	FMN	C4-C4A-N5	2.34	121.56	118.23
32	W	201	EHZ	O2-C9-S1	-2.33	119.58	122.61
29	I	301	3PE	O31-C31-O32	-2.31	117.76	123.59
30	P	401	NDP	N9A-C8A-N7A	-2.30	110.76	113.91
30	P	401	NDP	C6A-C5A-N7A	2.17	136.06	132.02
33	q	201	CDL	OA8-CA7-OA9	-2.10	118.30	123.59
30	P	401	NDP	C3D-C2D-C1D	2.07	105.36	101.43
28	F	501	FMN	C4A-C4-N3	2.06	118.42	113.19
28	F	501	FMN	C4A-C10-N10	2.06	119.49	116.48
28	F	501	FMN	C10-N1-C2	2.03	120.97	116.90
32	W	201	EHZ	C5-C6-C7	-2.02	109.03	114.85

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	B	303	PC1	C1-O11-P-O12
26	B	303	PC1	C1-O11-P-O14
26	B	303	PC1	C1-O11-P-O13
26	B	303	PC1	C22-C21-O21-C2
28	F	501	FMN	C5'-O5'-P-O2P
28	F	501	FMN	C5'-O5'-P-O3P
29	I	301	3PE	O22-C21-O21-C2
29	I	301	3PE	C22-C21-O21-C2
30	P	401	NDP	C5D-O5D-PN-O1N
32	W	201	EHZ	O1-C7-C8-C9
32	W	201	EHZ	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
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	CA3-OA5-PA1-OA2
33	q	201	CDL	CA3-OA5-PA1-OA3
33	q	201	CDL	CA3-OA5-PA1-OA4
26	B	303	PC1	O22-C21-O21-C2
25	H	400	UQ9	C25-C24-C26-C27
25	H	400	UQ9	C20-C19-C21-C22
25	H	400	UQ9	C12-C11-C9-C10
25	H	400	UQ9	C23-C24-C26-C27
25	H	400	UQ9	C18-C19-C21-C22
25	H	400	UQ9	C12-C11-C9-C8
32	W	201	EHZ	C2-C3-C4-C5
29	I	301	3PE	C1-O11-P-O13
29	I	301	3PE	C11-O13-P-O11
33	q	201	CDL	C11-CA5-OA6-CA4
32	W	201	EHZ	C18-C17-C20-O6
33	q	201	CDL	OA7-CA5-OA6-CA4
32	W	201	EHZ	C13-C14-N2-C15
32	W	201	EHZ	C5-C6-C7-O1
32	W	201	EHZ	C1-C2-C3-C4
29	I	301	3PE	C32-C31-O31-C3
33	q	201	CDL	C51-CB5-OB6-CB4
33	q	201	CDL	OB7-CB5-OB6-CB4
33	q	201	CDL	CA2-OA2-PA1-OA5
25	B	302	UQ9	C11-C12-C13-C14
32	W	201	EHZ	C21-C1-C2-C3
29	I	301	3PE	O32-C31-O31-C3
28	F	501	FMN	C5'-O5'-P-O1P
29	I	301	3PE	C29-C2A-C2B-C2C
32	W	201	EHZ	C5-C6-C7-C8
26	B	303	PC1	C2-C1-O11-P
32	W	201	EHZ	C3-C4-C5-C6
26	B	303	PC1	C32-C33-C34-C35
29	I	301	3PE	C35-C36-C37-C38
33	q	201	CDL	OB5-CB3-CB4-OB6
26	B	303	PC1	C32-C31-O31-C3

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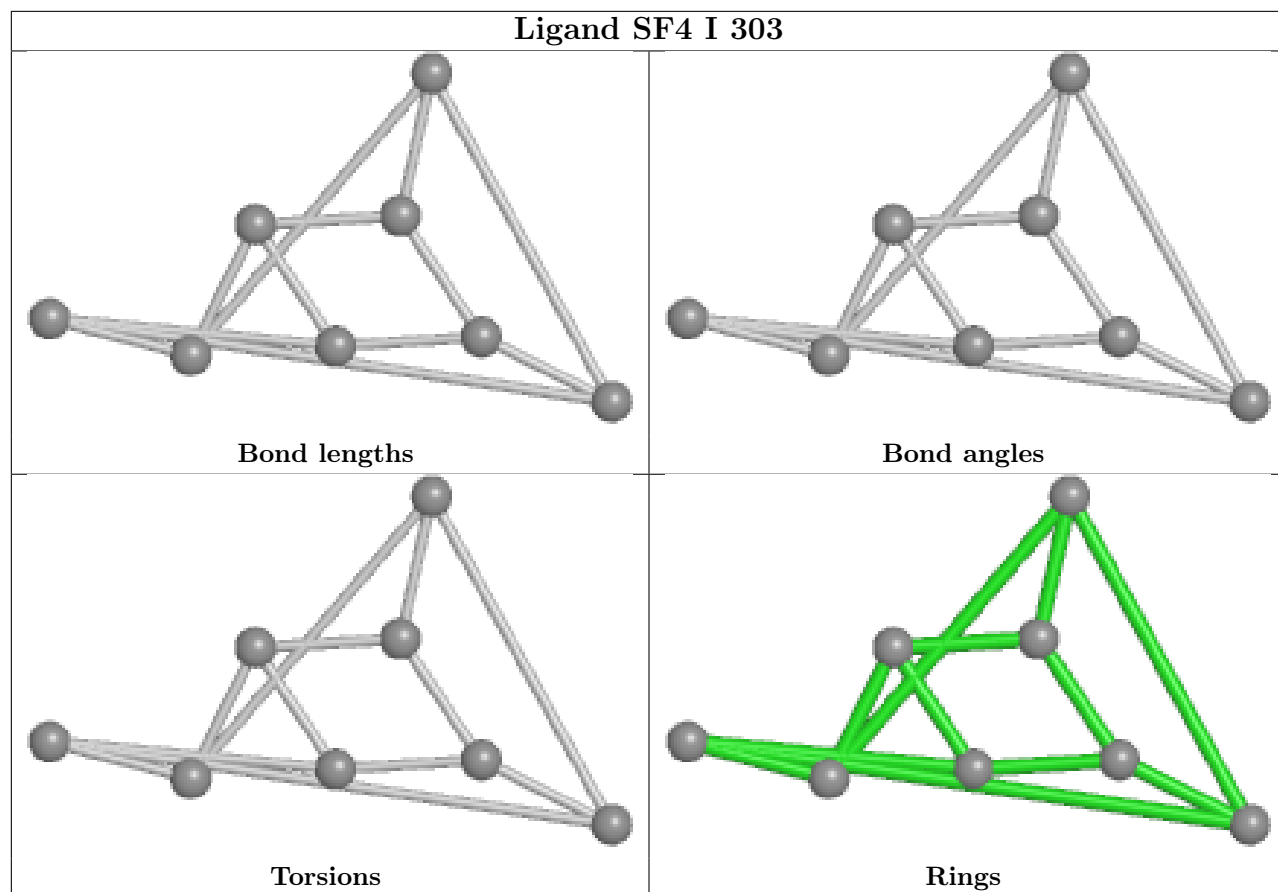
Mol	Chain	Res	Type	Atoms
29	I	301	3PE	C21-C22-C23-C24
33	q	201	CDL	CB4-CB3-OB5-PB2
32	W	201	EHZ	O2-C9-S1-C10
30	P	401	NDP	C2B-O2B-P2B-O1X
32	W	201	EHZ	C8-C9-S1-C10
32	W	201	EHZ	C12-C13-C14-N2
26	B	303	PC1	O32-C31-O31-C3
30	P	401	NDP	PN-O3-PA-O2A
30	P	401	NDP	O4D-C1D-N1N-C6N
33	q	201	CDL	C13-C14-C15-C16
29	I	301	3PE	C1-O11-P-O12
29	I	301	3PE	C1-O11-P-O14
29	I	301	3PE	C11-O13-P-O14
32	W	201	EHZ	C6-C7-C8-C9
28	F	501	FMN	N10-C1'-C2'-O2'
26	B	303	PC1	O13-C11-C12-N
32	W	201	EHZ	O3-C12-C13-C14
29	I	301	3PE	C33-C34-C35-C36
33	q	201	CDL	CB2-OB2-PB2-OB5
26	B	303	PC1	C34-C35-C36-C37
32	W	201	EHZ	C2-C1-C21-C22
32	W	201	EHZ	N1-C12-C13-C14
29	I	301	3PE	C28-C29-C2A-C2B
29	I	301	3PE	O21-C2-C3-O31
30	P	401	NDP	PN-O3-PA-O1A
29	I	301	3PE	C1-C2-C3-O31
25	B	302	UQ9	C5-C4-O4-C4M
33	q	201	CDL	OB5-CB3-CB4-CB6
33	q	201	CDL	C18-C19-C20-C21
32	W	201	EHZ	C10-C11-N1-C12
30	P	401	NDP	C5D-O5D-PN-O3
33	q	201	CDL	C71-CB7-OB8-CB6
25	H	400	UQ9	C6-C7-C8-C9
29	I	301	3PE	C11-O13-P-O12
33	q	201	CDL	CA2-OA2-PA1-OA3
33	q	201	CDL	CB2-OB2-PB2-OB3
29	I	301	3PE	C12-C11-O13-P
33	q	201	CDL	OB9-CB7-OB8-CB6
32	W	201	EHZ	S1-C10-C11-N1

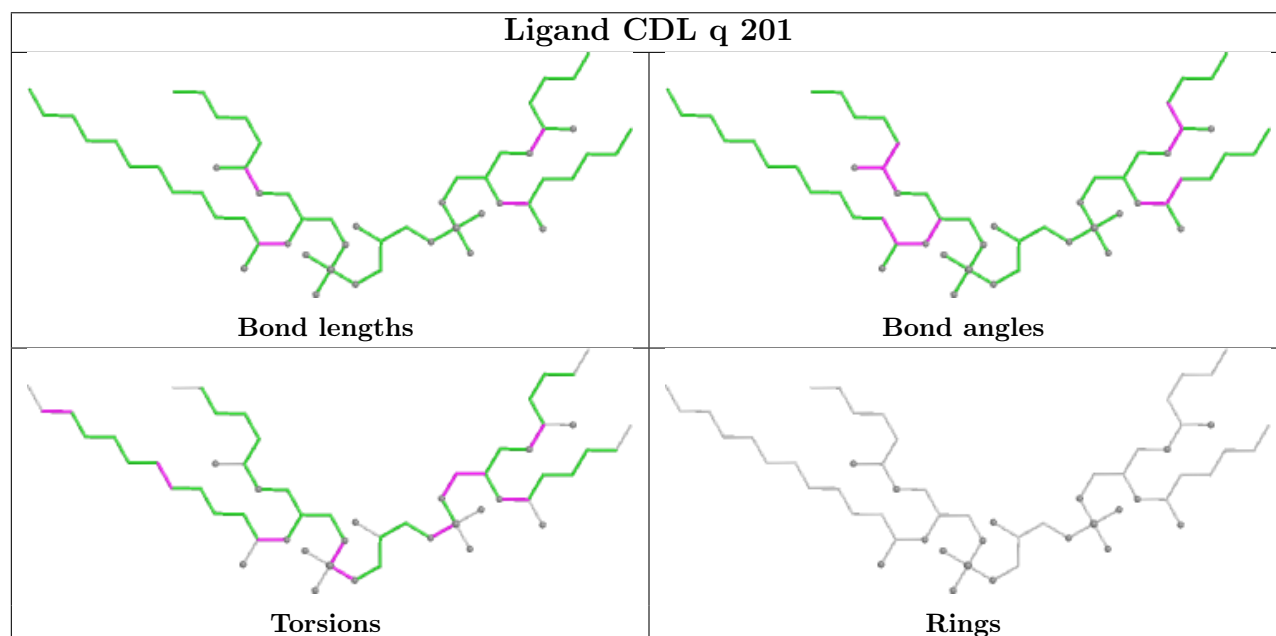
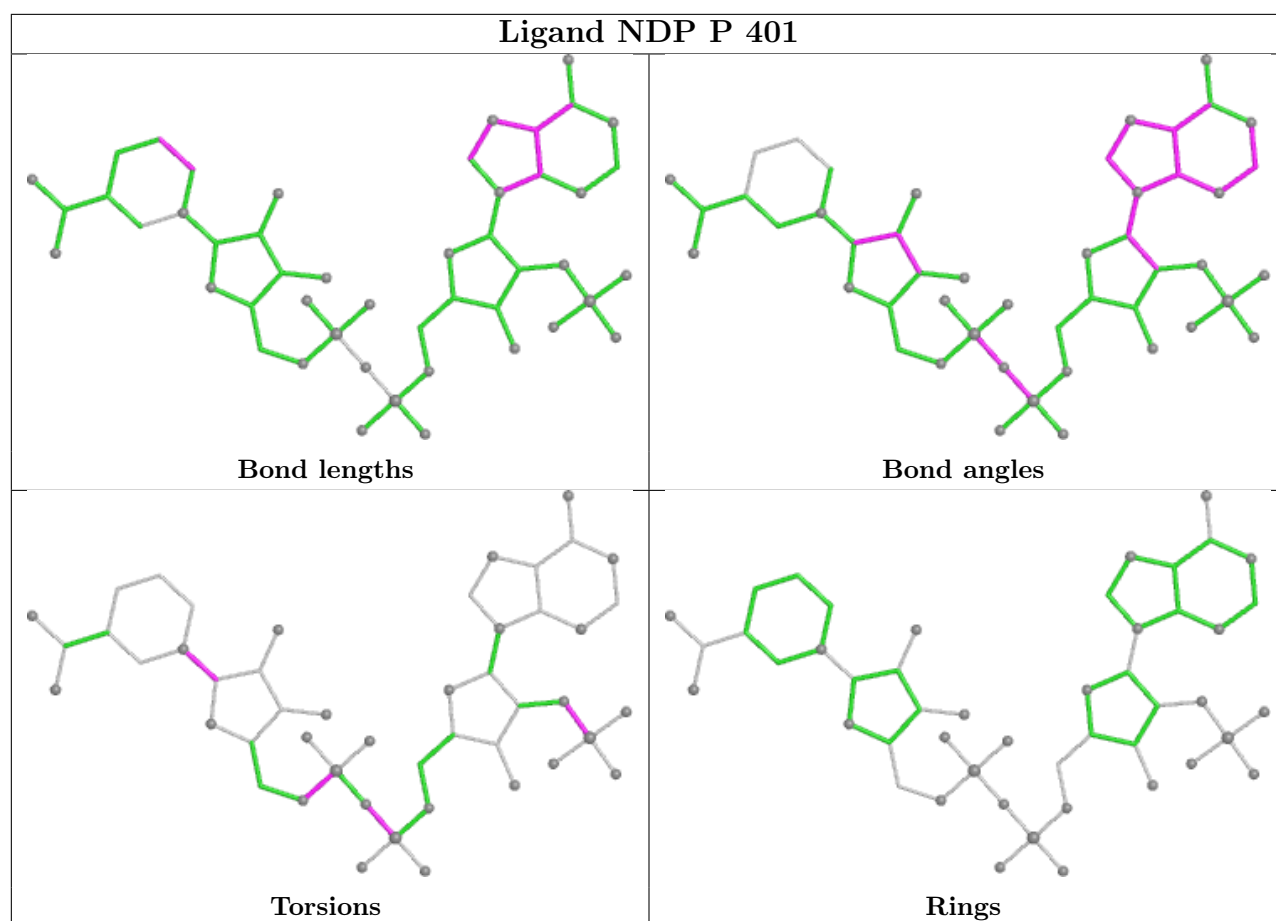
There are no ring outliers.

14 monomers are involved in 124 short contacts:

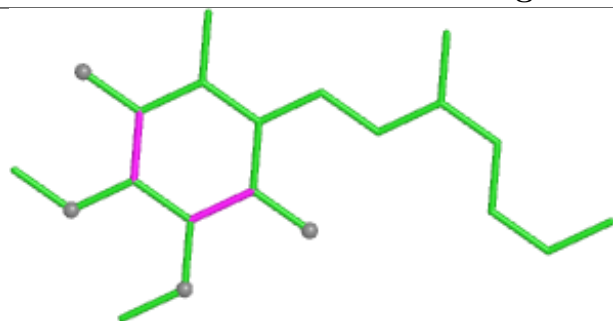
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	I	303	SF4	2	0
30	P	401	NDP	6	0
33	q	201	CDL	21	0
25	B	302	UQ9	12	0
25	H	400	UQ9	13	0
27	G	803	FES	4	0
29	I	301	3PE	23	0
24	G	802	SF4	8	0
24	I	302	SF4	6	0
24	F	502	SF4	10	0
24	B	301	SF4	7	0
27	E	301	FES	3	0
28	F	501	FMN	4	0
26	B	303	PC1	6	0

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.

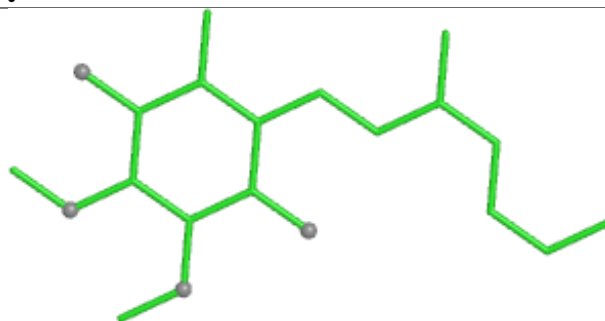




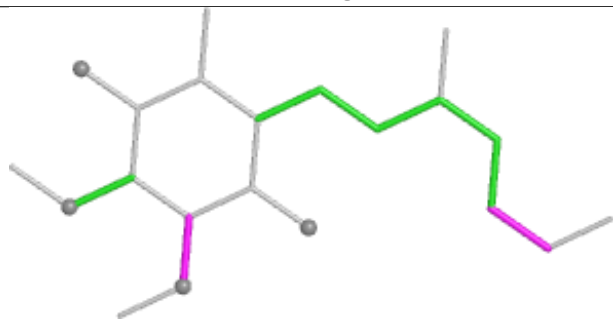
Ligand UQ9 B 302



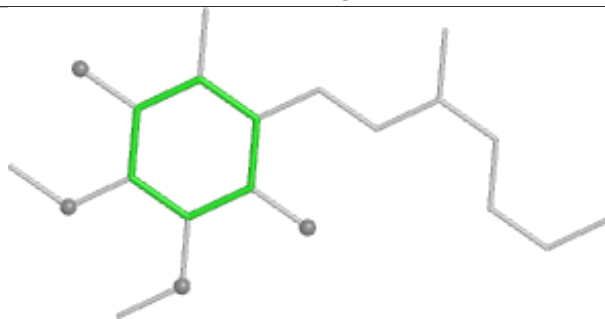
Bond lengths



Bond angles

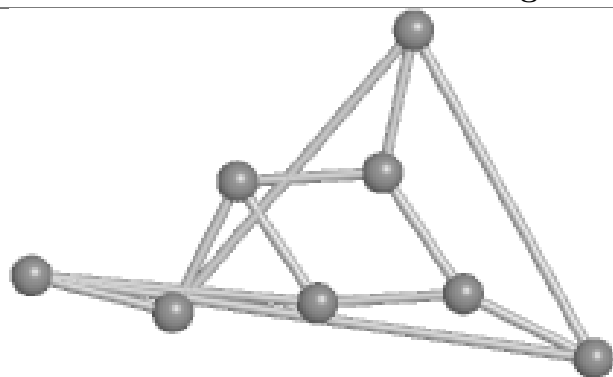


Torsions

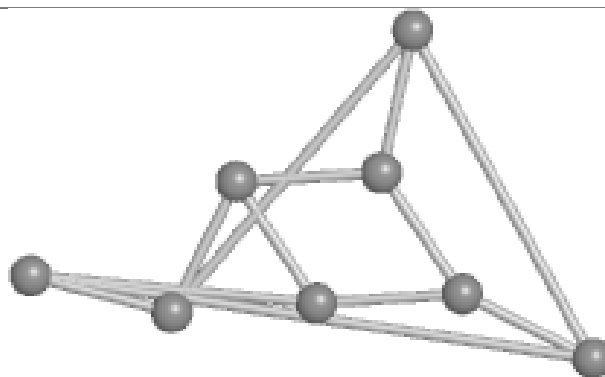


Rings

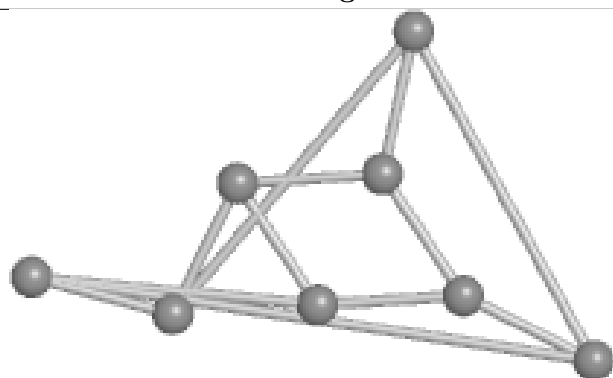
Ligand SF4 G 801



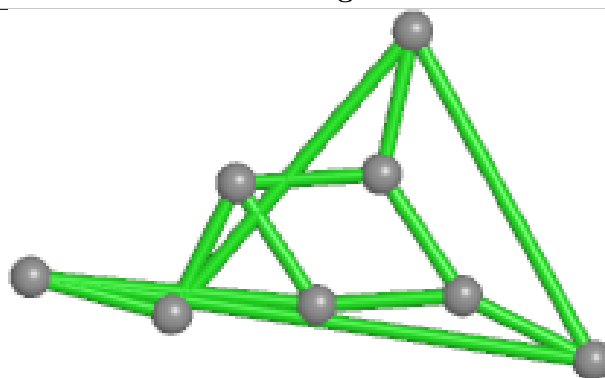
Bond lengths



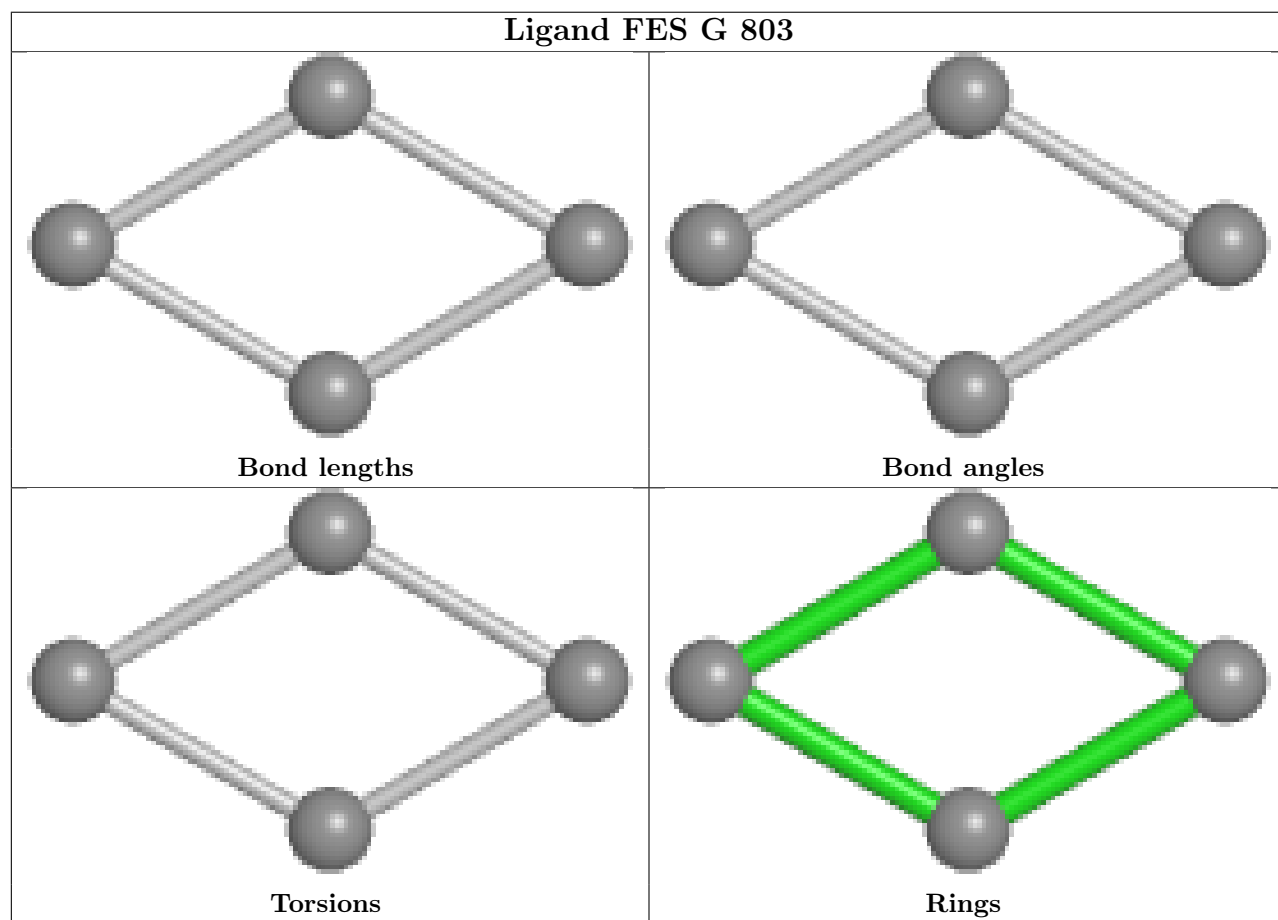
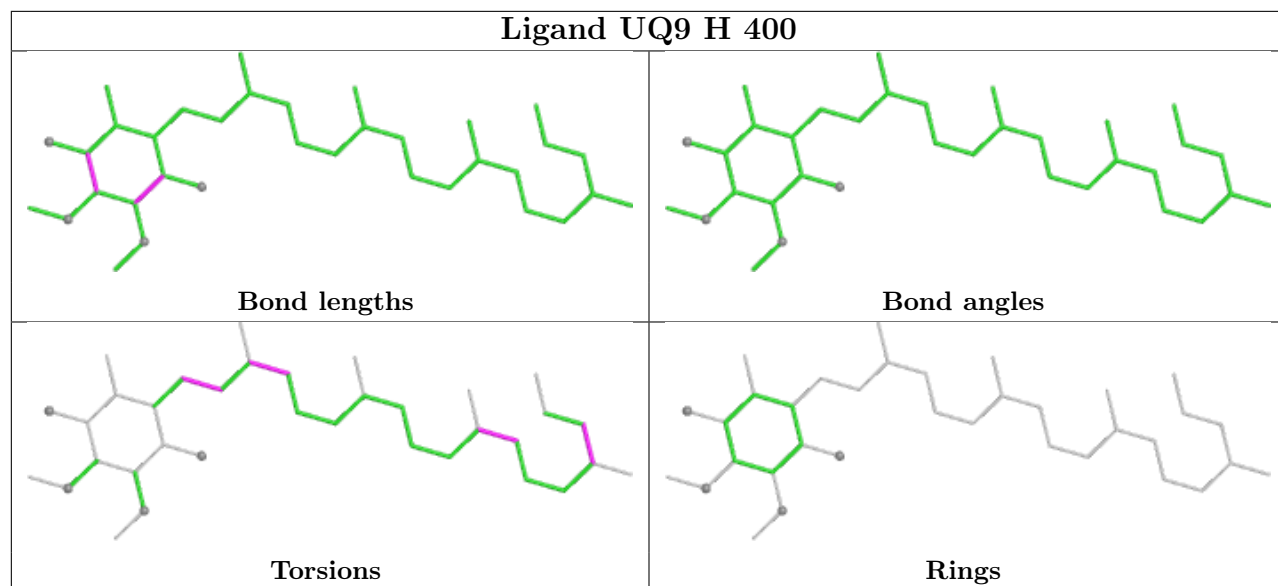
Bond angles

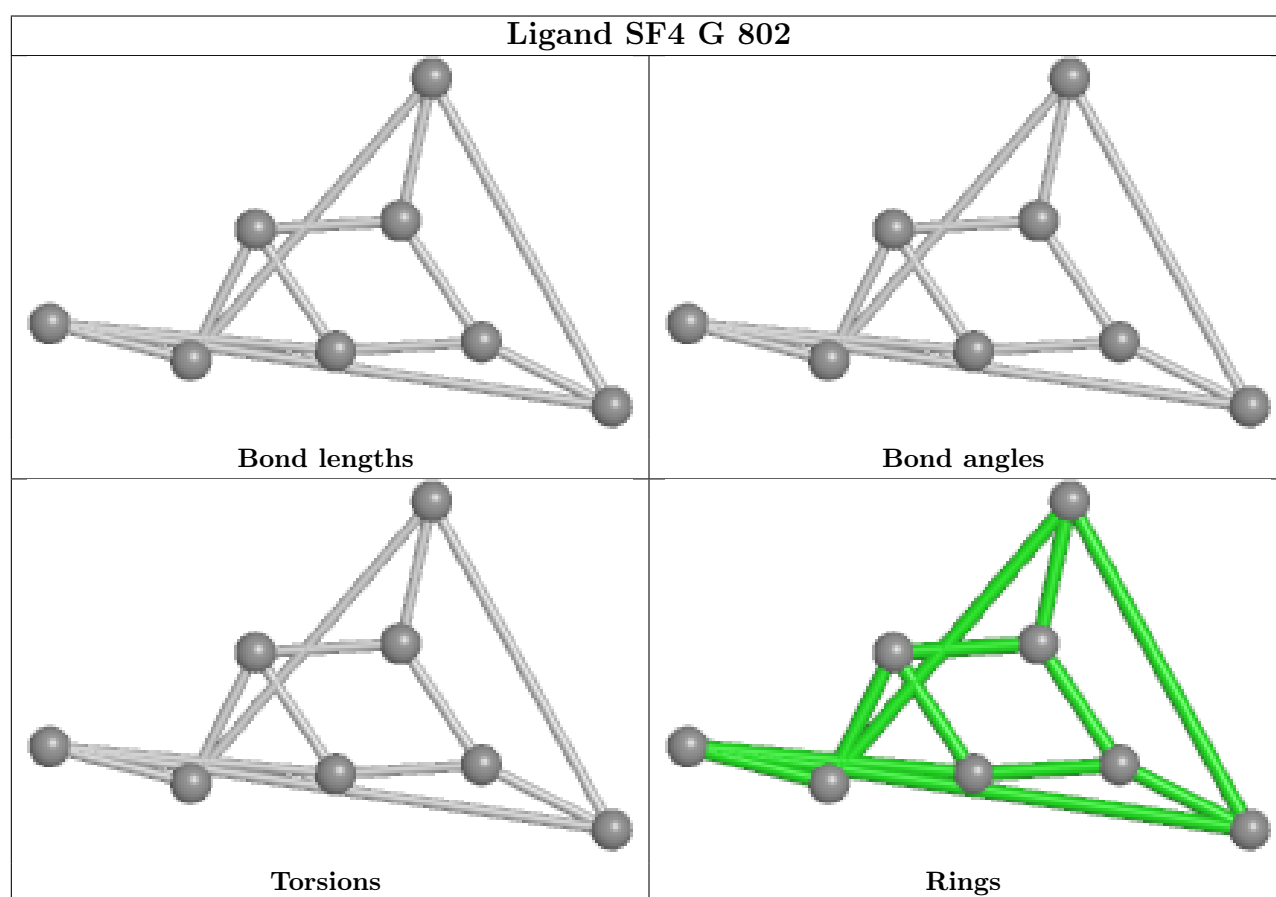
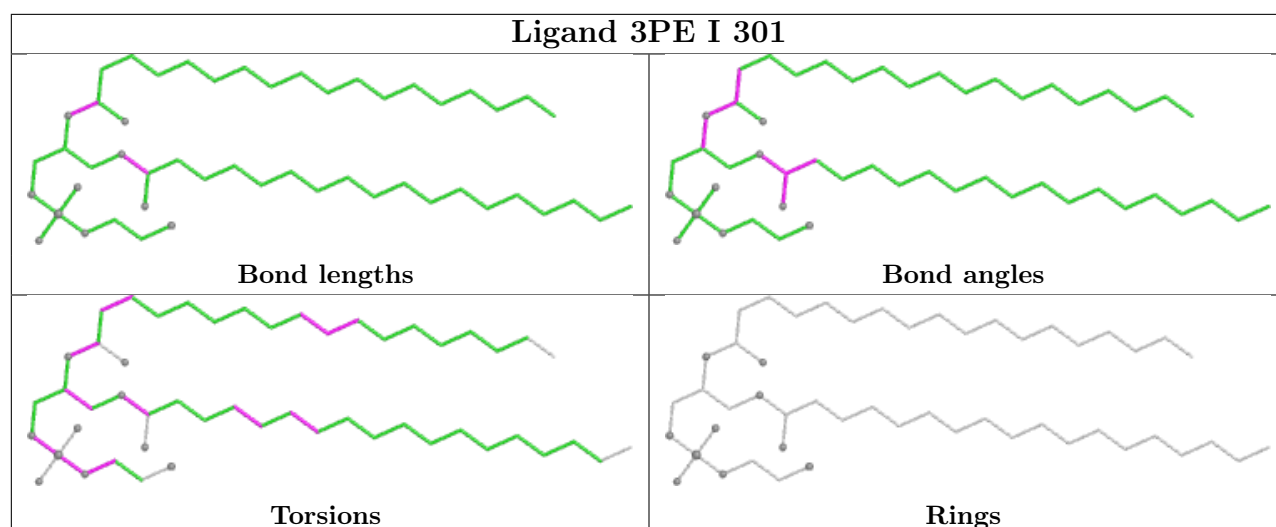


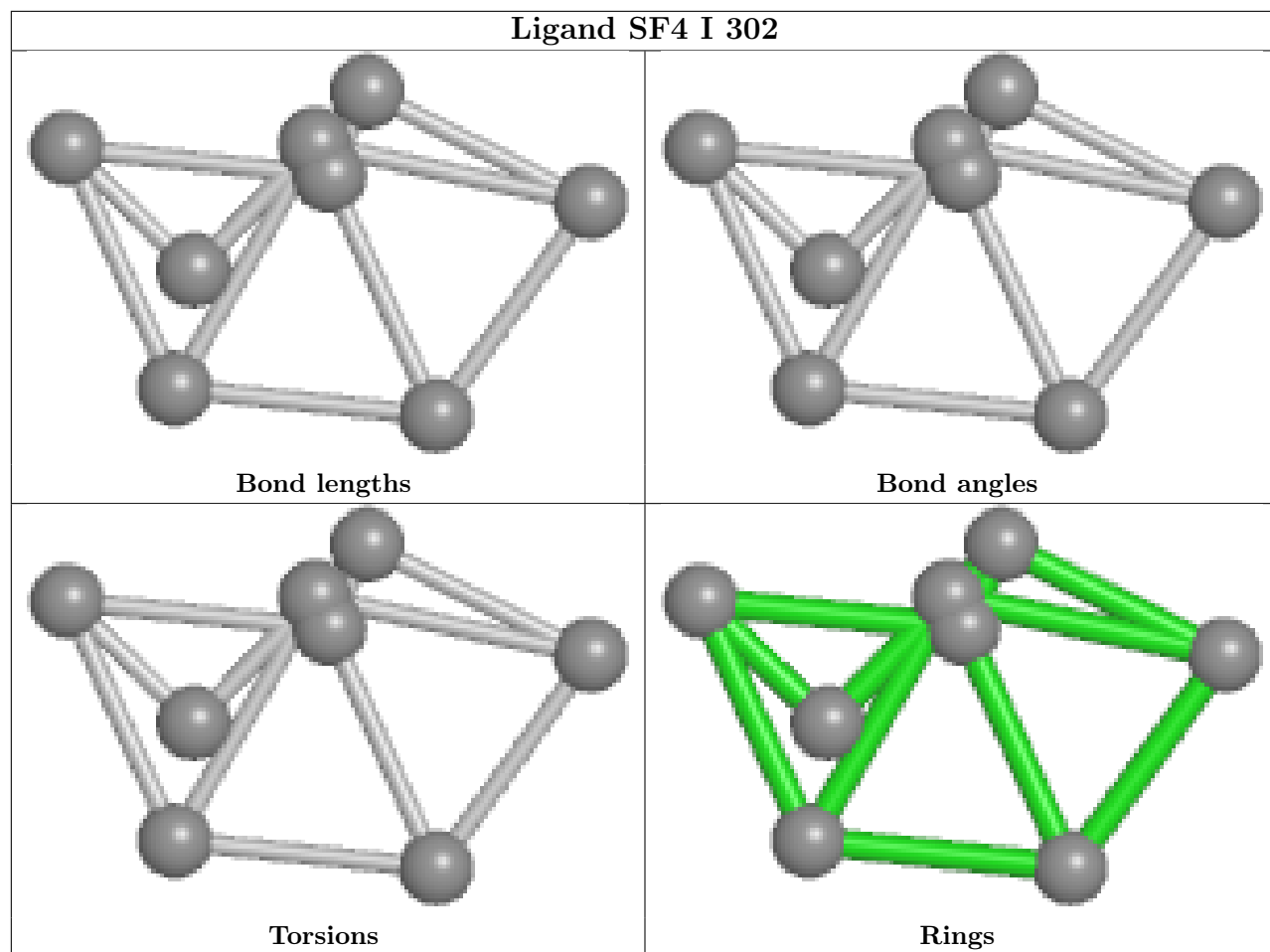
Torsions

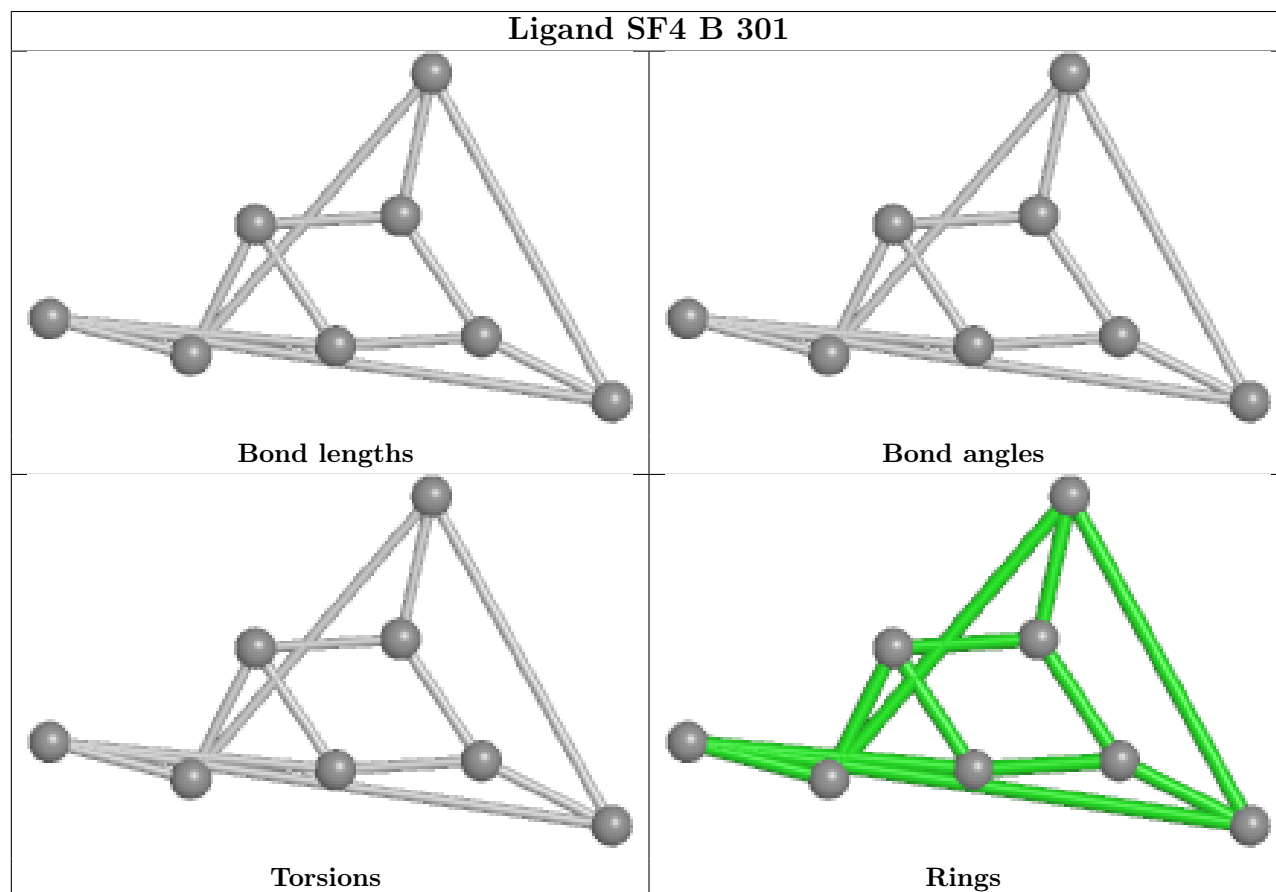
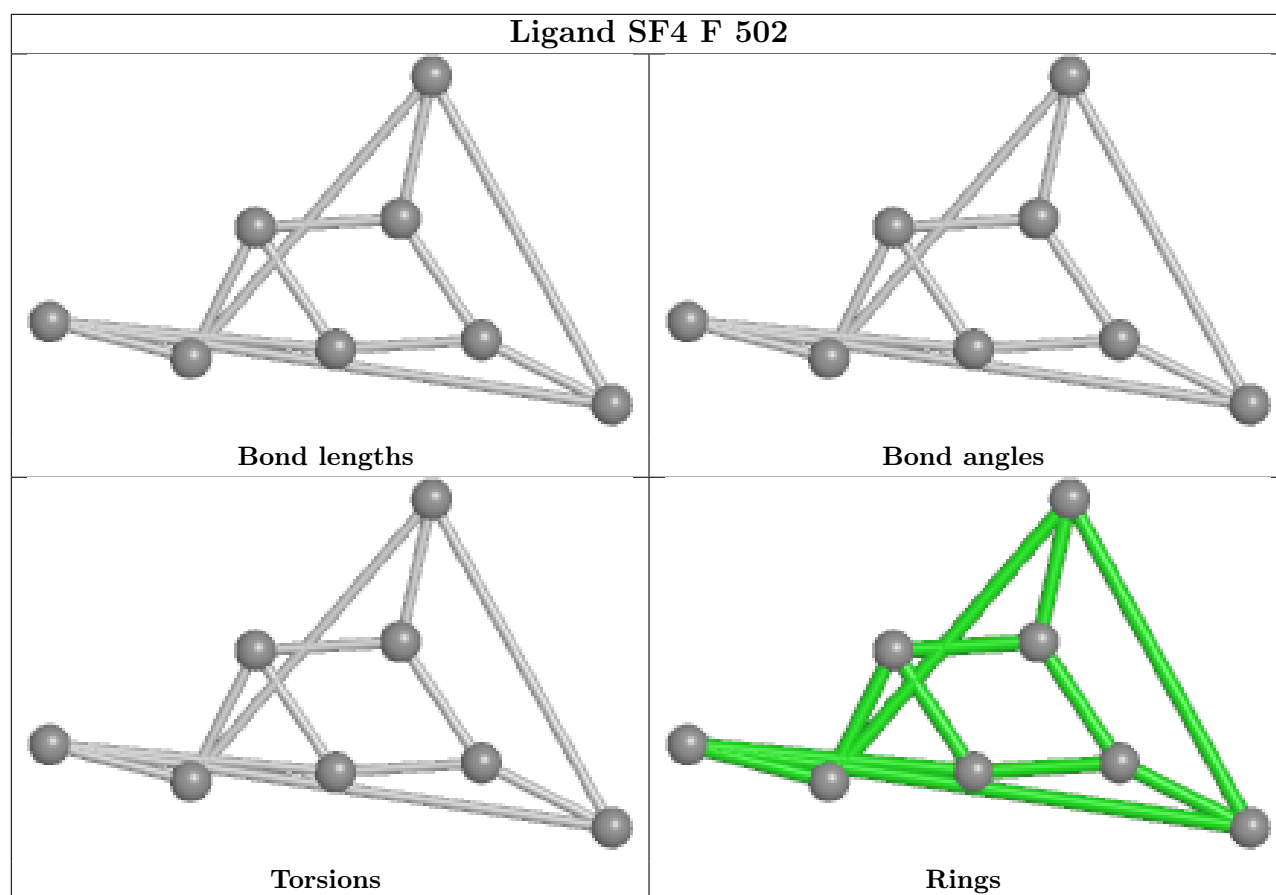


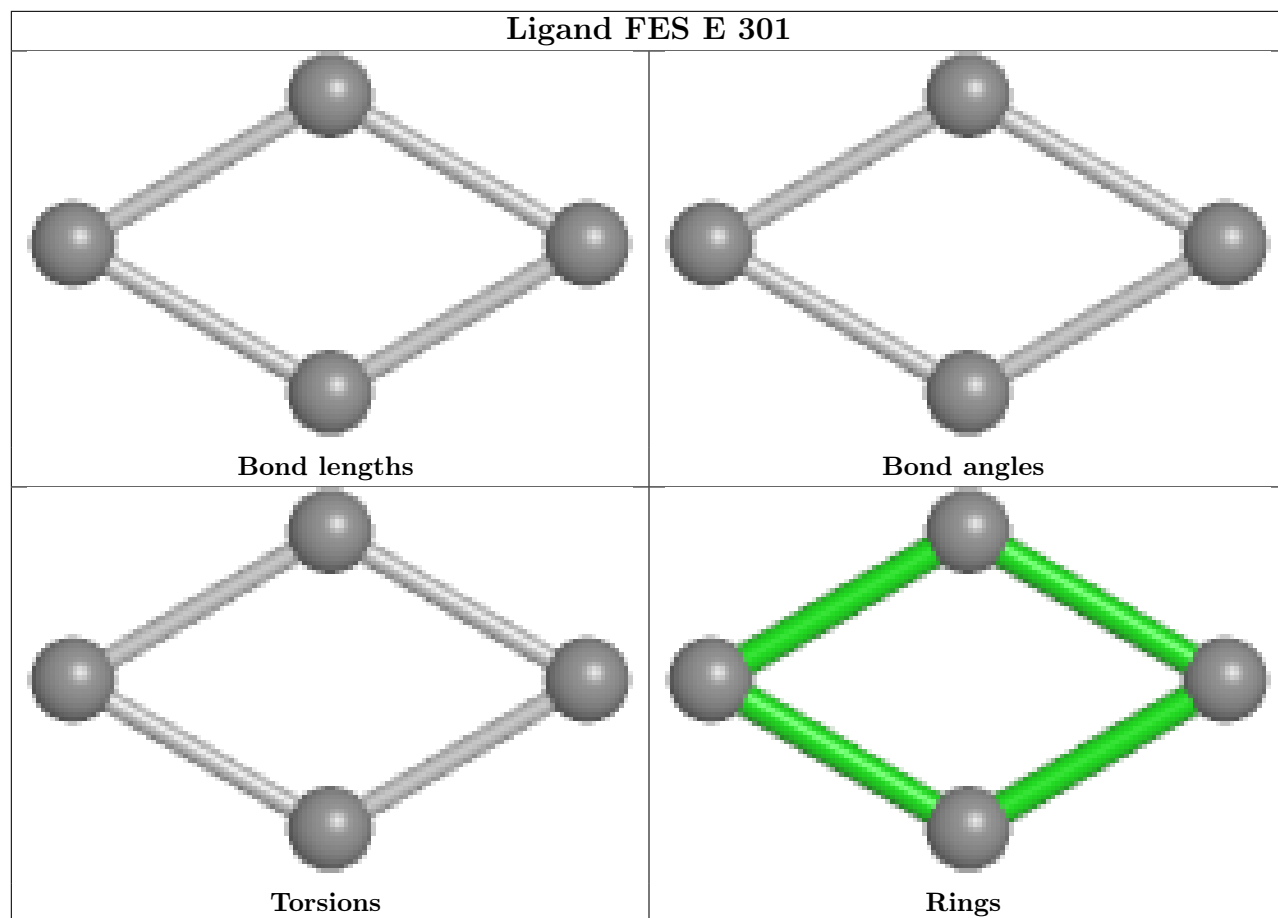
Rings

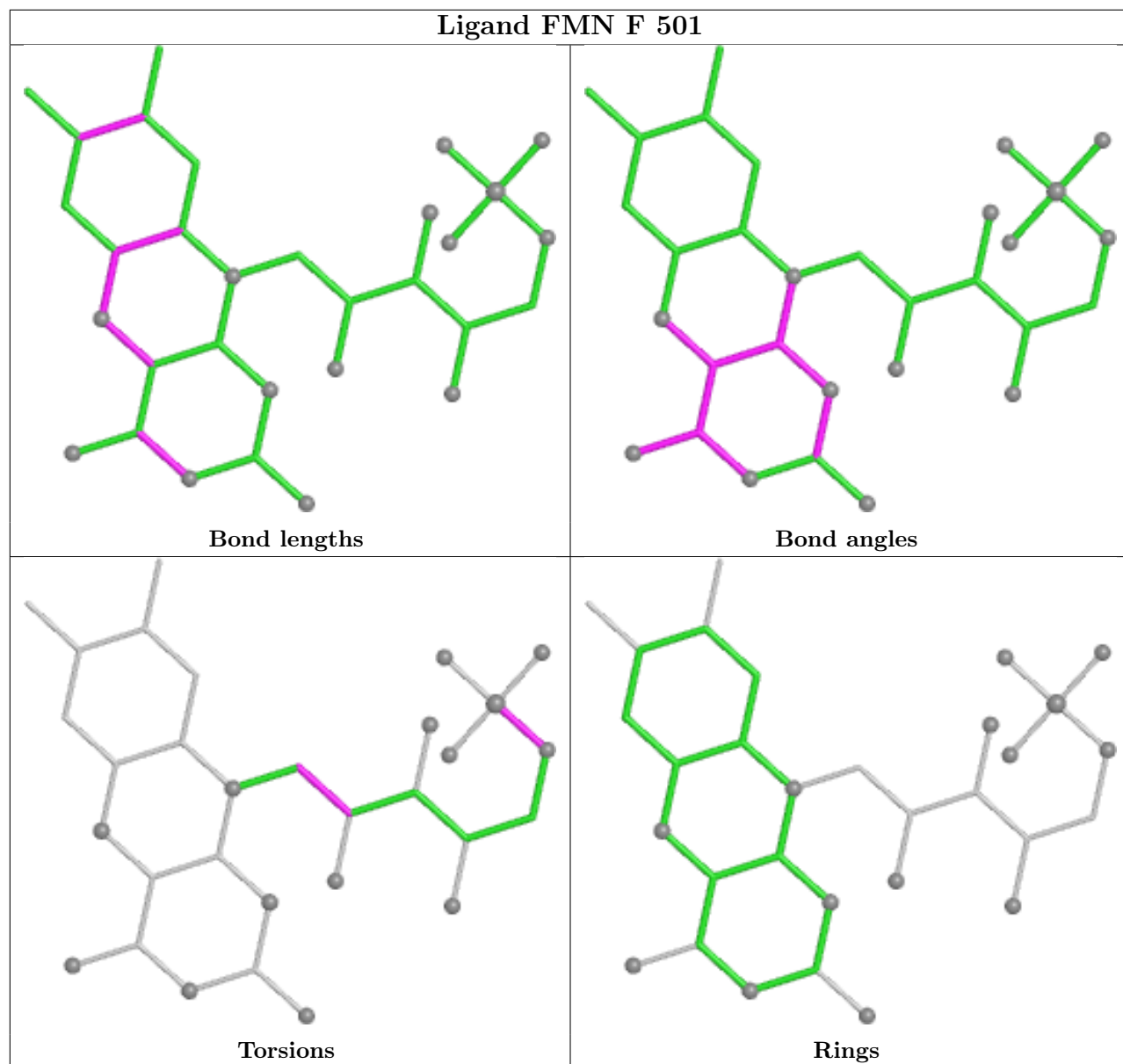


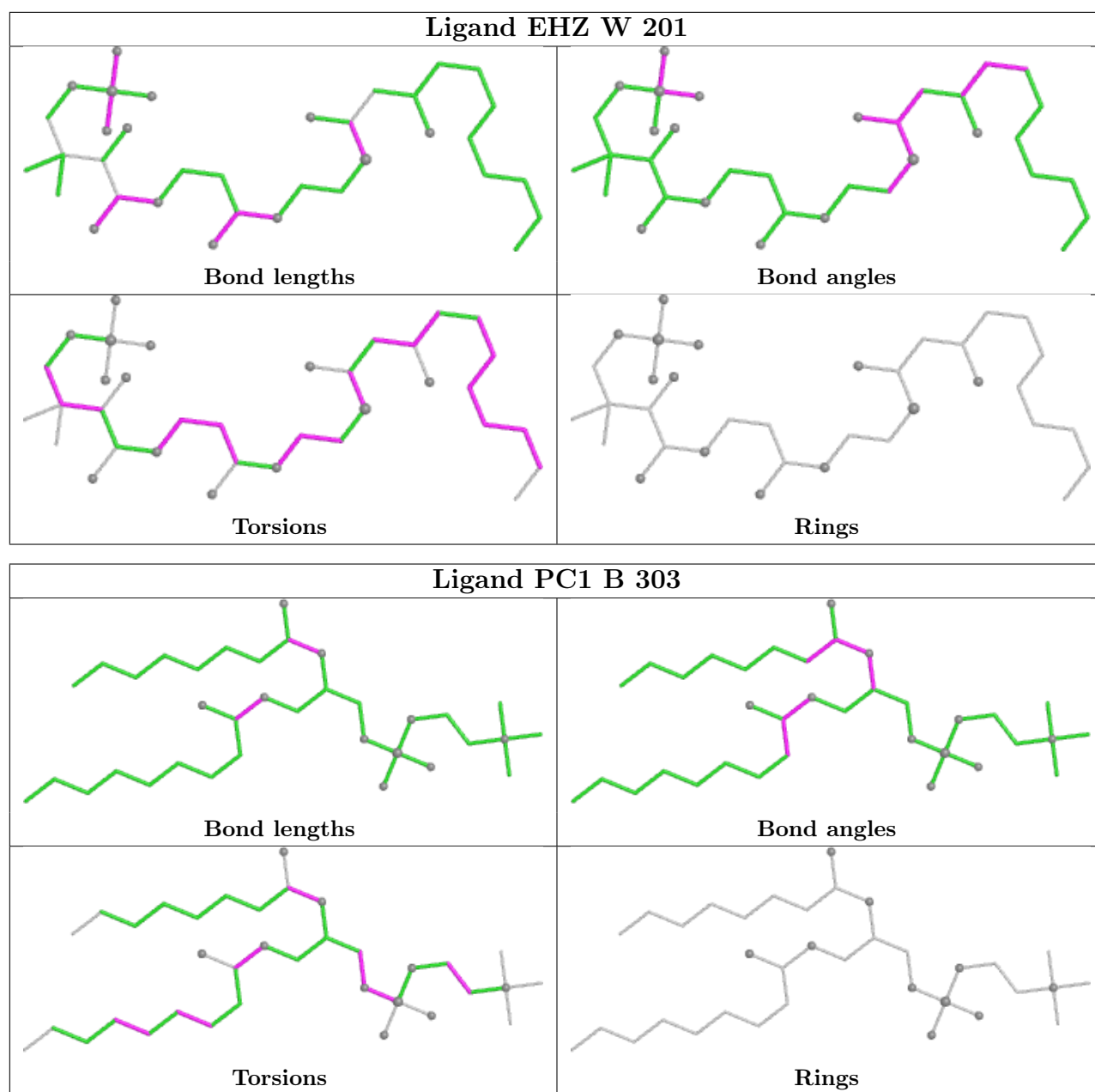












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

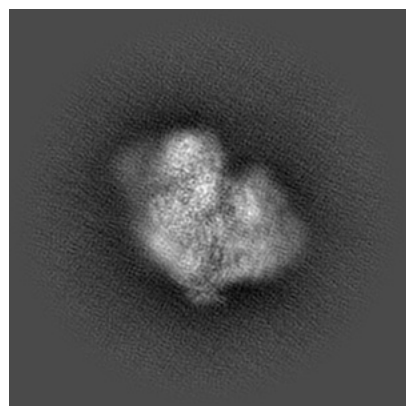
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38517. These allow visual inspection of the internal detail of the map and identification of artifacts.

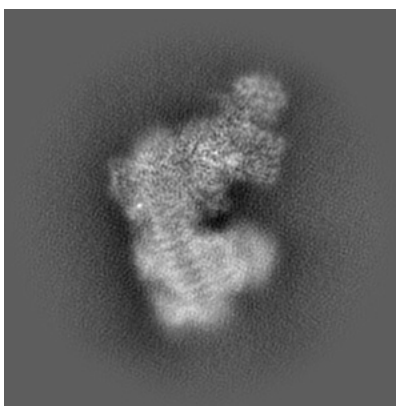
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

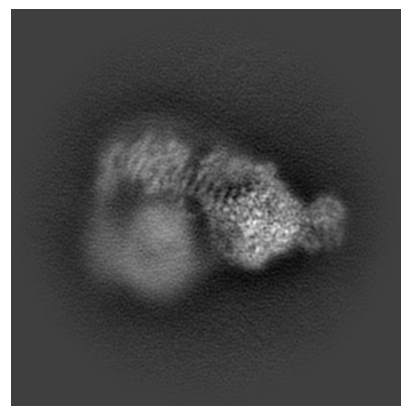
6.1.1 Primary map



X

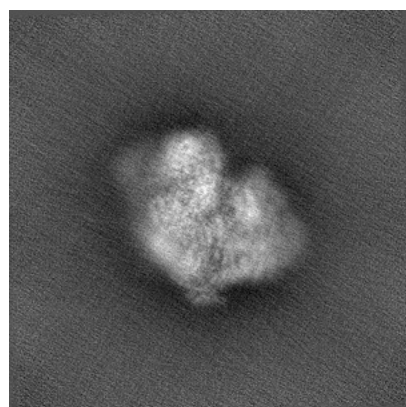


Y

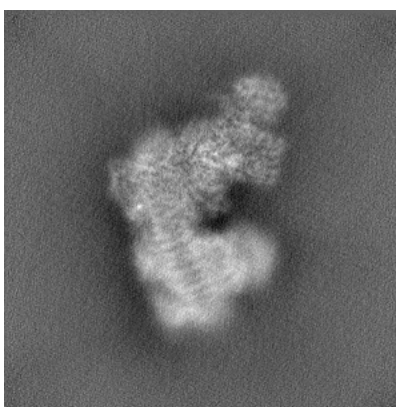


Z

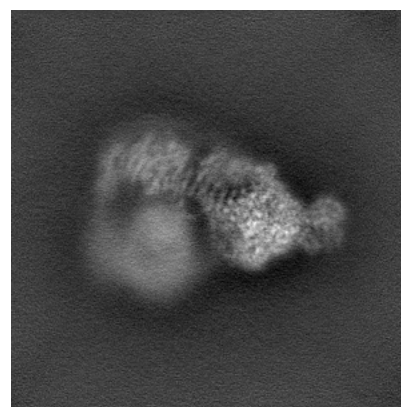
6.1.2 Raw map



X



Y

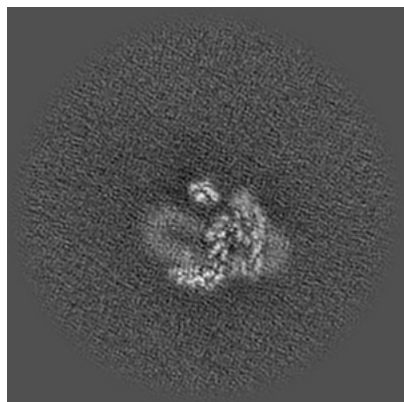


Z

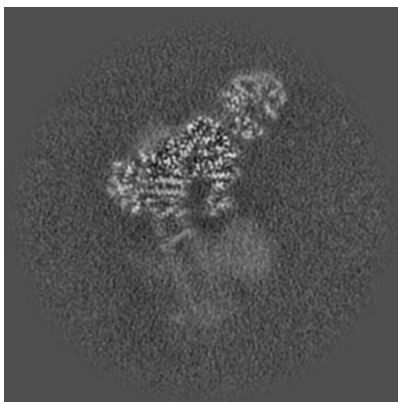
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

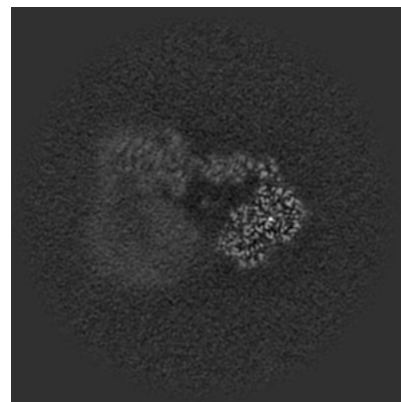
6.2.1 Primary map



X Index: 192

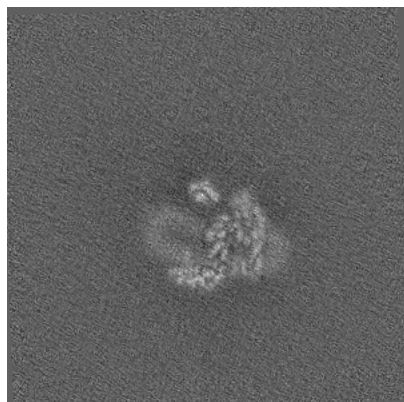


Y Index: 192

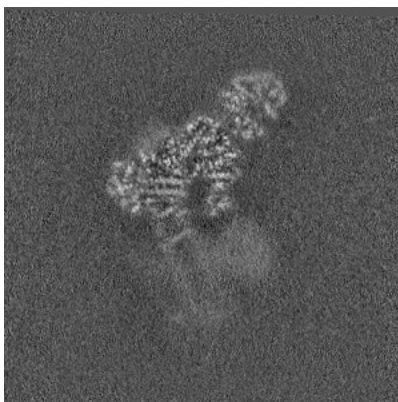


Z Index: 192

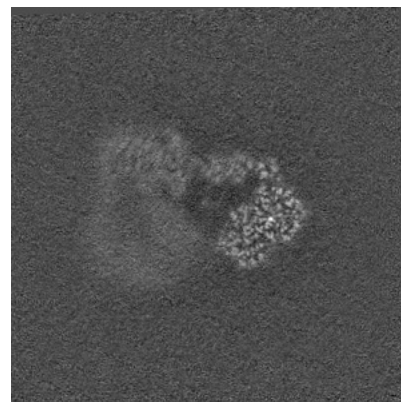
6.2.2 Raw map



X Index: 192



Y Index: 192

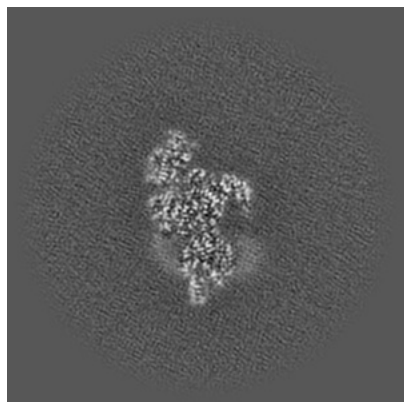


Z Index: 192

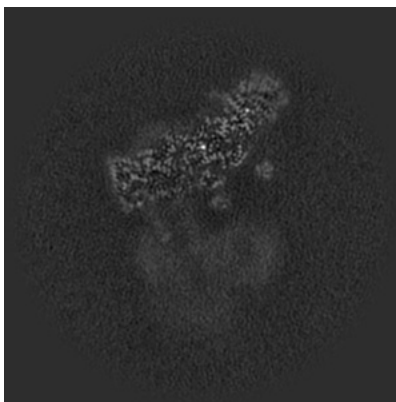
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

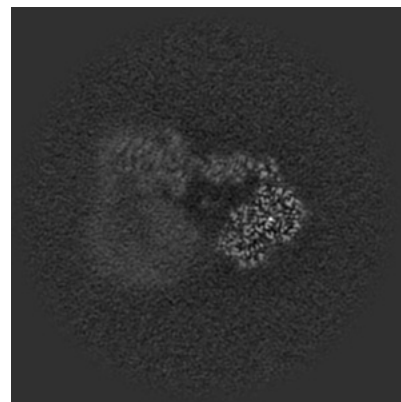
6.3.1 Primary map



X Index: 235

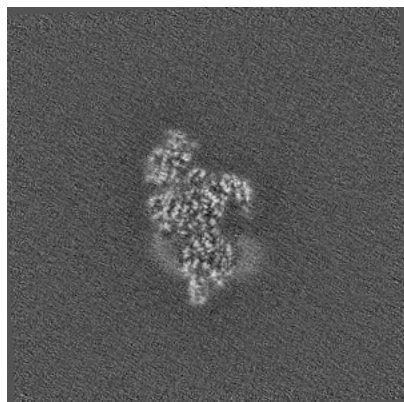


Y Index: 180

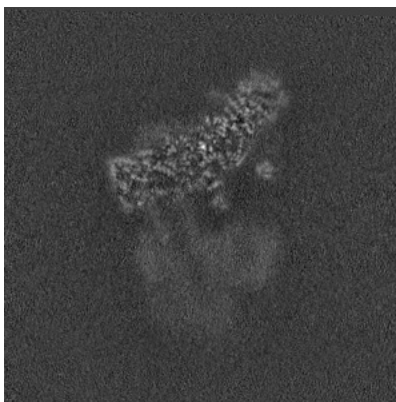


Z Index: 192

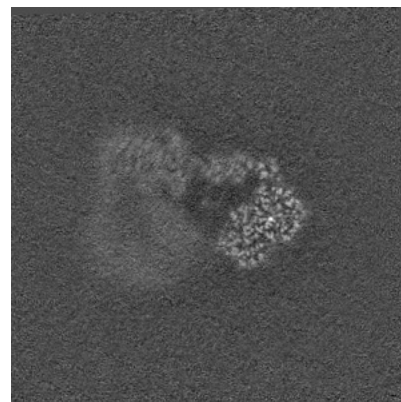
6.3.2 Raw map



X Index: 235



Y Index: 179

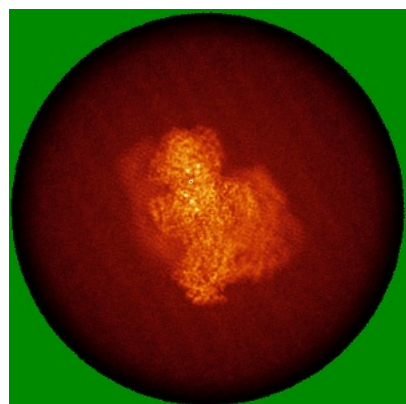


Z Index: 192

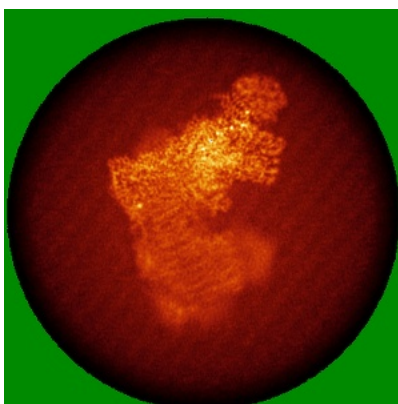
The images above show the largest variance slices of the map in three orthogonal directions.

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

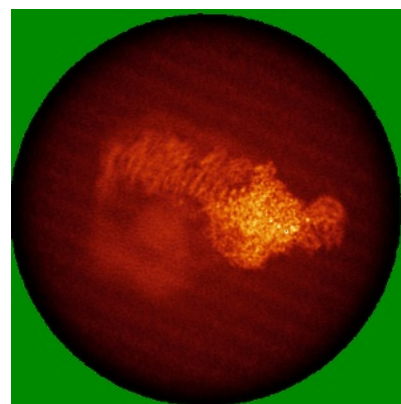
6.4.1 Primary map



X

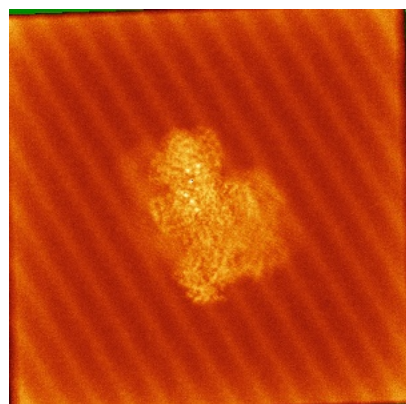


Y

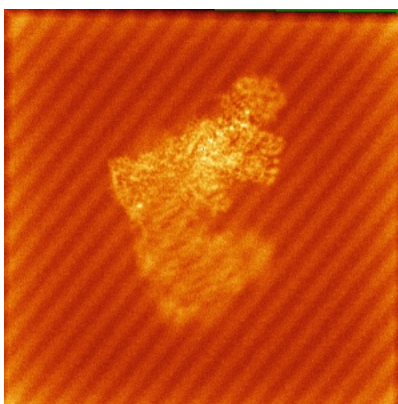


Z

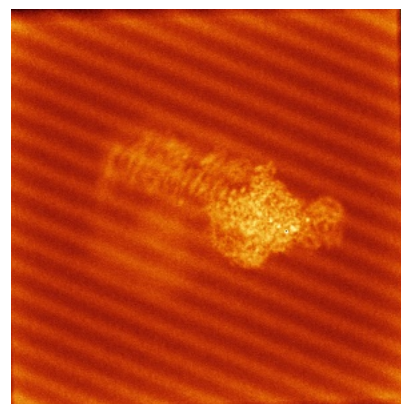
6.4.2 Raw map



X



Y

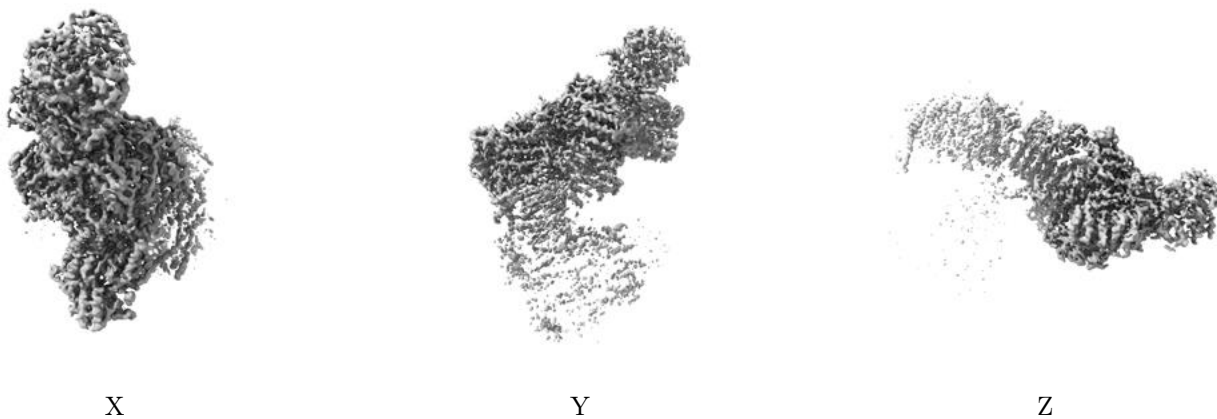


Z

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

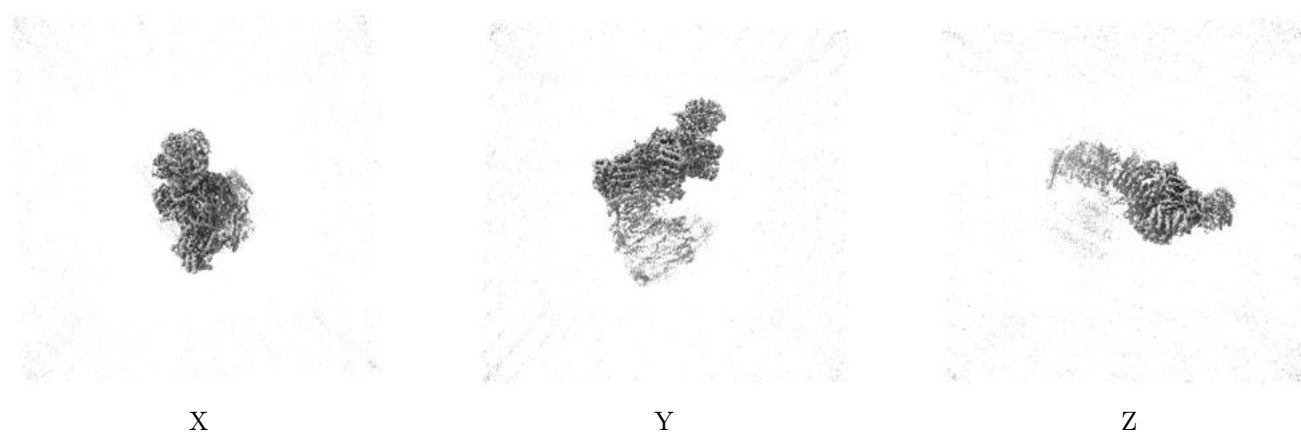
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

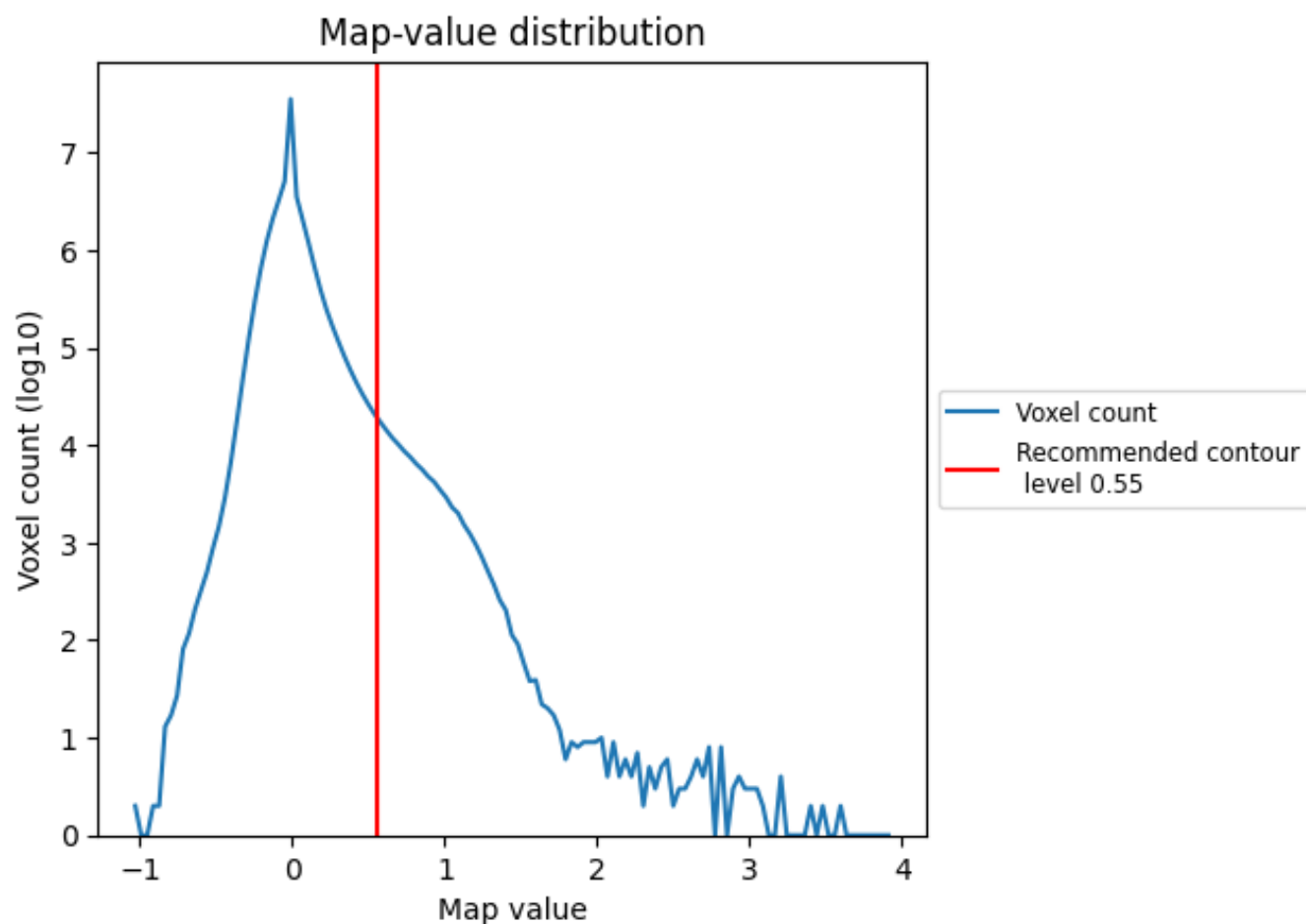
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

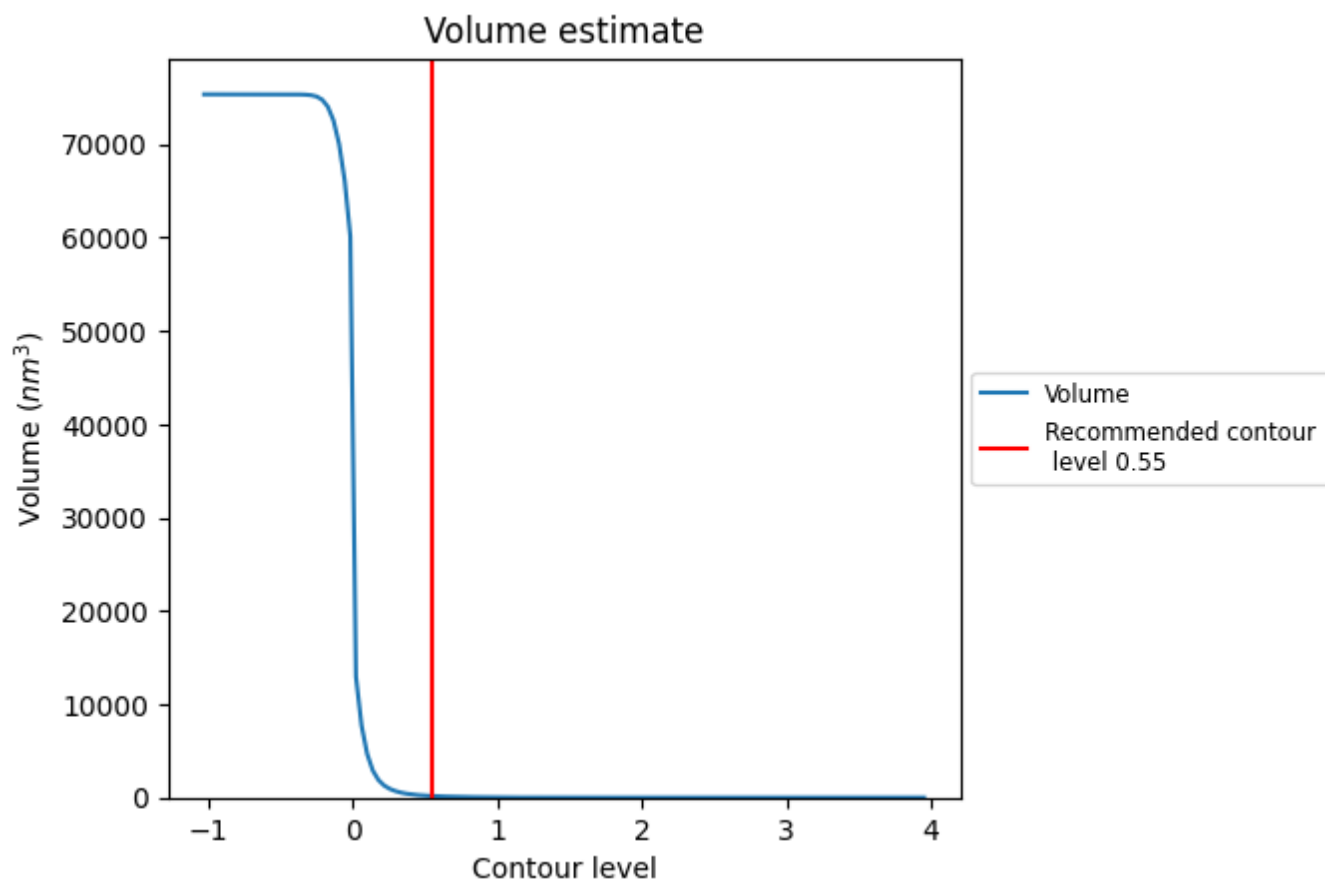
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

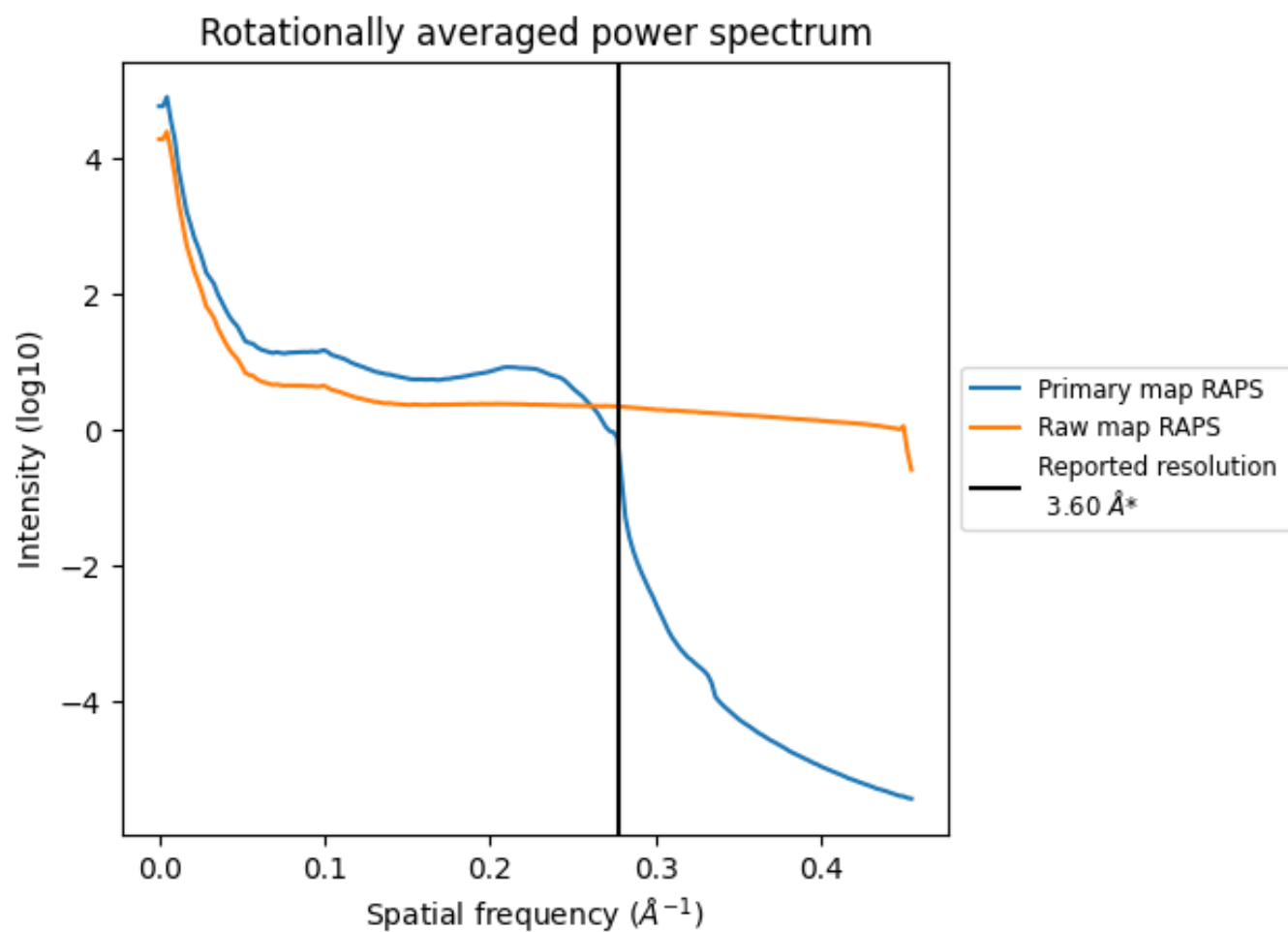
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm³; this corresponds to an approximate mass of 147 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

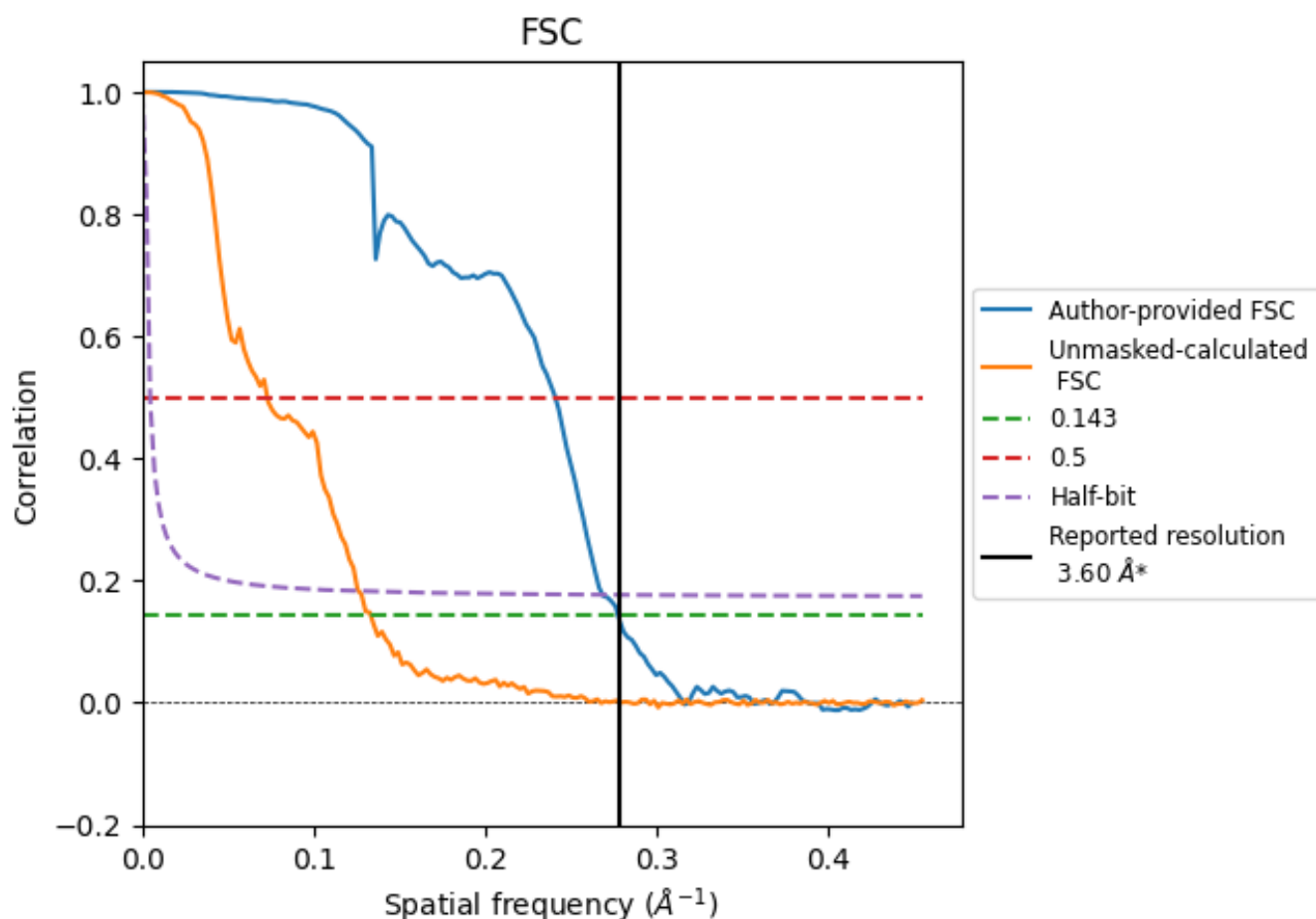


*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

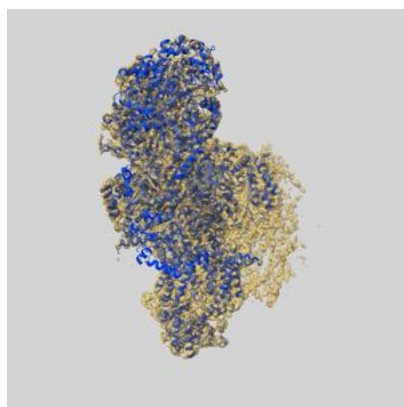
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.61	4.15	3.73
Unmasked-calculated*	7.51	13.72	7.92

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

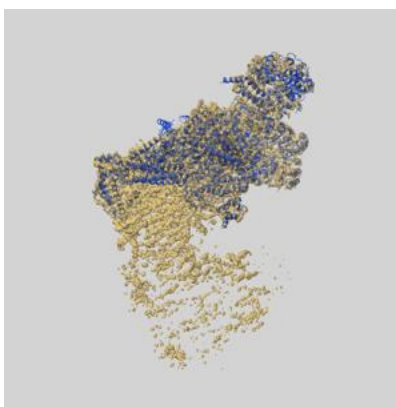
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38517 and PDB model 8XNW. Per-residue inclusion information can be found in section [3](#) on page [15](#).

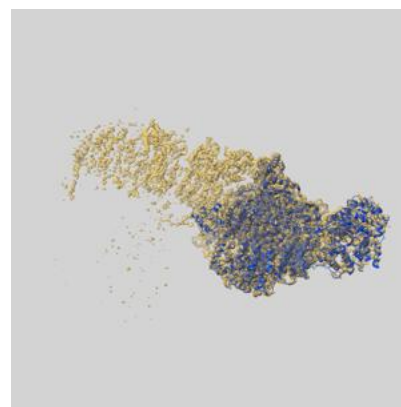
9.1 Map-model overlay [i](#)



X



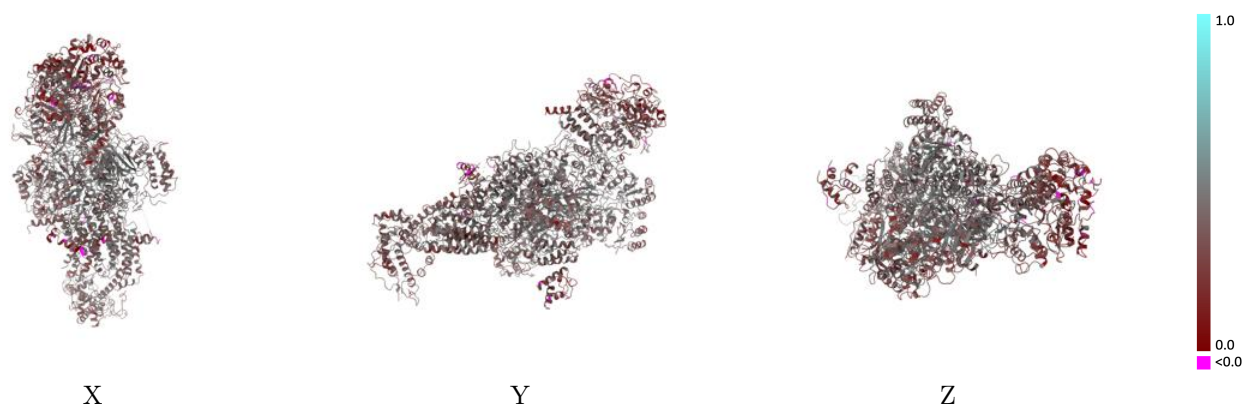
Y



Z

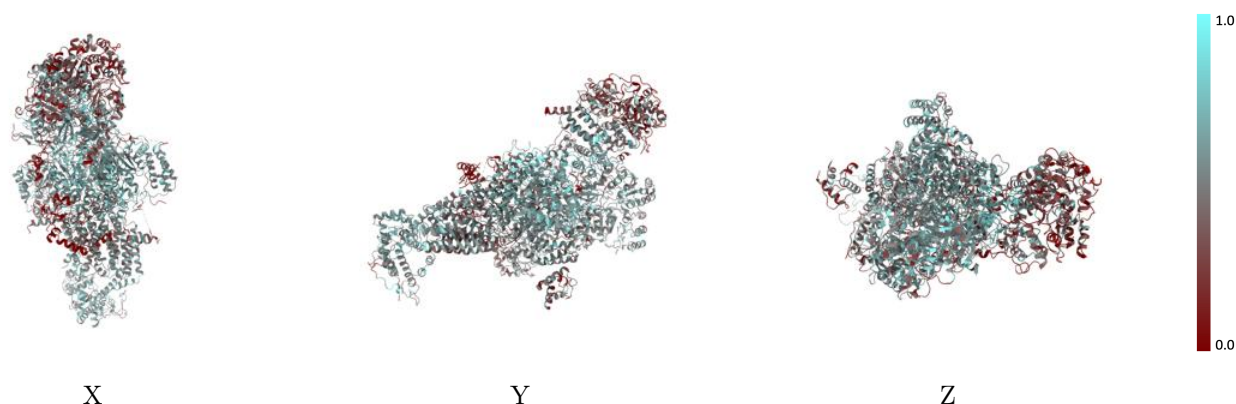
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



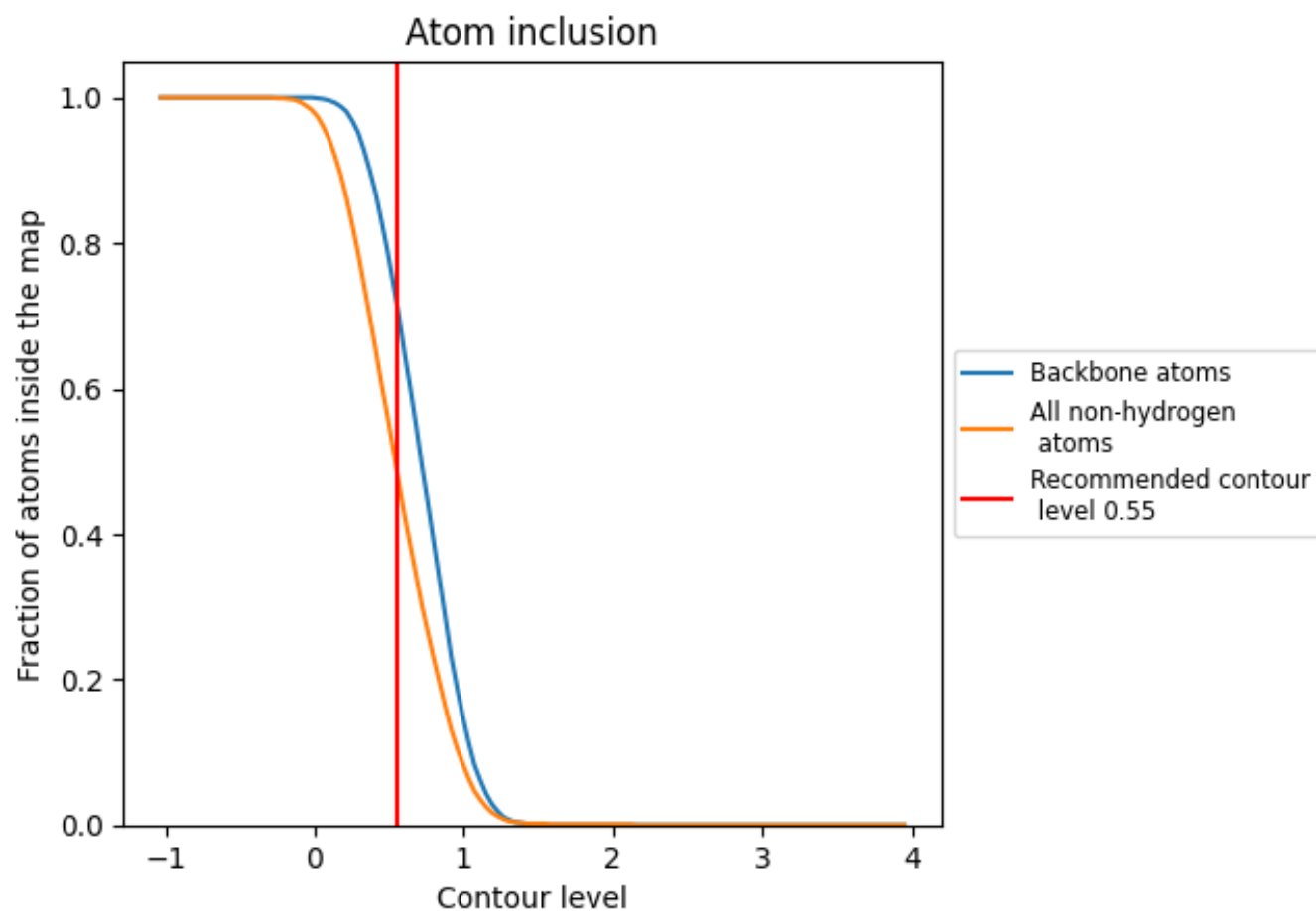
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 49% 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	 0.4890	 0.3740
A	 0.4450	 0.3970
B	 0.5880	 0.4340
C	 0.6040	 0.4440
D	 0.6150	 0.4450
E	 0.3180	 0.2820
F	 0.3630	 0.3010
G	 0.5570	 0.3990
H	 0.5000	 0.3850
I	 0.6230	 0.4240
P	 0.4840	 0.3620
Q	 0.4580	 0.4240
R	 0.2060	 0.3070
S	 0.5460	 0.3560
T	 0.3490	 0.2720
V	 0.5850	 0.3880
W	 0.5030	 0.3910
X	 0.5650	 0.3620
Z	 0.5300	 0.3560
a	 0.5860	 0.3870
b	 0.5170	 0.3590
q	 0.0690	 0.2780
r	 0.2580	 0.3060
s	 0.0260	 0.1960

