



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 11:48 AM UTC

PDB ID : 8XNU / pdb_00008xnu
EMDB ID : EMD-38515
Title : Respiratory complex Peripheral Arm of CI, open form A, focus-refined map of type IB, 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:

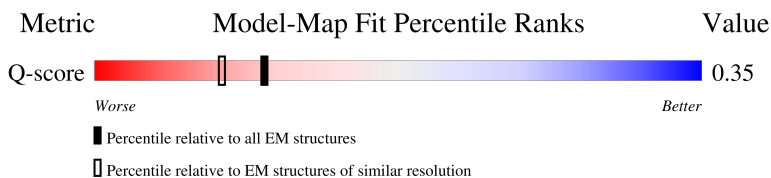
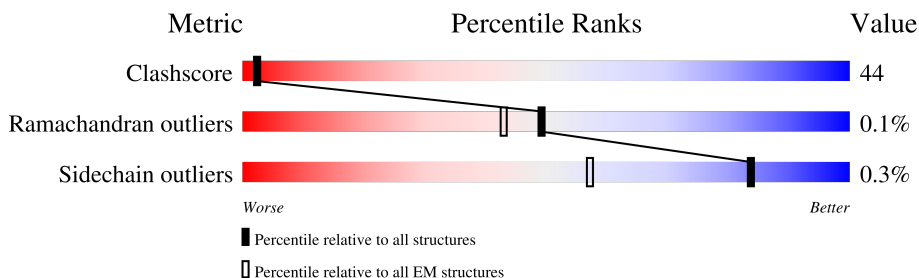
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



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

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

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

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

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

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

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

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 33733 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	93	Total	C	N	O	S	0	0
			762	528	108	120	6		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	384	Total	C	N	O	S	0	0
			3080	1966	531	560	23		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	312	Total	C	N	O	S	0	0
			2495	1679	378	416	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	174	Total	C	N	O	S	0	0
			1398	880	240	266	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	340	Total	C	N	O	S	0	0
			2730	1765	479	479	7		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	66	Total	C	N	O	S	0	0
			540	351	96	90	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	120	Total	C	N	O	S	0	0
			1004	645	178	177	4		

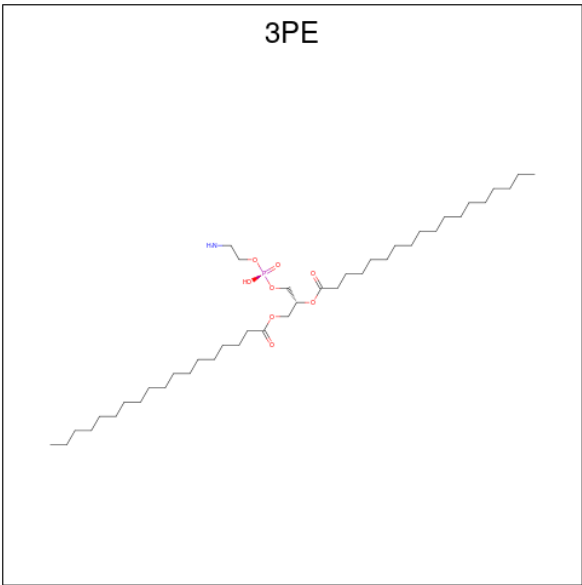
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	50	Total	C	N	O	S	0	0
			413	263	77	72	1		

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

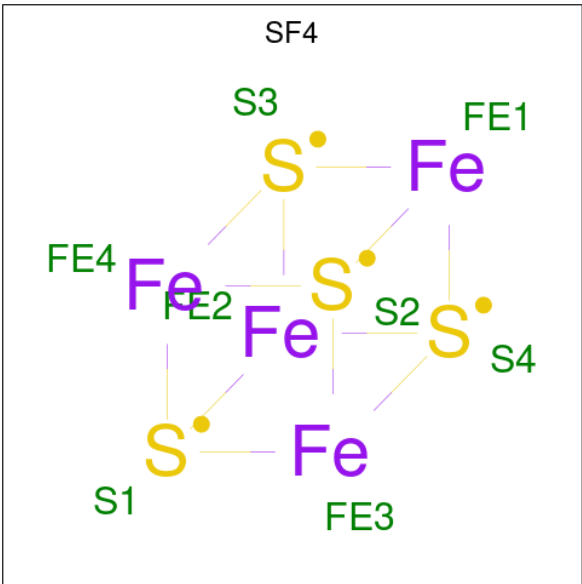
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	26	Total	C	N	O	0	0
			226	147	38	41		

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



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	I	1	Total	C	N	O	P	0
			29	19	1	8	1	

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



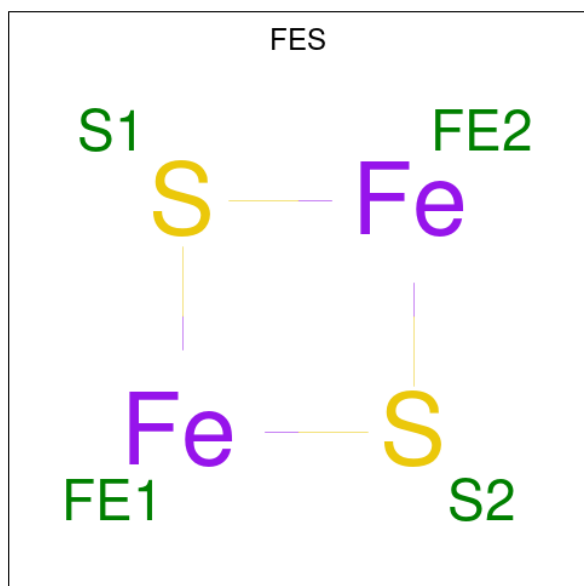
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	Fe	S	0
			8	4	4	

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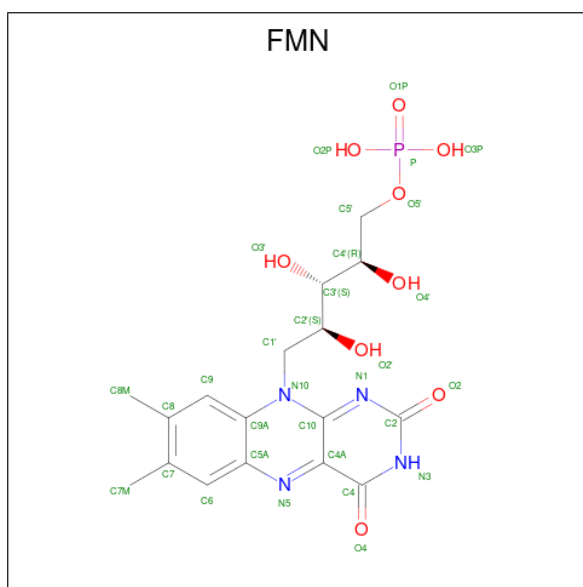
Mol	Chain	Residues	Atoms			AltConf
25	F	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	

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



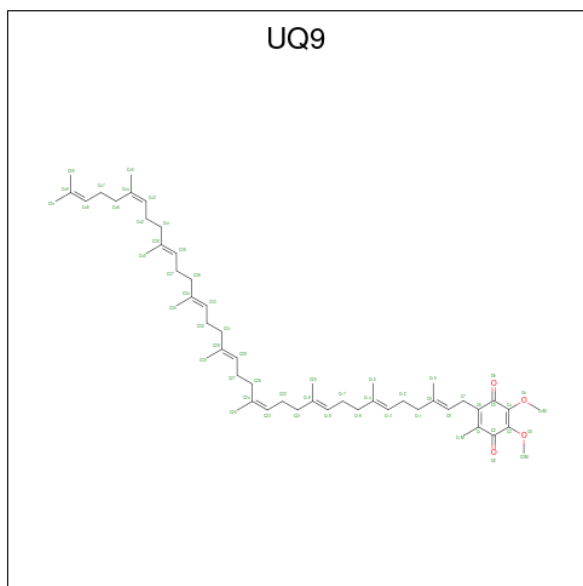
Mol	Chain	Residues	Atoms			AltConf
26	E	1	Total	Fe	S	0
			4	2	2	
26	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 27 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



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

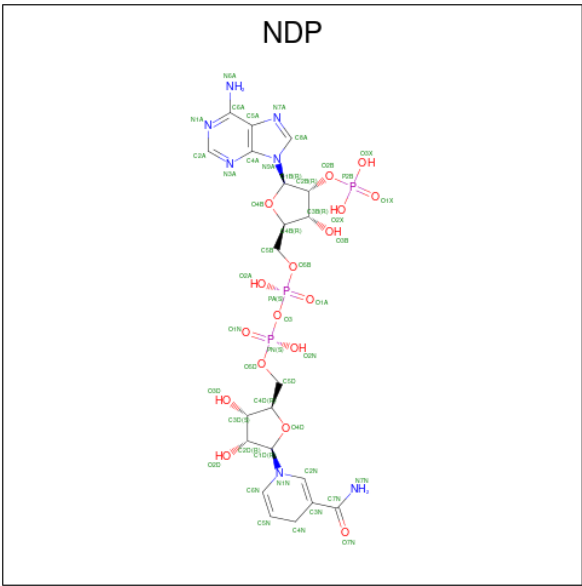
- Molecule 28 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is 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).

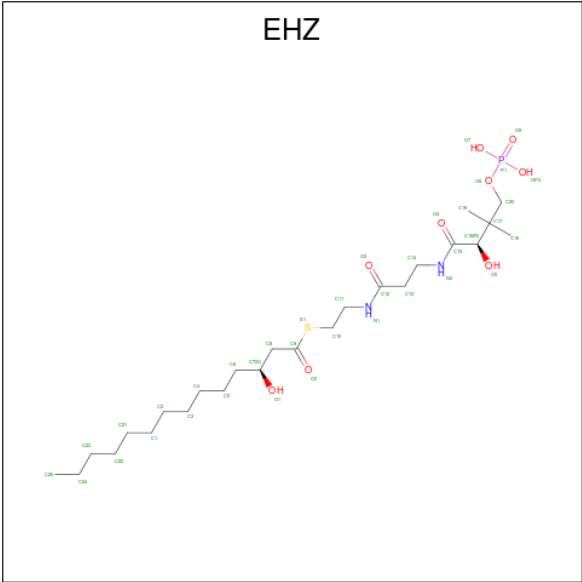


Mol	Chain	Residues	Atoms					AltConf
29	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 31 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).

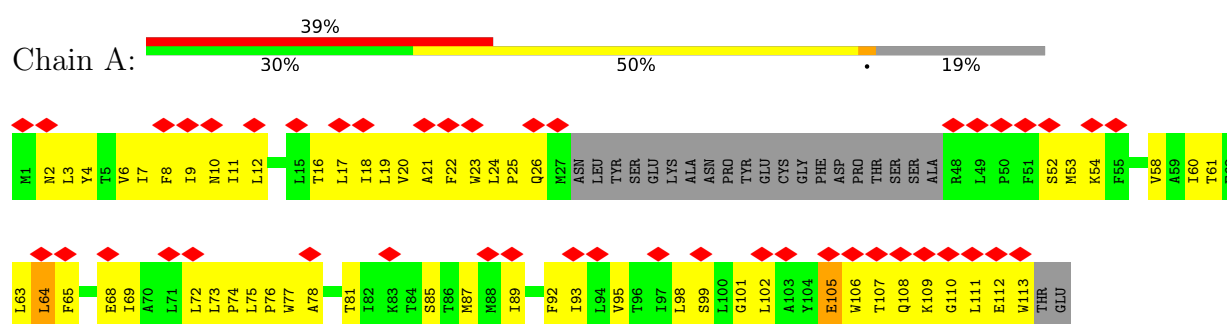


Mol	Chain	Residues	Atoms					AltConf	
31	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

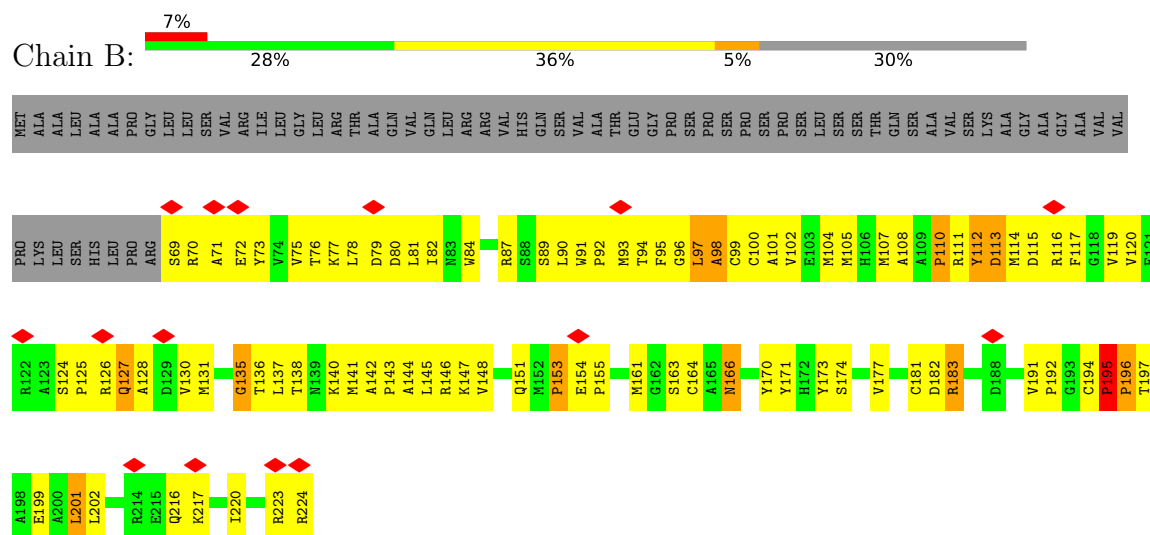
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

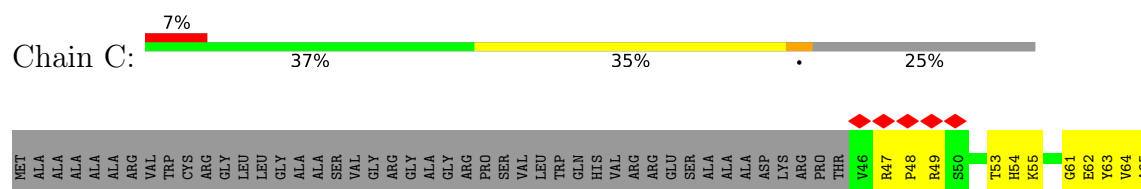
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

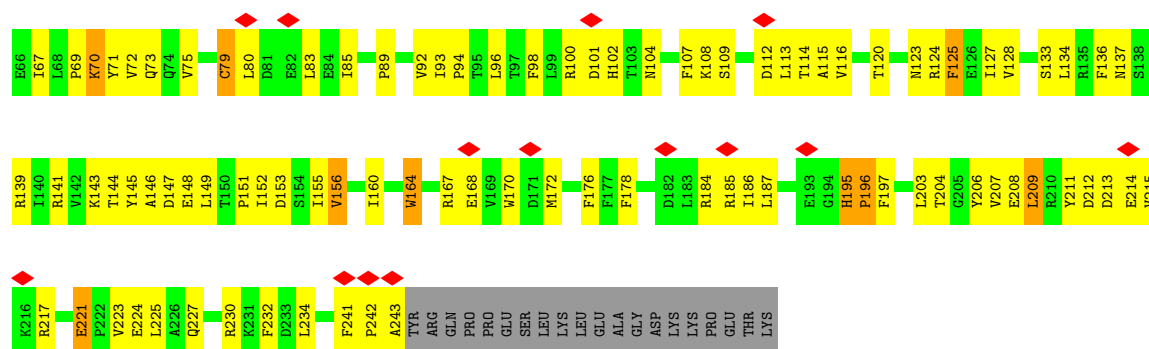


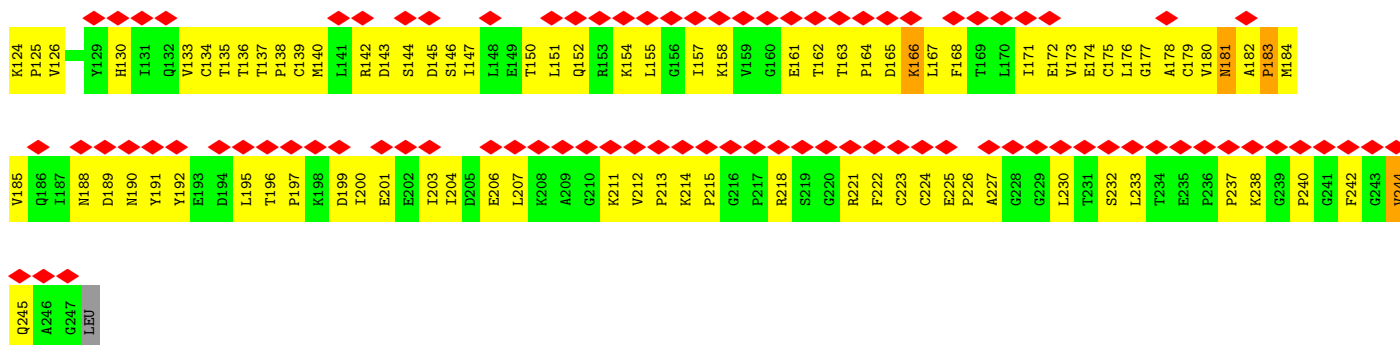
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



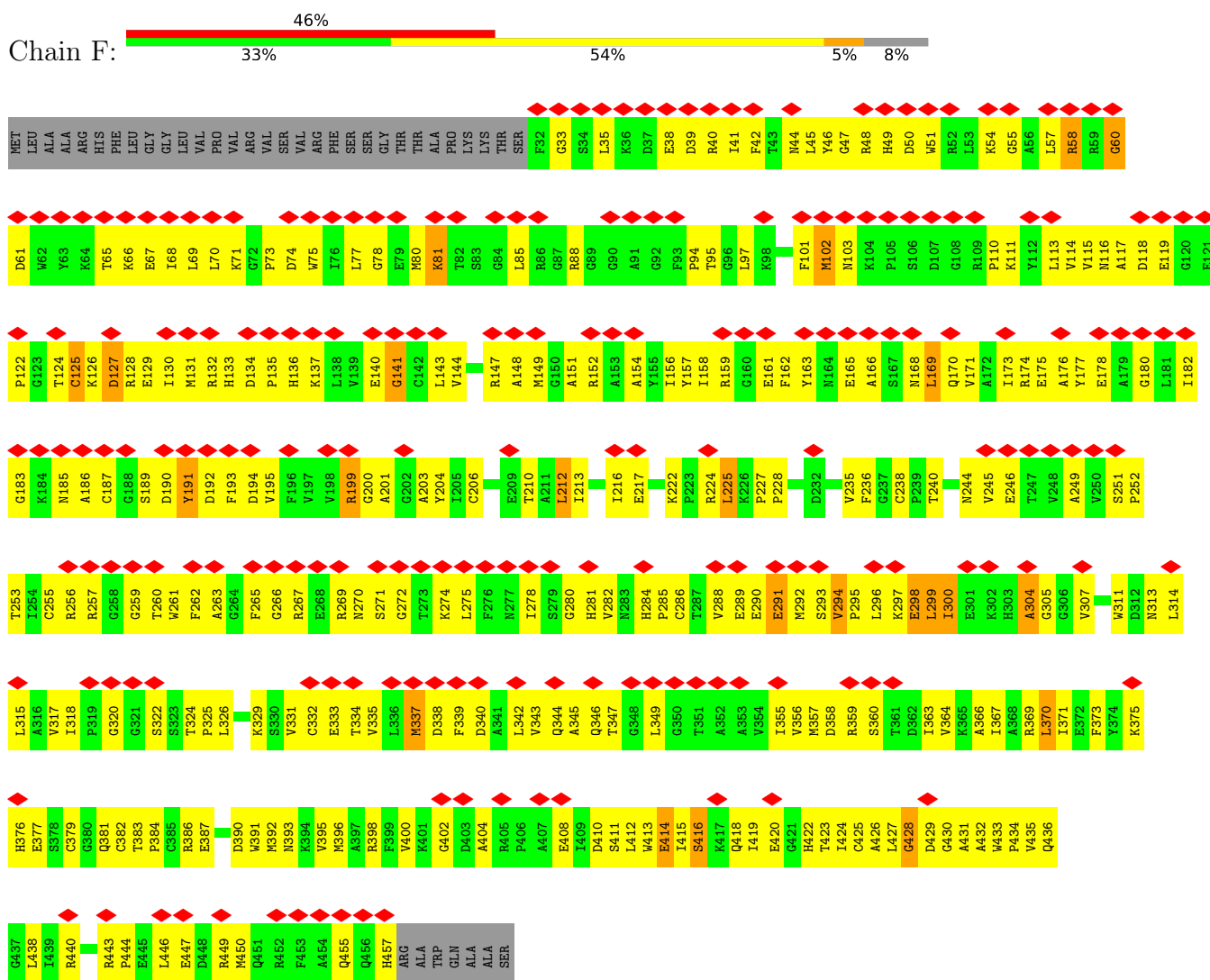
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



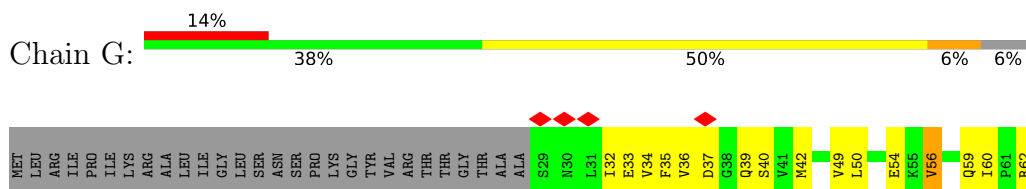


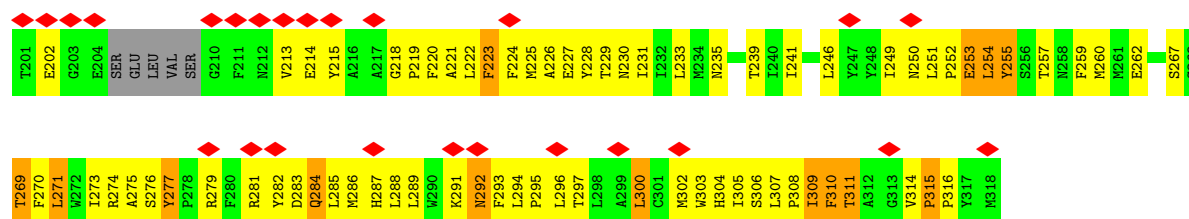


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

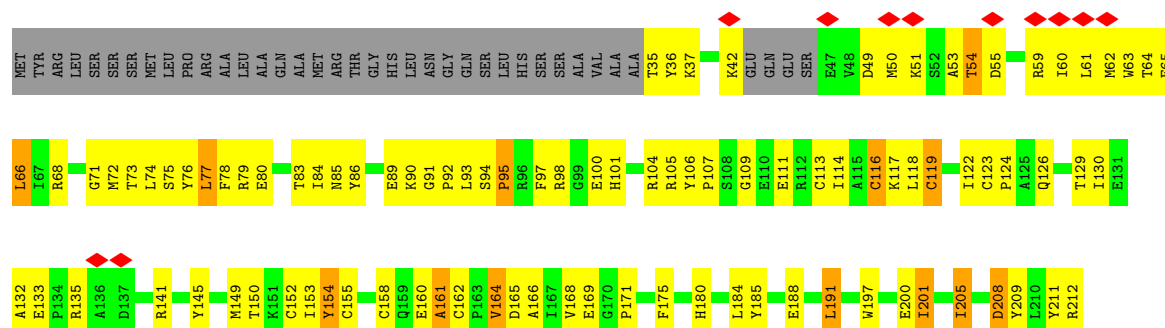


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

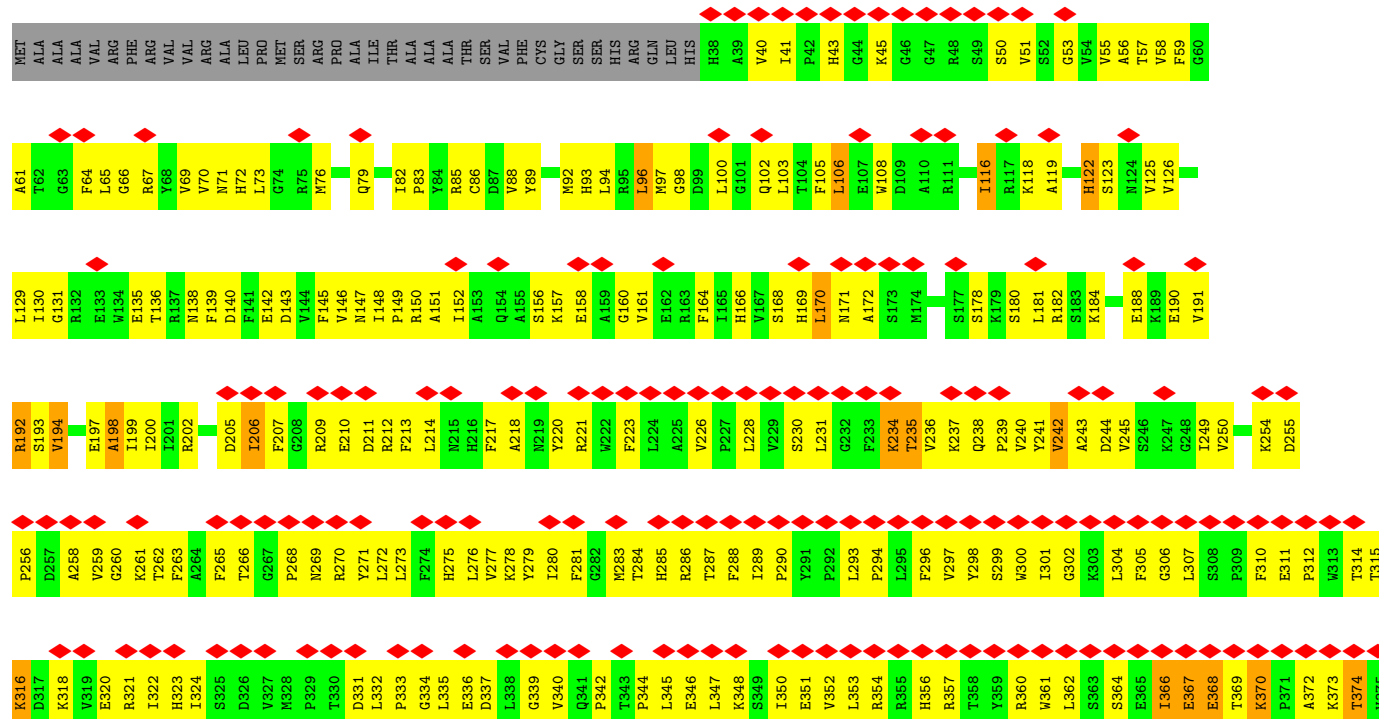




- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

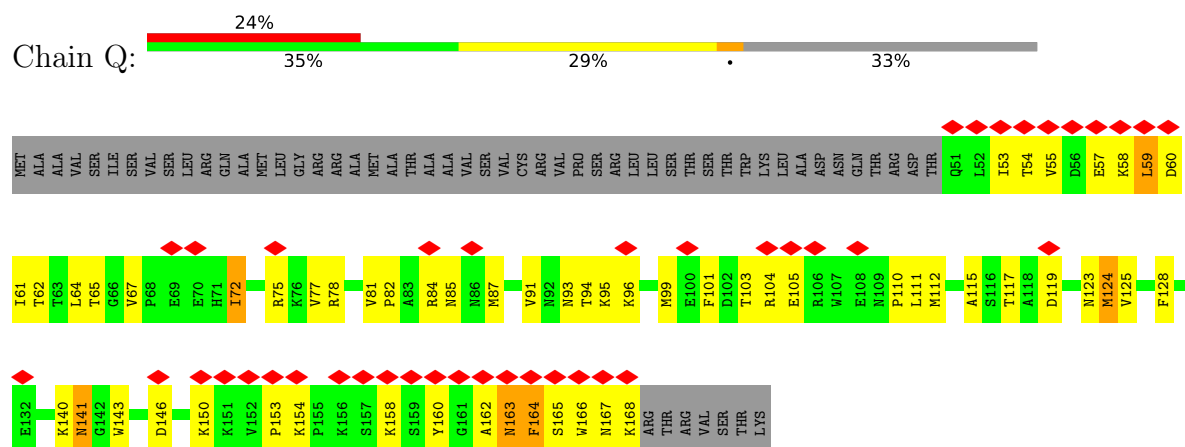


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

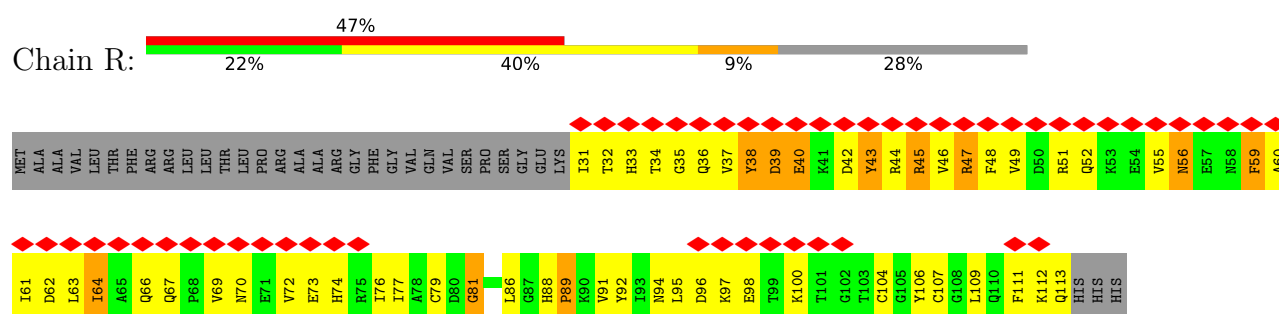




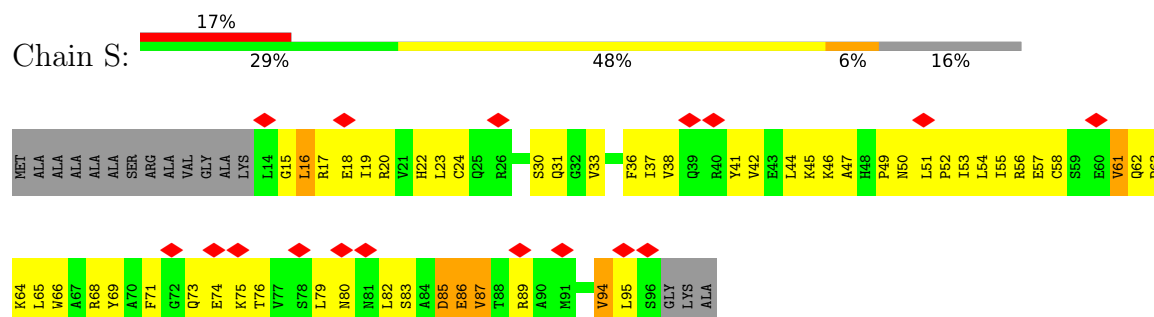
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



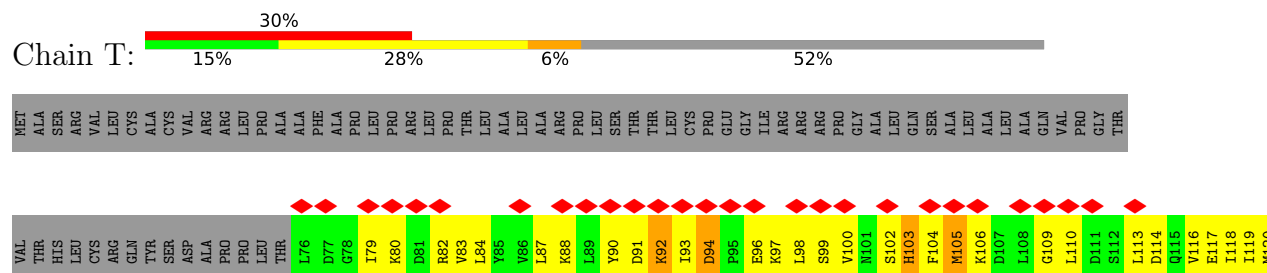
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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

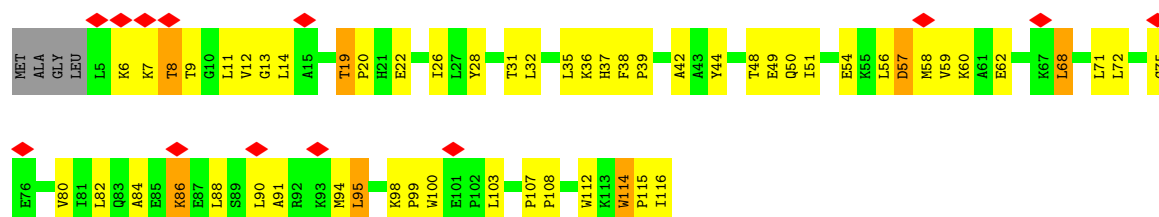


- Molecule 14: Acyl carrier protein, mitochondrial

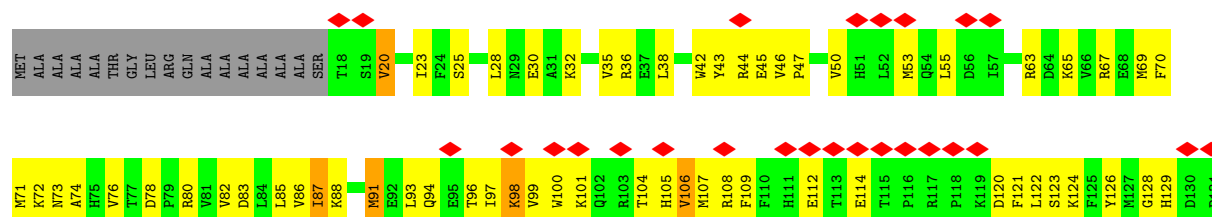
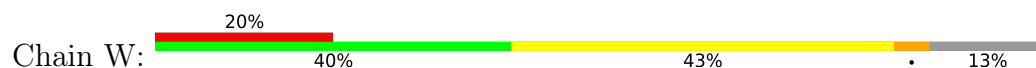




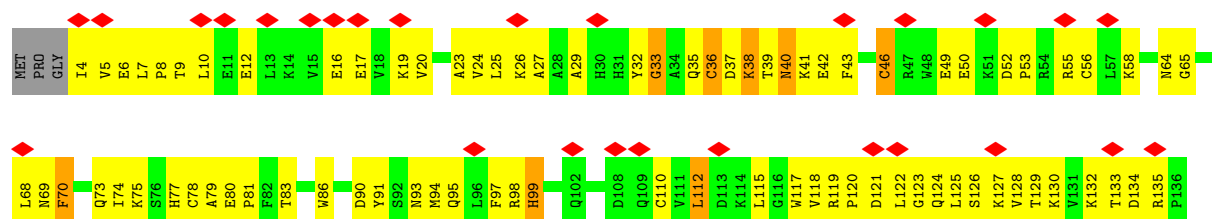
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



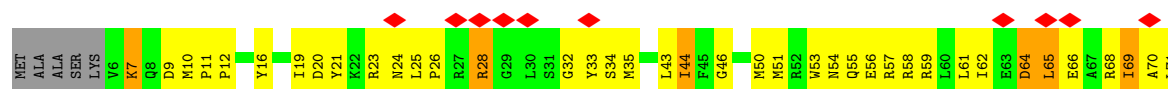
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

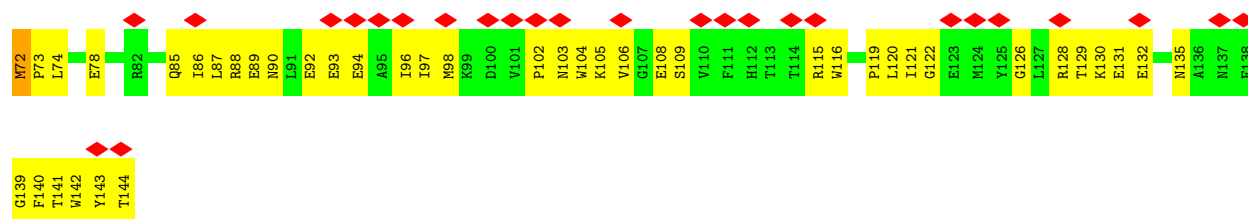


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

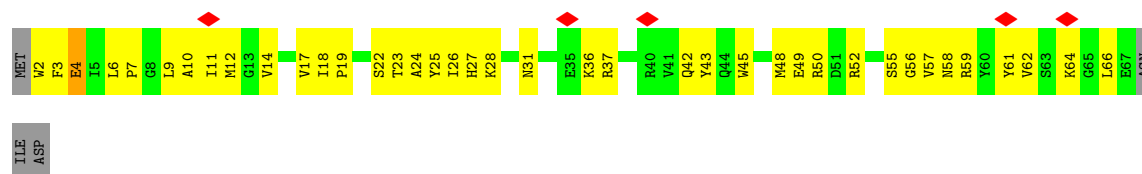


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

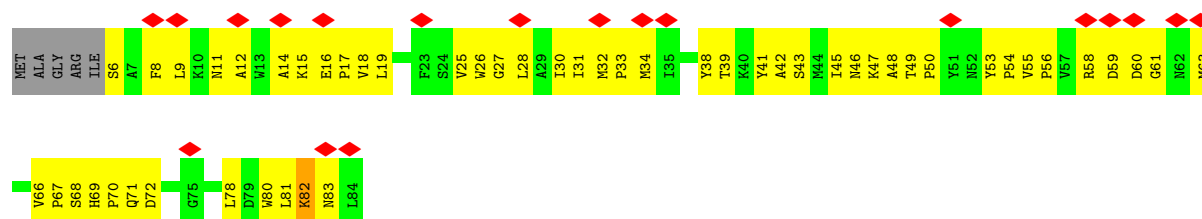




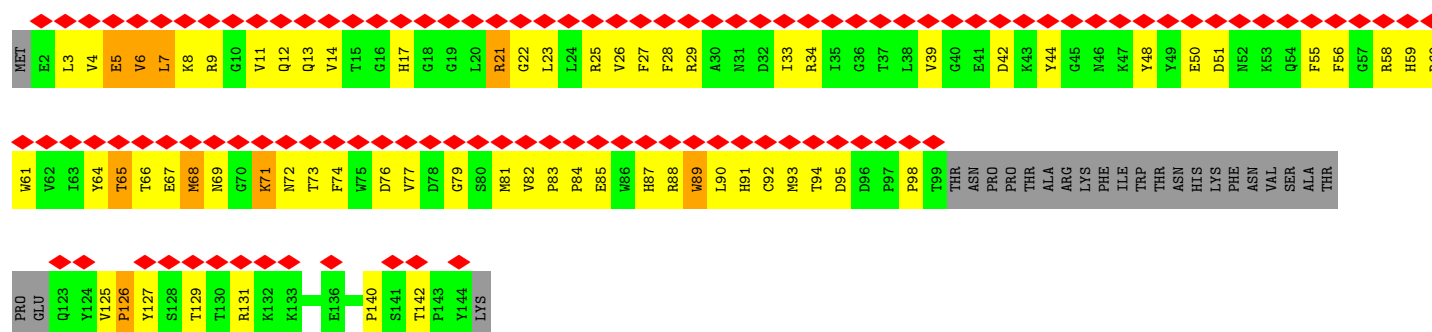
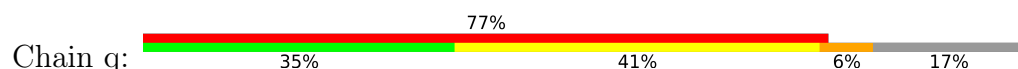
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



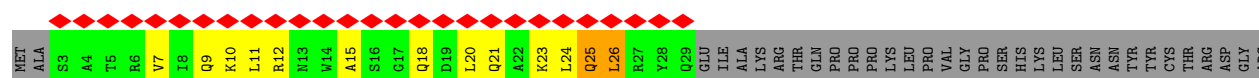
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

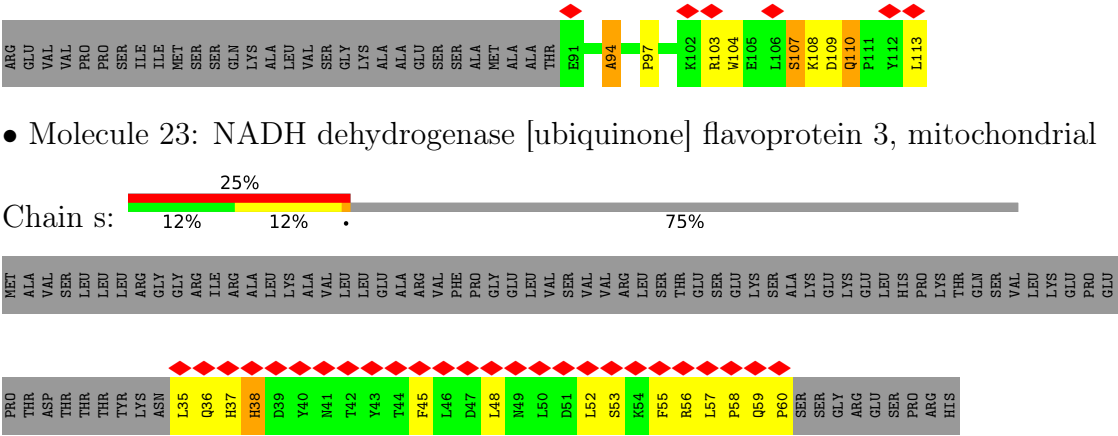


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25905	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.221	Depositor
Minimum map value	-1.104	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.5	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: UQ9, EH3, FMN, FES, NDP, ZN, 3PE, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.81	0/782	1.20	6/1066 (0.6%)
2	B	0.97	1/1278 (0.1%)	1.37	13/1730 (0.8%)
3	C	0.90	1/1687 (0.1%)	1.30	14/2297 (0.6%)
4	D	0.94	5/3154 (0.2%)	1.42	30/4265 (0.7%)
5	E	0.77	1/1675 (0.1%)	1.17	9/2282 (0.4%)
6	F	0.87	2/3363 (0.1%)	1.43	47/4543 (1.0%)
7	G	0.89	6/5374 (0.1%)	1.58	102/7281 (1.4%)
8	H	0.92	1/2570 (0.0%)	1.48	52/3509 (1.5%)
9	I	0.90	0/1427	1.52	19/1927 (1.0%)
10	P	0.77	1/2804 (0.0%)	1.22	27/3802 (0.7%)
11	Q	0.87	1/980 (0.1%)	1.28	12/1324 (0.9%)
12	R	0.87	4/671 (0.6%)	1.34	11/903 (1.2%)
13	S	0.85	0/678	1.44	10/915 (1.1%)
14	T	0.92	0/613	1.51	10/826 (1.2%)
15	V	0.86	0/937	1.46	14/1270 (1.1%)
16	W	0.84	1/993 (0.1%)	1.16	8/1335 (0.6%)
17	X	0.78	0/1191	1.34	18/1605 (1.1%)
18	Z	0.78	0/1183	1.22	13/1597 (0.8%)
19	a	0.88	0/553	1.21	4/745 (0.5%)
20	b	0.74	0/643	0.95	1/884 (0.1%)
21	q	0.88	1/1037 (0.1%)	1.34	15/1408 (1.1%)
22	r	0.87	1/421 (0.2%)	1.38	8/566 (1.4%)
23	s	0.43	0/233	0.75	1/317 (0.3%)
All	All	0.87	26/34247 (0.1%)	1.38	444/46397 (1.0%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	W	106	VAL	C-N	-8.67	1.22	1.33
12	R	39	ASP	CA-C	7.90	1.64	1.53
11	Q	53	ILE	C-O	7.83	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	40	GLU	N-CA	7.70	1.56	1.46
7	G	203	ASP	CA-C	6.79	1.63	1.52
7	G	600	GLU	CA-C	6.53	1.61	1.52
4	D	106	VAL	C-N	-6.49	1.24	1.33
4	D	266	ARG	C-O	-6.37	1.16	1.24
7	G	127	ASP	CA-C	6.25	1.62	1.52
7	G	76	ARG	CA-C	6.12	1.61	1.53
2	B	110	PRO	C-O	-6.10	1.16	1.24
5	E	93	PRO	N-CD	-5.92	1.39	1.47
7	G	361	VAL	CA-C	5.85	1.60	1.52
8	H	60	PRO	N-CD	5.76	1.55	1.47
22	r	25	GLN	CA-C	5.76	1.60	1.52
6	F	225	LEU	C-O	5.70	1.31	1.23
12	R	59	PHE	CA-C	-5.69	1.45	1.52
4	D	107	ARG	C-N	5.58	1.40	1.33
6	F	414	GLU	C-O	-5.54	1.17	1.24
4	D	392	PRO	C-O	-5.46	1.20	1.24
7	G	683	PRO	N-CD	-5.41	1.40	1.47
21	q	126	PRO	N-CD	5.37	1.55	1.47
10	P	235	THR	CA-C	5.30	1.59	1.53
4	D	266	ARG	CA-C	-5.18	1.45	1.52
3	C	61	GLY	C-N	-5.05	1.27	1.33
12	R	89	PRO	N-CD	-5.02	1.40	1.47

All (444) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	142	VAL	N-CA-CB	19.32	132.48	110.65
4	D	142	VAL	N-CA-C	-18.99	92.57	110.42
7	G	174	THR	N-CA-C	-16.84	89.05	114.64
6	F	125	CYS	N-CA-C	-15.62	93.49	113.17
7	G	251	ILE	N-CA-C	13.32	126.82	108.17
7	G	77	MET	N-CA-C	-13.04	97.34	113.38
7	G	500	ILE	N-CA-C	-12.48	98.80	110.53
10	P	106	LEU	N-CA-C	12.16	128.65	109.07
7	G	204	MET	N-CA-C	-11.62	91.47	109.25
6	F	449	ARG	N-CA-C	-11.62	98.70	111.36
6	F	171	VAL	N-CA-C	-11.47	99.41	110.42
11	Q	60	ASP	N-CA-C	-11.30	90.36	109.24
7	G	599	THR	N-CA-C	11.23	126.08	112.38
16	W	87	ILE	N-CA-C	-11.08	99.78	110.42
8	H	259	PHE	N-CA-C	-11.00	99.37	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	57	ASP	N-CA-C	-10.98	99.32	111.07
9	I	164	VAL	N-CA-C	-10.61	100.17	113.22
9	I	77	LEU	N-CA-C	-10.48	99.66	111.71
14	T	139	MET	N-CA-C	-10.40	97.45	113.89
2	B	195	PRO	N-CA-C	-10.36	98.07	110.70
7	G	280	ASP	N-CA-C	10.30	122.50	111.28
4	D	140	ASP	CB-CA-C	-10.19	98.07	111.42
4	D	337	MET	N-CA-C	-10.18	100.17	111.07
19	a	4	GLU	N-CA-C	10.17	124.79	112.38
9	I	161	ALA	N-CA-C	10.16	122.35	111.28
7	G	414	PHE	N-CA-C	-10.14	101.41	113.88
10	P	366	ILE	N-CA-C	10.14	120.96	110.62
14	T	135	ALA	N-CA-C	-10.06	100.32	111.28
6	F	178	GLU	N-CA-C	-9.84	99.30	111.11
9	I	166	ALA	N-CA-C	-9.84	100.82	113.12
6	F	103	ASN	N-CA-C	-9.82	100.98	113.16
7	G	325	ARG	N-CA-C	-9.82	100.27	110.97
6	F	141	GLY	N-CA-C	-9.77	101.17	112.50
6	F	144	VAL	N-CA-C	-9.74	101.38	110.53
7	G	654	VAL	N-CA-C	9.71	123.23	111.09
8	H	52	ALA	N-CA-C	-9.60	100.80	111.07
7	G	337	ALA	N-CA-C	-9.58	100.80	114.12
6	F	418	GLN	N-CA-C	-9.58	100.79	111.14
17	X	70	PHE	N-CA-C	-9.55	99.65	111.11
12	R	38	TYR	N-CA-C	-9.44	96.36	110.24
17	X	112	LEU	N-CA-C	-9.44	100.95	111.14
4	D	427	PRO	N-CA-C	-9.41	95.73	110.50
7	G	692	LYS	N-CA-C	-9.30	100.51	112.23
10	P	367	GLU	N-CA-C	9.29	122.60	111.82
7	G	694	PHE	N-CA-C	9.27	121.39	111.28
14	T	133	ILE	N-CA-C	9.27	119.81	110.82
10	P	369	THR	N-CA-CB	9.24	123.48	110.17
18	Z	69	ILE	N-CA-C	-9.23	100.67	110.36
7	G	640	ASP	N-CA-C	-9.17	101.37	111.36
7	G	389	THR	N-CA-C	-9.13	96.27	109.96
5	E	85	ALA	N-CA-C	-9.10	101.44	111.36
19	a	57	VAL	N-CA-C	-9.01	105.15	113.71
7	G	133	GLN	N-CA-CB	8.80	121.54	110.45
7	G	212	LYS	N-CA-C	-8.76	94.62	108.90
9	I	154	TYR	N-CA-CB	-8.67	99.22	111.62
16	W	20	VAL	N-CA-C	8.66	120.74	108.36
8	H	60	PRO	N-CA-CB	8.65	108.53	102.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	365	ASN	N-CA-C	-8.65	102.28	112.92
10	P	96	LEU	N-CA-C	8.62	121.63	111.71
13	S	86	GLU	N-CA-C	-8.49	102.10	111.36
10	P	373	LYS	N-CA-C	8.49	121.90	110.35
16	W	100	TRP	N-CA-C	-8.48	99.82	112.04
13	S	18	GLU	N-CA-C	8.47	123.21	109.40
3	C	70	LYS	N-CA-C	8.47	121.58	111.33
8	H	141	SER	N-CA-C	-8.43	102.05	111.07
17	X	99	HIS	N-CA-C	-8.41	102.19	111.36
3	C	108	LYS	N-CA-C	8.38	120.04	111.07
7	G	452	LEU	N-CA-C	-8.34	102.19	111.28
11	Q	54	THR	N-CA-C	8.32	123.28	109.46
8	H	311	THR	N-CA-C	-8.27	102.50	112.59
7	G	558	GLN	N-CA-C	-8.26	102.23	111.07
6	F	171	VAL	N-CA-CB	8.24	120.20	110.55
8	H	196	ALA	N-CA-C	8.23	127.99	109.81
3	C	196	PRO	N-CA-C	8.19	124.92	113.53
6	F	298	GLU	N-CA-C	8.19	120.20	111.28
7	G	534	VAL	N-CA-C	-8.18	104.64	111.91
7	G	691	ILE	N-CA-C	8.17	123.66	111.89
1	A	64	LEU	N-CA-C	-8.17	102.33	111.07
16	W	96	THR	N-CA-C	-8.17	102.32	111.14
6	F	191	TYR	N-CA-C	8.12	121.69	110.24
7	G	484	ASP	N-CA-C	8.12	121.04	111.71
15	V	86	LYS	N-CA-C	-8.06	102.44	111.14
13	S	76	THR	N-CA-C	8.04	122.01	108.90
7	G	500	ILE	N-CA-CB	8.03	120.85	110.57
9	I	201	ILE	N-CA-C	-8.03	102.61	110.72
2	B	110	PRO	N-CA-C	8.02	124.48	113.65
8	H	271	LEU	N-CA-C	-8.00	102.50	111.14
16	W	98	LYS	N-CA-C	-7.99	101.58	113.72
17	X	46	CYS	N-CA-C	-7.98	102.66	111.36
17	X	43	PHE	N-CA-C	-7.98	102.53	111.07
21	q	67	GLU	CB-CA-C	-7.96	99.57	112.06
7	G	651	PRO	CB-CA-C	-7.94	98.45	111.56
1	A	9	ILE	N-CA-C	-7.94	102.52	110.62
10	P	206	ILE	N-CA-C	7.92	120.90	108.87
8	H	311	THR	N-CA-CB	7.88	123.52	110.92
9	I	160	GLU	N-CA-C	7.85	124.24	111.37
15	V	6	LYS	N-CA-C	-7.85	100.17	110.53
10	P	235	THR	CB-CA-C	-7.82	100.03	112.07
7	G	270	VAL	N-CA-CB	-7.80	100.71	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	74	LEU	N-CA-C	-7.79	102.79	111.28
7	G	389	THR	N-CA-CB	7.78	121.45	109.85
17	X	58	LYS	N-CA-C	-7.75	102.77	111.07
12	R	47	ARG	N-CA-C	7.75	120.71	111.33
4	D	141	TYR	CA-C-N	7.73	130.16	120.72
4	D	141	TYR	C-N-CA	7.73	130.16	120.72
21	q	44	TYR	N-CA-C	-7.71	98.87	110.28
8	H	253	GLU	N-CA-C	7.70	121.94	112.54
6	F	58	ARG	N-CA-C	-7.67	103.00	111.36
4	D	361	ALA	N-CA-C	-7.64	103.05	112.38
21	q	89	TRP	N-CA-C	-7.64	102.89	111.14
2	B	153	PRO	CB-CA-C	-7.63	98.97	111.56
4	D	83	ASN	N-CA-C	-7.62	96.85	108.67
7	G	56	VAL	N-CA-C	-7.61	103.03	110.72
7	G	569	GLN	N-CA-C	7.57	121.93	108.24
12	R	74	HIS	N-CA-C	7.54	121.12	110.50
7	G	277	MET	N-CA-C	7.53	120.67	109.59
9	I	119	CYS	N-CA-C	-7.53	103.15	111.36
7	G	467	LYS	N-CA-C	-7.51	102.24	111.33
8	H	223	PHE	CB-CA-C	-7.51	99.09	110.88
2	B	183	ARG	N-CA-C	-7.48	104.39	113.97
9	I	158	CYS	N-CA-C	-7.47	103.14	111.28
7	G	510	TRP	N-CA-CB	7.44	120.94	109.85
6	F	430	GLY	N-CA-C	7.39	121.60	112.73
7	G	303	THR	N-CA-C	7.38	123.00	113.18
4	D	350	LYS	CB-CA-C	-7.38	101.00	111.85
12	R	39	ASP	N-CA-C	7.37	121.28	110.59
15	V	57	ASP	N-CA-CB	7.36	120.68	110.01
8	H	309	ILE	N-CA-C	7.34	117.42	110.30
8	H	50	ALA	N-CA-C	7.31	118.89	111.07
7	G	384	ASN	N-CA-C	-7.30	103.35	111.82
3	C	195	HIS	CB-CA-C	7.29	117.39	110.17
13	S	94	VAL	N-CA-C	7.28	117.41	110.42
7	G	661	GLU	N-CA-C	7.28	118.90	110.97
10	P	370	LYS	N-CA-C	7.26	119.34	109.24
7	G	374	THR	CB-CA-C	-7.22	99.87	111.28
14	T	105	MET	N-CA-C	7.20	119.21	111.36
8	H	139	THR	N-CA-CB	7.18	120.42	110.01
8	H	254	LEU	N-CA-C	-7.17	103.50	111.82
7	G	461	SER	N-CA-C	7.15	119.98	111.33
7	G	497	VAL	N-CA-C	-7.13	103.35	110.62
7	G	465	VAL	N-CA-CB	7.13	118.42	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	217	GLU	N-CA-C	-7.12	101.65	110.41
6	F	73	PRO	N-CA-C	-7.11	103.87	113.40
6	F	81	LYS	N-CA-C	-7.11	103.61	111.36
15	V	68	LEU	N-CA-C	-7.10	103.55	111.28
6	F	169	LEU	N-CA-C	7.07	118.99	111.28
10	P	235	THR	CA-C-O	7.07	128.25	121.67
7	G	148	SER	N-CA-C	7.06	120.91	109.40
7	G	150	ARG	N-CA-C	7.06	119.66	109.14
6	F	455	GLN	N-CA-C	7.06	118.62	111.07
11	Q	162	ALA	N-CA-C	7.05	118.96	111.28
6	F	78	GLY	N-CA-C	-7.03	104.29	112.73
15	V	95	LEU	N-CA-C	-7.02	103.62	111.28
8	H	176	LEU	CA-C-N	-6.99	113.60	120.52
8	H	176	LEU	C-N-CA	-6.99	113.60	120.52
6	F	428	GLY	N-CA-C	-6.98	103.84	112.77
12	R	45	ARG	N-CA-C	-6.97	104.64	113.01
7	G	294	TYR	N-CA-C	-6.97	104.59	113.23
2	B	166	ASN	N-CA-C	-6.96	103.38	110.97
6	F	418	GLN	N-CA-CB	6.95	120.15	110.07
6	F	103	ASN	N-CA-CB	6.94	121.06	110.44
18	Z	34	SER	N-CA-C	-6.94	103.65	111.07
5	E	152	GLN	N-CA-C	-6.92	103.67	111.07
7	G	582	VAL	N-CA-C	6.91	118.43	108.48
16	W	87	ILE	N-CA-CB	6.91	118.63	110.55
6	F	246	GLU	N-CA-C	-6.90	103.76	111.28
8	H	292	ASN	N-CA-C	6.90	118.88	111.36
18	Z	28	ARG	N-CA-C	6.89	119.75	108.52
7	G	362	ASP	N-CA-C	6.88	125.45	110.80
7	G	300	GLN	N-CA-CB	6.87	122.46	112.08
8	H	300	LEU	N-CA-C	-6.87	104.16	112.54
6	F	148	ALA	N-CA-C	-6.87	103.88	111.36
14	T	145	VAL	N-CA-C	-6.84	103.81	110.72
7	G	268	GLY	N-CA-C	6.79	124.74	115.30
12	R	56	ASN	N-CA-C	6.78	119.96	108.90
7	G	133	GLN	N-CA-C	-6.78	101.26	110.68
8	H	305	ILE	N-CA-C	-6.76	103.44	113.39
15	V	114	TRP	N-CA-CB	6.73	120.33	110.30
6	F	244	ASN	N-CA-C	-6.72	101.02	110.50
7	G	434	SER	N-CA-C	-6.71	101.03	110.29
15	V	8	THR	N-CA-C	6.71	119.06	108.79
9	I	208	ASP	N-CA-C	6.70	121.61	113.17
8	H	8	THR	N-CA-C	-6.68	101.26	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	W	105	HIS	N-CA-C	-6.68	104.95	113.23
8	H	93	HIS	CB-CA-C	6.66	117.88	108.76
7	G	640	ASP	N-CA-CB	6.66	120.01	110.16
3	C	79	CYS	N-CA-C	-6.65	101.71	110.43
7	G	601	GLY	N-CA-C	6.65	124.88	115.30
10	P	116	ILE	N-CA-C	-6.64	104.01	110.72
3	C	125	PHE	N-CA-CB	-6.64	100.61	110.17
3	C	69	PRO	N-CA-C	-6.61	104.34	113.53
4	D	184	ILE	N-CA-C	-6.60	103.88	110.62
7	G	287	SER	N-CA-C	6.60	119.25	110.53
8	H	182	ALA	N-CA-C	-6.60	104.01	111.07
11	Q	141	ASN	N-CA-CB	6.58	120.78	110.46
15	V	86	LYS	N-CA-CB	6.58	119.60	110.07
17	X	129	THR	N-CA-C	6.57	120.75	110.17
18	Z	65	LEU	N-CA-C	-6.56	104.20	111.36
7	G	435	PRO	N-CA-C	-6.56	100.20	110.50
8	H	267	SER	N-CA-C	-6.56	104.21	111.36
2	B	97	LEU	N-CA-C	-6.54	101.46	110.35
8	H	223	PHE	N-CA-C	-6.52	104.09	111.07
4	D	388	GLY	N-CA-C	6.52	119.64	110.38
17	X	98	ARG	N-CA-C	6.51	120.48	112.54
4	D	140	ASP	N-CA-C	-6.48	96.41	107.23
7	G	605	GLN	N-CA-C	6.47	119.08	108.52
13	S	16	LEU	N-CA-C	-6.47	98.35	108.90
7	G	250	SER	N-CA-C	6.46	116.81	108.34
22	r	24	LEU	N-CA-C	6.46	119.61	110.50
8	H	255	TYR	N-CA-CB	6.45	119.36	110.01
9	I	66	LEU	N-CA-C	-6.45	104.33	111.36
8	H	177	PRO	N-CA-C	-6.42	101.56	111.13
15	V	49	GLU	N-CA-C	-6.42	104.29	111.28
12	R	81	GLY	N-CA-C	-6.41	106.88	115.21
7	G	95	PRO	N-CA-C	-6.41	101.12	110.80
3	C	125	PHE	N-CA-C	6.41	119.53	110.50
6	F	178	GLU	N-CA-CB	6.40	119.48	109.94
6	F	370	LEU	N-CA-C	-6.39	104.39	111.36
8	H	271	LEU	N-CA-CB	6.39	119.34	110.07
11	Q	59	LEU	N-CA-C	-6.39	100.72	110.30
9	I	205	ILE	N-CA-C	-6.37	104.28	110.72
7	G	273	ILE	N-CA-C	-6.36	98.36	107.77
7	G	176	CYS	N-CA-C	6.35	119.69	110.42
15	V	71	LEU	N-CA-C	6.34	118.19	111.28
21	q	28	PHE	N-CA-C	6.34	117.85	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	91	ALA	N-CA-C	-6.34	104.37	111.28
6	F	144	VAL	N-CA-CB	6.30	118.63	110.57
7	G	383	SER	N-CA-C	-6.29	106.83	114.75
17	X	99	HIS	N-CA-CB	6.29	119.46	110.16
1	A	101	GLY	N-CA-C	-6.27	105.23	112.50
11	Q	141	ASN	N-CA-C	-6.27	105.63	113.28
7	G	356	ASP	N-CA-CB	6.26	119.33	110.12
8	H	52	ALA	N-CA-CB	6.25	119.07	110.01
4	D	141	TYR	N-CA-C	6.25	120.90	113.16
4	D	233	HIS	N-CA-C	6.24	119.01	111.40
2	B	113	ASP	N-CA-CB	6.22	119.49	109.28
6	F	101	PHE	N-CA-C	6.21	118.84	111.33
21	q	69	ASN	N-CA-CB	6.19	121.32	111.66
10	P	368	GLU	N-CA-CB	6.19	119.83	110.30
13	S	61	VAL	N-CA-C	-6.19	99.57	108.42
22	r	26	LEU	N-CA-CB	-6.19	101.13	110.35
7	G	420	LYS	N-CA-C	6.18	118.81	111.33
19	a	26	ILE	N-CA-C	-6.18	104.66	113.07
7	G	451	ILE	N-CA-C	-6.17	104.97	113.00
6	F	192	ASP	N-CA-C	6.17	119.00	109.07
18	Z	69	ILE	N-CA-CB	6.17	117.36	110.51
10	P	118	LYS	N-CA-C	6.16	118.96	111.82
8	H	269	THR	N-CA-C	6.15	117.99	111.28
4	D	291	VAL	N-CA-C	-6.13	103.42	111.09
6	F	415	ILE	N-CA-C	-6.13	104.37	110.62
7	G	418	ILE	N-CA-C	-6.12	103.47	112.04
6	F	212	LEU	N-CA-C	-6.12	104.61	111.28
7	G	325	ARG	N-CA-CB	6.10	118.82	109.91
8	H	185	TRP	N-CA-C	-6.09	103.99	112.45
8	H	7	LEU	N-CA-C	-6.07	104.30	111.03
8	H	276	SER	N-CA-C	6.06	118.85	111.82
13	S	87	VAL	N-CA-C	-6.06	104.44	110.62
7	G	353	ALA	N-CA-C	-6.05	104.60	112.23
8	H	103	LEU	N-CA-C	-6.03	104.79	111.36
7	G	508	ALA	N-CA-C	6.02	117.84	111.28
8	H	24	GLU	N-CA-C	-6.01	104.09	112.45
22	r	108	LYS	N-CA-C	6.01	117.92	111.36
7	G	638	THR	N-CA-C	-6.00	100.19	109.24
18	Z	65	LEU	N-CA-CB	6.00	119.03	110.16
17	X	38	LYS	N-CA-C	-5.99	104.66	111.07
18	Z	72	MET	CA-C-N	-5.99	113.01	119.24
18	Z	72	MET	C-N-CA	-5.99	113.01	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	196	PRO	N-CA-C	-5.97	101.84	111.03
7	G	387	LEU	CB-CA-C	-5.92	101.73	111.68
18	Z	44	ILE	N-CA-C	-5.92	104.74	110.42
17	X	97	PHE	N-CA-C	5.91	118.67	111.82
6	F	291	GLU	N-CA-C	5.91	118.17	110.43
9	I	116	CYS	N-CA-C	-5.90	105.57	112.89
14	T	94	ASP	N-CA-CB	-5.89	105.12	111.66
6	F	127	ASP	N-CA-C	5.88	118.47	111.71
8	H	116	ILE	N-CA-C	-5.87	104.78	110.42
10	P	122	HIS	N-CA-C	5.87	120.14	112.92
6	F	255	CYS	N-CA-C	-5.85	104.49	111.69
13	S	86	GLU	N-CA-CB	5.85	118.81	110.16
8	H	315	PRO	O-C-N	5.84	123.90	121.15
15	V	19	THR	N-CA-CB	5.83	120.76	110.37
7	G	639	LEU	N-CA-C	5.83	118.58	111.82
7	G	672	ALA	N-CA-C	-5.82	104.93	111.28
21	q	65	THR	N-CA-C	5.82	119.17	110.14
3	C	209	LEU	N-CA-CB	-5.82	100.71	110.83
6	F	102	MET	CB-CA-C	-5.82	101.34	110.94
2	B	135	GLY	CA-C-O	-5.81	117.93	122.52
10	P	367	GLU	CB-CA-C	-5.80	99.53	110.67
21	q	7	LEU	N-CA-C	-5.80	104.87	111.07
7	G	480	ALA	N-CA-C	-5.79	105.05	111.36
11	Q	164	PHE	N-CA-CB	5.79	119.81	110.42
17	X	36	CYS	CB-CA-C	-5.78	102.55	111.74
4	D	258	VAL	N-CA-C	-5.78	104.03	110.62
4	D	414	ASP	N-CA-C	-5.77	101.42	110.36
4	D	352	PRO	N-CA-C	5.75	117.72	110.70
12	R	34	THR	N-CA-C	-5.74	106.88	112.97
10	P	234	LYS	CB-CA-C	-5.74	103.42	111.80
1	A	105	GLU	N-CA-C	-5.74	105.03	111.28
5	E	119	THR	N-CA-C	-5.72	105.79	112.89
12	R	35	GLY	N-CA-C	5.71	121.82	113.48
7	G	289	LYS	N-CA-C	5.71	117.50	111.28
10	P	119	ALA	N-CA-C	-5.70	104.98	111.14
13	S	73	GLN	N-CA-C	-5.70	100.41	109.59
6	F	299	LEU	N-CA-C	5.70	118.43	111.82
8	H	252	PRO	N-CA-CB	-5.69	98.05	103.51
6	F	393	ASN	N-CA-C	-5.69	104.98	111.07
11	Q	124	MET	CA-C-N	-5.68	114.91	122.98
11	Q	124	MET	C-N-CA	-5.68	114.91	122.98
6	F	176	ALA	N-CA-C	5.68	118.20	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	272	LEU	N-CA-C	-5.68	101.88	110.28
7	G	540	ASN	CA-C-N	-5.68	114.53	120.38
7	G	540	ASN	C-N-CA	-5.68	114.53	120.38
7	G	59	GLN	N-CA-C	5.66	118.01	107.99
8	H	126	LYS	N-CA-C	5.66	117.45	111.28
6	F	457	HIS	N-CA-CB	-5.65	100.89	110.50
9	I	191	LEU	N-CA-C	-5.64	105.22	111.36
17	X	40	ASN	N-CA-C	-5.63	104.83	110.97
6	F	416	SER	N-CA-C	5.63	117.87	111.11
12	R	52	GLN	N-CA-C	5.62	117.95	110.53
7	G	599	THR	CA-C-N	-5.62	114.18	122.83
7	G	599	THR	C-N-CA	-5.62	114.18	122.83
6	F	304	ALA	CB-CA-C	-5.62	110.08	116.54
8	H	76	THR	N-CA-C	-5.61	104.54	111.33
2	B	112	TYR	N-CA-C	5.61	122.75	110.80
21	q	142	THR	N-CA-CB	5.59	119.91	109.68
18	Z	64	ASP	N-CA-C	5.59	119.82	112.89
2	B	201	LEU	N-CA-C	-5.57	105.11	111.07
22	r	94	ALA	N-CA-C	-5.57	101.61	109.96
5	E	183	PRO	N-CA-C	-5.56	102.19	111.26
7	G	530	TYR	N-CA-C	-5.55	102.06	110.28
7	G	615	LEU	N-CA-C	-5.55	106.28	113.16
21	q	68	MET	N-CA-C	5.55	119.31	112.54
6	F	294	VAL	CA-C-N	-5.54	114.05	119.76
6	F	294	VAL	C-N-CA	-5.54	114.05	119.76
6	F	118	ASP	N-CA-C	-5.53	102.09	110.28
4	D	200	PHE	CA-CB-CG	5.52	119.32	113.80
19	a	25	TYR	N-CA-C	-5.51	107.80	114.75
4	D	132	ALA	N-CA-C	-5.50	106.56	113.72
10	P	86	CYS	N-CA-C	-5.48	103.15	110.55
7	G	313	LEU	N-CA-C	5.48	118.49	109.72
21	q	71	LYS	N-CA-C	5.48	119.95	113.16
7	G	363	SER	N-CA-C	-5.47	100.27	109.07
2	B	98	ALA	CB-CA-C	-5.46	108.68	115.89
7	G	127	ASP	CA-C-O	5.46	128.93	121.89
8	H	141	SER	N-CA-CB	5.45	117.92	110.01
18	Z	50	MET	N-CA-C	-5.45	105.34	111.28
7	G	404	GLY	N-CA-C	5.44	121.42	113.48
4	D	141	TYR	N-CA-CB	-5.43	102.13	110.44
4	D	231	GLY	N-CA-C	-5.43	103.09	110.43
7	G	150	ARG	N-CA-CB	-5.43	102.82	111.62
14	T	135	ALA	N-CA-CB	5.41	118.08	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	27	ALA	N-CA-C	-5.40	105.05	111.69
7	G	682	ASP	CA-C-N	-5.39	114.21	119.76
7	G	682	ASP	C-N-CA	-5.39	114.21	119.76
7	G	420	LYS	N-CA-CB	-5.39	101.98	110.06
14	T	92	LYS	N-CA-C	-5.38	106.30	112.92
4	D	391	VAL	CA-C-N	-5.38	115.79	119.66
4	D	391	VAL	C-N-CA	-5.38	115.79	119.66
10	P	374	THR	N-CA-C	5.38	117.49	108.73
7	G	510	TRP	N-CA-C	-5.37	101.91	109.96
5	E	48	PRO	N-CA-C	5.36	120.81	113.84
11	Q	163	ASN	CB-CA-C	-5.35	99.30	109.95
6	F	199	ARG	N-CA-C	5.34	117.44	109.59
8	H	94	PRO	N-CA-C	5.33	118.68	111.22
7	G	362	ASP	CA-CB-CG	5.33	117.92	112.60
18	Z	55	GLN	N-CA-C	-5.32	105.48	111.28
4	D	201	PHE	N-CA-C	-5.32	105.56	111.36
8	H	284	GLN	N-CA-C	-5.31	105.57	111.36
8	H	310	PHE	N-CA-C	5.31	119.38	113.01
10	P	339	GLY	N-CA-C	5.31	122.64	115.00
8	H	252	PRO	CA-N-CD	5.30	119.43	112.00
21	q	131	ARG	N-CA-C	5.29	117.66	110.35
9	I	54	THR	N-CA-C	-5.29	104.93	111.33
11	Q	164	PHE	N-CA-C	-5.29	106.80	113.20
9	I	160	GLU	N-CA-CB	-5.28	100.74	109.72
5	E	74	GLN	N-CA-C	-5.28	107.50	114.04
22	r	25	GLN	N-CA-C	5.26	118.96	112.54
17	X	33	GLY	N-CA-C	-5.26	107.80	114.16
15	V	84	ALA	N-CA-C	5.25	116.69	111.07
6	F	300	ILE	N-CA-CB	5.25	119.33	110.56
11	Q	72	ILE	N-CA-C	-5.24	108.39	113.53
21	q	6	VAL	CB-CA-C	-5.24	105.06	112.14
7	G	63	PHE	CA-C-O	-5.24	114.98	121.06
7	G	600	GLU	CB-CA-C	-5.23	102.95	111.06
4	D	363	VAL	N-CA-C	5.23	116.31	111.81
7	G	435	PRO	CB-CA-C	-5.23	105.86	111.56
7	G	356	ASP	N-CA-C	-5.23	105.58	111.28
13	S	85	ASP	N-CA-C	5.23	117.89	111.82
5	E	48	PRO	CB-CA-C	-5.23	104.43	111.85
7	G	277	MET	N-CA-CB	-5.23	101.66	109.71
8	H	46	LEU	N-CA-C	-5.22	106.68	113.16
10	P	260	GLY	N-CA-C	-5.22	108.41	115.36
3	C	164	TRP	N-CA-C	5.22	117.05	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	q	21	ARG	N-CA-C	5.21	117.63	111.33
22	r	107	SER	N-CA-C	-5.21	102.15	109.96
8	H	146	MET	N-CA-C	-5.20	105.50	111.07
8	H	101	GLY	N-CA-C	5.20	118.53	112.50
10	P	316	LYS	N-CA-C	-5.19	104.89	111.11
4	D	391	VAL	N-CA-C	5.18	113.84	109.02
10	P	194	VAL	N-CA-CB	5.18	118.35	110.58
1	A	2	ASN	CA-C-N	-5.17	112.95	120.29
1	A	2	ASN	C-N-CA	-5.17	112.95	120.29
7	G	556	THR	N-CA-C	-5.17	101.55	109.41
7	G	713	ALA	N-CA-C	-5.17	105.54	111.07
10	P	198	ALA	N-CA-C	-5.17	100.10	108.52
7	G	172	ILE	N-CA-C	-5.16	98.61	109.34
7	G	458	GLY	N-CA-C	-5.15	108.22	115.32
16	W	91	MET	N-CA-C	-5.13	105.86	111.82
8	H	277	TYR	N-CA-C	5.13	117.95	110.10
3	C	156	VAL	N-CA-C	-5.13	104.10	111.17
22	r	110	GLN	CA-C-N	-5.13	113.64	118.97
22	r	110	GLN	C-N-CA	-5.13	113.64	118.97
20	b	82	LYS	N-CA-C	-5.12	103.77	110.53
7	G	569	GLN	CB-CA-C	-5.12	104.26	112.05
5	E	181	ASN	N-CA-C	-5.11	99.46	108.20
7	G	387	LEU	N-CA-C	-5.11	98.37	107.98
23	s	38	HIS	N-CA-C	5.11	118.61	112.38
8	H	196	ALA	CA-C-N	-5.11	113.50	119.32
8	H	196	ALA	C-N-CA	-5.11	113.50	119.32
21	q	5	GLU	N-CA-C	5.11	116.53	111.07
6	F	60	GLY	N-CA-C	-5.10	106.01	114.48
2	B	98	ALA	N-CA-C	5.10	117.59	109.02
3	C	109	SER	N-CA-C	5.09	118.11	109.76
7	G	393	GLY	N-CA-C	-5.09	107.72	115.66
5	E	166	LYS	N-CA-C	-5.08	104.63	111.54
17	X	112	LEU	N-CA-CB	5.08	117.44	110.07
9	I	95	PRO	N-CA-C	5.08	121.17	113.81
7	G	280	ASP	N-CA-CB	-5.08	102.66	110.12
8	H	254	LEU	N-CA-CB	5.08	118.15	110.28
3	C	221	GLU	N-CA-C	-5.07	102.37	108.25
21	q	140	PRO	N-CA-C	-5.07	102.28	110.55
4	D	224	ALA	N-CA-C	5.07	117.19	111.11
17	X	140	ASN	CA-C-N	-5.06	114.56	119.78
17	X	140	ASN	C-N-CA	-5.06	114.56	119.78
10	P	376	ASN	CB-CA-C	-5.06	102.25	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	170	LEU	N-CA-C	5.05	117.05	110.43
18	Z	130	LYS	N-CA-C	-5.05	105.67	111.07
12	R	43	TYR	N-CA-CB	-5.04	103.19	110.70
9	I	160	GLU	CB-CA-C	5.03	119.19	110.84
4	D	224	ALA	CA-C-O	-5.02	115.53	120.90
14	T	140	CYS	N-CA-C	5.02	116.67	109.04
14	T	140	CYS	CB-CA-C	-5.02	104.13	109.85
3	C	208	GLU	CA-C-O	-5.01	115.74	121.40
8	H	193	THR	N-CA-C	-5.00	106.48	112.59

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	762	0	823	79	0
2	B	1247	0	1258	156	0
3	C	1641	0	1596	137	0
4	D	3080	0	3053	342	0
5	E	1635	0	1626	176	0
6	F	3288	0	3243	344	0
7	G	5287	0	5323	547	0
8	H	2495	0	2582	341	0
9	I	1398	0	1359	169	0
10	P	2730	0	2747	228	0
11	Q	957	0	949	81	0
12	R	660	0	639	87	0
13	S	667	0	683	71	0
14	T	604	0	596	89	0
15	V	915	0	954	83	0
16	W	970	0	991	88	0
17	X	1164	0	1154	116	0
18	Z	1152	0	1148	145	0
19	a	540	0	550	49	0
20	b	620	0	617	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	q	1004	0	962	80	0
22	r	413	0	429	40	0
23	s	226	0	214	13	0
24	A	46	0	69	11	0
24	I	29	0	32	8	0
25	B	8	0	0	5	0
25	F	8	0	0	11	0
25	G	16	0	0	7	0
25	I	16	0	0	16	0
26	E	4	0	0	5	0
26	G	4	0	0	5	0
27	F	31	0	19	4	0
28	H	35	0	43	18	0
29	P	48	0	26	4	0
30	R	1	0	0	0	0
31	W	32	0	0	7	0
All	All	33733	0	33685	2995	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 44.

All (2995) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:142:VAL:HG21	4:D:185:MET:SD	1.68	1.34
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.28
4:D:142:VAL:CG2	4:D:185:MET:SD	2.23	1.25
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.21
10:P:93:HIS:CD2	10:P:94:LEU:HD12	1.75	1.21
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.17
15:V:44:TYR:CE1	15:V:48:THR:HG21	1.77	1.17
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.40	1.17
8:H:251:LEU:HD12	8:H:251:LEU:O	1.41	1.16
6:F:382:CYS:SG	25:F:502:SF4:FE3	1.38	1.13
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.12
9:I:123:CYS:SG	25:I:302:SF4:FE1	1.40	1.11
6:F:379:CYS:SG	25:F:502:SF4:FE4	1.43	1.09
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.09
12:R:88:HIS:HB2	12:R:89:PRO:HD2	1.08	1.08
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.08
13:S:23:LEU:HD12	13:S:23:LEU:O	1.54	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:4:ILE:HG22	17:X:5:VAL:H	0.96	1.08
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.31	1.07
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.27	1.07
11:Q:160:TYR:CZ	11:Q:164:PHE:HZ	1.72	1.07
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.07
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.06
12:R:88:HIS:CB	12:R:89:PRO:HD2	1.84	1.06
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.06
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.06
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.06
4:D:86:PRO:HD2	4:D:87:GLN:OE1	1.56	1.05
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.38	1.05
15:V:44:TYR:CE1	15:V:48:THR:CG2	2.39	1.05
2:B:82:ILE:HG23	8:H:57:MET:SD	1.97	1.05
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.33	1.05
9:I:152:CYS:SG	25:I:302:SF4:FE2	1.46	1.05
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.04
3:C:102:HIS:HE1	15:V:48:THR:HG22	1.22	1.04
6:F:266:GLY:CA	6:F:271:SER:HA	1.86	1.04
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.04
14:T:138:LEU:HD12	14:T:138:LEU:O	1.55	1.04
9:I:208:ASP:O	9:I:208:ASP:OD1	1.75	1.04
5:E:179:CYS:SG	26:E:301:FES:FE2	1.48	1.03
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.22	1.03
8:H:142:TYR:CD1	8:H:289:LEU:HD12	1.94	1.03
7:G:401:LEU:HD11	7:G:466:LEU:HD21	1.40	1.03
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.92	1.03
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.02
16:W:32:LYS:HG2	31:W:201:EHZ:C19	1.90	1.02
21:q:66:THR:HG22	21:q:74:PHE:HB2	1.39	1.02
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.02
11:Q:160:TYR:CZ	11:Q:164:PHE:CZ	2.49	1.01
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.96	1.00
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.86	1.00
9:I:155:CYS:SG	25:I:302:SF4:FE4	1.52	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.00
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	1.00
2:B:105:MET:HE2	4:D:200:PHE:HE2	1.24	1.00
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:266:GLY:HA3	6:F:271:SER:CA	1.90	0.99
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.99
15:V:44:TYR:CZ	15:V:48:THR:HG21	1.97	0.99
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	0.99
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.99
2:B:82:ILE:HG12	8:H:57:MET:CE	1.93	0.98
8:H:93:HIS:CD2	19:a:27:HIS:HD1	1.80	0.97
8:H:249:ILE:HD13	17:X:99:HIS:CG	1.98	0.97
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.97
17:X:4:ILE:HG22	17:X:5:VAL:N	1.77	0.97
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.78	0.97
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.97
9:I:152:CYS:HG	25:I:302:SF4:FE2	0.70	0.97
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.97
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.97
13:S:16:LEU:HD11	13:S:51:LEU:HD11	1.46	0.97
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.47	0.97
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.97
10:P:376:ASN:OD1	10:P:377:TYR:N	1.98	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
16:W:55:LEU:HB3	16:W:107:MET:CE	1.94	0.96
7:G:92:CYS:SG	26:G:803:FES:S1	2.62	0.96
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.96
12:R:38:TYR:HE2	21:q:127:TYR:HB2	1.30	0.96
5:E:240:PRO:HA	6:F:60:GLY:HA3	1.44	0.96
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	0.96
6:F:379:CYS:HG	25:F:502:SF4:FE4	0.73	0.96
11:Q:160:TYR:CE2	11:Q:164:PHE:CE2	2.53	0.96
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.96
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.96
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.96
2:B:100:CYS:SG	25:B:301:SF4:FE4	1.59	0.95
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.95
8:H:249:ILE:HG21	17:X:99:HIS:CE1	2.00	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.95
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.95
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.95
5:E:179:CYS:HG	26:E:301:FES:FE2	0.74	0.95
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.95
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:88:HIS:HB2	12:R:89:PRO:CD	1.97	0.94
8:H:224:PHE:CE2	28:H:400:UQ9:H13	2.02	0.94
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.32	0.94
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.44	0.94
4:D:142:VAL:HG22	4:D:185:MET:SD	2.03	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	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
9:I:113:CYS:SG	25:I:303:SF4:FE3	1.59	0.94
11:Q:160:TYR:CE2	11:Q:164:PHE:HE2	1.86	0.94
10:P:333:PRO:HB2	10:P:337:ASP:HB2	1.47	0.94
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.93
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.93
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.93
15:V:75:GLY:HA2	22:r:103:ARG:HD2	1.51	0.93
10:P:93:HIS:CD2	10:P:94:LEU:CD1	2.52	0.92
22:r:9:GLN:HA	22:r:12:ARG:HD3	1.50	0.92
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.92
6:F:128:ARG:HA	6:F:131:MET:HE2	1.49	0.92
17:X:53:PRO:HD2	18:Z:116:TRP:CD1	2.03	0.92
17:X:4:ILE:CG2	17:X:5:VAL:H	1.82	0.91
4:D:86:PRO:HB3	4:D:96:ARG:HG2	1.51	0.91
10:P:262:THR:H	10:P:332:LEU:HD12	1.34	0.91
16:W:55:LEU:HB3	16:W:107:MET:HE1	1.52	0.91
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.91
18:Z:86:ILE:HG23	18:Z:128:ARG:HE	1.33	0.91
6:F:382:CYS:HG	25:F:502:SF4:FE3	0.63	0.90
7:G:176:CYS:HG	25:G:802:SF4:FE4	0.62	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
7:G:226:CYS:HG	25:G:802:SF4:FE1	0.70	0.90
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.89
10:P:93:HIS:NE2	10:P:94:LEU:CD1	2.35	0.89
10:P:192:ARG:HH22	10:P:198:ALA:HB3	1.35	0.89
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.34	0.89
6:F:110:PRO:HB3	6:F:152:ARG:CZ	2.03	0.89
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.86	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
13:S:16:LEU:HD22	13:S:19:ILE:HD11	1.53	0.89
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.89
10:P:96:LEU:HD12	10:P:97:MET:N	1.88	0.89
6:F:266:GLY:HA3	6:F:271:SER:HA	0.94	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
17:X:29:ALA:HB2	18:Z:71:LEU:HD11	1.54	0.88
7:G:32:ILE:HG23	7:G:98:LYS:HD2	1.54	0.88
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.88
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.88
7:G:97:MET:HB2	7:G:100:TRP:CD1	2.09	0.88
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.88
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.55	0.88
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.09	0.88
20:b:60:ASP:OD1	20:b:61:GLY:N	2.07	0.88
2:B:81:LEU:HG	8:H:53:MET:HE1	1.53	0.87
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.88	0.87
14:T:79:ILE:HB	14:T:145:VAL:HG13	1.55	0.87
6:F:292:MET:HG2	6:F:338:ASP:OD1	1.75	0.87
6:F:425:CYS:HG	25:F:502:SF4:FE1	0.60	0.87
13:S:16:LEU:HD12	13:S:16:LEU:O	1.76	0.86
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.86
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.86
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.86
7:G:78:CYS:SG	26:G:803:FES:FE2	1.68	0.86
6:F:300:ILE:HD13	6:F:307:VAL:H	1.41	0.86
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.86
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.86
16:W:55:LEU:HD22	16:W:107:MET:HE2	1.57	0.86
9:I:162:CYS:SG	25:I:303:SF4:FE4	1.68	0.85
6:F:44:ASN:HD21	6:F:51:TRP:HA	1.41	0.85
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.56	0.85
10:P:192:ARG:NH2	10:P:198:ALA:HB3	1.92	0.85
7:G:78:CYS:HG	26:G:803:FES:FE2	0.57	0.85
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.85
12:R:32:THR:HG22	12:R:36:GLN:H	1.40	0.85
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.59	0.85
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.85
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.59	0.85
4:D:266:ARG:HB2	9:I:65:GLU:OE2	1.77	0.85
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.95	0.85
8:H:224:PHE:CE2	28:H:400:UQ9:C13	2.60	0.85
2:B:105:MET:CE	4:D:200:PHE:HE2	1.90	0.84
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.84
15:V:56:LEU:HD12	15:V:57:ASP:N	1.92	0.84
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.07	0.84
9:I:54:THR:HG21	18:Z:33:TYR:CZ	2.13	0.84
12:R:38:TYR:CE2	21:q:127:TYR:HB2	2.13	0.84
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.84
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.84
7:G:126:LEU:CD1	12:R:89:PRO:HB2	2.07	0.84
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.84
10:P:206:ILE:H	29:P:401:NDP:H71N	1.25	0.83
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
4:D:92:HIS:HB3	4:D:458:PHE:HE2	1.43	0.83
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.83
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.83
2:B:89:SER:O	8:H:54:LYS:HD3	1.79	0.82
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.79	0.82
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.92	0.82
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.82
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.60	0.82
8:H:249:ILE:HD13	17:X:99:HIS:ND1	1.93	0.82
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.82
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.45	0.82
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.61	0.82
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.82
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.62	0.81
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.81
6:F:117:ALA:HB1	6:F:131:MET:SD	2.19	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
2:B:105:MET:HE2	4:D:200:PHE:CE2	2.14	0.81
3:C:217:ARG:NH1	16:W:112:GLU:HB2	1.95	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.81
8:H:251:LEU:O	8:H:251:LEU:CD1	2.27	0.81
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.63	0.81
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.96	0.81
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.81
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:401:LEU:CD1	7:G:466:LEU:HD21	2.09	0.81
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.11	0.81
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.81
16:W:55:LEU:CD2	16:W:107:MET:HE2	2.09	0.81
1:A:25:PRO:HG3	8:H:60:PRO:HD3	1.63	0.81
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.81
13:S:36:PHE:HZ	13:S:44:LEU:HD11	1.45	0.81
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.46	0.81
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.80
14:T:113:LEU:HD22	16:W:71:MET:HE2	1.63	0.80
17:X:130:LYS:HE3	20:b:67:PRO:HB3	1.61	0.80
4:D:348:LEU:O	18:Z:11:PRO:HB3	1.81	0.80
21:q:71:LYS:O	21:q:72:ASN:OD1	1.99	0.80
3:C:102:HIS:CE1	15:V:48:THR:HG22	2.14	0.80
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.63	0.80
8:H:181:MET:CE	8:H:304:HIS:ND1	2.45	0.80
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.80
12:R:51:ARG:HH21	21:q:125:VAL:HG12	1.44	0.80
6:F:342:LEU:HB3	6:F:347:THR:HG23	1.63	0.80
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.80
9:I:162:CYS:HG	25:I:303:SF4:FE4	0.51	0.80
13:S:20:ARG:HG3	13:S:54:LEU:HB2	1.64	0.80
6:F:174:ARG:HA	23:s:52:LEU:HD21	1.64	0.79
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.79
8:H:142:TYR:OH	8:H:288:LEU:HD22	1.82	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.65	0.79
14:T:93:ILE:HG21	14:T:110:LEU:HD22	1.63	0.79
2:B:89:SER:O	8:H:54:LYS:CD	2.29	0.79
16:W:42:TRP:CZ2	16:W:93:LEU:HB2	2.16	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
7:G:73:GLY:HA2	26:G:803:FES:S1	2.21	0.79
4:D:280:ALA:CB	15:V:11:LEU:HG	2.13	0.79
21:q:55:PHE:CD1	22:r:26:LEU:HD22	2.17	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.23	0.79
20:b:66:VAL:HG13	20:b:72:ASP:HB2	1.65	0.79
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.78
18:Z:69:ILE:HG23	20:b:54:PRO:HD3	1.65	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.66	0.78
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.65	0.78
14:T:87:LEU:HD21	14:T:104:PHE:HZ	1.47	0.78
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.78
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.18	0.78
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.65	0.78
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.65	0.78
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
17:X:130:LYS:CE	20:b:67:PRO:HB3	2.12	0.78
4:D:260:GLU:HG3	18:Z:25:LEU:HD22	1.66	0.78
4:D:259:GLU:HB3	18:Z:25:LEU:HD11	1.64	0.78
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.78
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.63	0.78
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.78
14:T:87:LEU:HD22	14:T:104:PHE:CE1	2.19	0.78
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.77
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
5:E:178:ALA:HA	6:F:125:CYS:SG	2.24	0.77
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.77
2:B:96:GLY:HA2	2:B:101:ALA:HB2	1.67	0.77
8:H:17:MET:SD	8:H:229:THR:OG1	2.41	0.77
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.67	0.77
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
14:T:83:VAL:CG2	14:T:126:PHE:HZ	1.97	0.77
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.77
9:I:113:CYS:HG	25:I:303:SF4:FE3	0.49	0.77
8:H:91:MET:O	8:H:92:PRO:C	2.26	0.77
18:Z:58:ARG:NH2	20:b:49:THR:HG21	1.99	0.77
3:C:217:ARG:HH12	16:W:112:GLU:HB2	1.50	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.77
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.50	0.77
21:q:9:ARG:HA	21:q:12:GLN:HG2	1.65	0.77
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.76
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.00	0.76
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.76
16:W:42:TRP:CD2	16:W:93:LEU:HD12	2.21	0.76
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:TYR:OH	9:I:91:GLY:CA	2.29	0.76
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.76
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.76
17:X:20:VAL:HG22	17:X:24:VAL:HG21	1.66	0.76
3:C:102:HIS:HE1	15:V:48:THR:CG2	1.99	0.76
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
13:S:51:LEU:HD13	13:S:95:LEU:HD21	1.68	0.76
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.76
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.13	0.76
12:R:89:PRO:HG3	12:R:106:TYR:CE1	2.20	0.76
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.76
14:T:93:ILE:HG23	14:T:110:LEU:HD13	1.66	0.76
4:D:271:ARG:HD2	8:H:279:ARG:O	1.86	0.75
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.75
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.75
10:P:336:GLU:HG3	10:P:342:PRO:HD3	1.67	0.75
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.75
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.50	0.75
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.75
14:T:117:GLU:HA	14:T:120:MET:HE3	1.67	0.75
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.67	0.75
13:S:19:ILE:HG13	13:S:95:LEU:HD11	1.69	0.75
16:W:55:LEU:HB3	16:W:107:MET:HE2	1.66	0.75
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
7:G:632:ILE:HG13	7:G:632:ILE:O	1.84	0.75
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.75
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.67	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.79	0.75
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.75
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.75
5:E:189:ASP:CG	6:F:163:TYR:HB3	2.11	0.75
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.68	0.75
10:P:143:ASP:HA	10:P:147:ASN:HB2	1.67	0.75
14:T:94:ASP:HB3	14:T:98:LEU:HB2	1.68	0.75
4:D:92:HIS:HB3	4:D:458:PHE:CE2	2.21	0.75
11:Q:167:ASN:O	11:Q:168:LYS:CD	2.35	0.75
16:W:28:LEU:HG	16:W:32:LYS:HE3	1.69	0.75
2:B:89:SER:O	8:H:54:LYS:HE2	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:31:ILE:HA	20:b:34:MET:HE2	1.69	0.74
7:G:651:PRO:HG3	13:S:57:GLU:H	1.51	0.74
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.74
9:I:123:CYS:HG	25:I:302:SF4:FE1	0.44	0.74
11:Q:160:TYR:CD2	11:Q:164:PHE:HE2	2.03	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.87	0.74
1:A:4:TYR:CE2	24:A:401:3PE:H231	2.22	0.74
6:F:210:THR:HB	6:F:224:ARG:HB2	1.70	0.74
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.74
7:G:674:LEU:HD11	13:S:46:LYS:HE2	1.69	0.74
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.70	0.74
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.74
17:X:123:GLY:HA2	18:Z:66:GLU:OE2	1.86	0.74
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.28	0.74
14:T:88:LYS:HG3	14:T:98:LEU:HD22	1.70	0.74
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.03	0.74
18:Z:93:GLU:O	18:Z:97:ILE:HG13	1.88	0.74
5:E:240:PRO:HG3	6:F:57:LEU:O	1.88	0.74
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.74
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.88	0.74
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.69	0.74
5:E:232:SER:HB3	6:F:288:VAL:HG23	1.69	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.27	0.74
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.74
2:B:91:TRP:CZ3	28:H:400:UQ9:H1M	2.22	0.74
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.68	0.73
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.67	0.73
4:D:87:GLN:HG2	4:D:87:GLN:O	1.88	0.73
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.73
14:T:103:HIS:CG	14:T:106:LYS:HD2	2.23	0.73
17:X:29:ALA:CB	18:Z:71:LEU:HD11	2.18	0.73
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.71	0.73
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.73
16:W:32:LYS:HE2	31:W:201:EHZ:C19	2.18	0.73
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.73
17:X:33:GLY:CA	18:Z:70:ALA:HB1	2.19	0.73
18:Z:65:LEU:O	18:Z:69:ILE:HG12	1.89	0.73
5:E:39:VAL:HG11	7:G:163:LYS:NZ	2.04	0.73
10:P:169:HIS:H	10:P:184:LYS:HE3	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:69:HIS:HD2	20:b:70:PRO:HD2	1.54	0.73
21:q:56:PHE:HA	21:q:59:HIS:CD2	2.24	0.73
17:X:33:GLY:HA3	18:Z:70:ALA:HB1	1.70	0.73
1:A:21:ALA:O	1:A:25:PRO:HD3	1.88	0.72
4:D:375:MET:HE1	7:G:126:LEU:HA	1.71	0.72
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
11:Q:167:ASN:O	11:Q:168:LYS:HD2	1.88	0.72
14:T:120:MET:HG2	16:W:44:ARG:HH11	1.54	0.72
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.24	0.72
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.72
7:G:176:CYS:SG	25:G:802:SF4:FE4	1.78	0.72
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.72
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.72
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.54	0.72
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.72
12:R:89:PRO:CG	12:R:106:TYR:CZ	2.72	0.72
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.72
21:q:56:PHE:HD1	21:q:59:HIS:HE2	1.35	0.72
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.70	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.20	0.72
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.69	0.72
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.72
9:I:200:GLU:OE2	21:q:93:MET:SD	2.48	0.72
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.72
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.72
12:R:89:PRO:HG3	12:R:106:TYR:CZ	2.23	0.72
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.71	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.71
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.24	0.71
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.55	0.71
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.71
16:W:101:LYS:NZ	16:W:109:PHE:CE2	2.58	0.71
4:D:266:ARG:CB	9:I:65:GLU:OE2	2.39	0.71
4:D:338:ARG:NH1	18:Z:23:ARG:HA	2.05	0.71
7:G:127:ASP:HA	12:R:106:TYR:OH	1.90	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.71
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
10:P:192:ARG:NH1	10:P:192:ARG:HA	2.05	0.71
5:E:240:PRO:CA	6:F:60:GLY:HA3	2.20	0.71
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.71
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.55	0.71
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.26	0.71
9:I:155:CYS:HG	25:I:302:SF4:FE4	1.08	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.73	0.70
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.70
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.56	0.70
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.73	0.70
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.55	0.70
7:G:64:CYS:SG	26:G:803:FES:FE1	1.83	0.70
12:R:67:GLN:HG2	12:R:109:LEU:CD2	2.21	0.70
17:X:7:LEU:O	18:Z:88:ARG:NH1	2.24	0.70
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.70
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.21	0.70
8:H:113:VAL:HG22	8:H:136:VAL:HG23	1.72	0.70
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.74	0.70
2:B:108:ALA:HA	2:B:114:MET:HG2	1.72	0.70
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	0.70
5:E:237:PRO:HG3	6:F:49:HIS:CD2	2.27	0.70
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.70
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.70
10:P:170:LEU:O	10:P:171:ASN:OD1	2.09	0.70
10:P:191:VAL:HA	10:P:194:VAL:HG22	1.73	0.70
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.27	0.70
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	2.06	0.70
18:Z:86:ILE:HG23	18:Z:128:ARG:NE	2.06	0.70
16:W:32:LYS:CG	31:W:201:EHZ:C19	2.69	0.70
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.74	0.70
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.70
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.70
15:V:56:LEU:HD12	15:V:56:LEU:C	2.16	0.70
21:q:3:LEU:HD12	21:q:6:VAL:CG2	2.22	0.70
2:B:89:SER:O	8:H:54:LYS:CE	2.40	0.69
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.69
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.69
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.74	0.69
2:B:95:PHE:HE2	2:B:131:MET:SD	2.15	0.69
4:D:253:LEU:HB2	22:r:23:LYS:CD	2.22	0.69
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.21	0.69
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.73	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
2:B:116:ARG:O	8:H:39:ILE:HG22	1.91	0.69
6:F:314:LEU:HB3	6:F:329:LYS:HD3	1.73	0.69
9:I:92:PRO:HA	21:q:91:HIS:O	1.93	0.69
14:T:100:VAL:HB	14:T:142:GLN:HB2	1.74	0.69
2:B:82:ILE:HA	8:H:57:MET:HE1	1.74	0.69
2:B:136:THR:HG21	2:B:177:VAL:HG22	1.73	0.69
3:C:107:PHE:CD1	3:C:133:SER:HB2	2.28	0.69
14:T:87:LEU:HD22	14:T:104:PHE:HE1	1.58	0.69
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.69
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.28	0.69
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.69
8:H:85:LEU:HD21	8:H:108:THR:HB	1.74	0.69
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.69
15:V:116:ILE:HG23	15:V:116:ILE:O	1.92	0.69
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.69
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.75	0.69
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.08	0.69
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.75	0.69
10:P:171:ASN:OD1	10:P:171:ASN:O	2.11	0.69
17:X:124:GLN:O	20:b:70:PRO:HB2	1.92	0.69
22:r:20:LEU:C	22:r:20:LEU:HD12	2.18	0.69
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.68
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.68
8:H:42:PRO:HD2	8:H:45:ILE:HG12	1.74	0.68
8:H:224:PHE:CZ	28:H:400:UQ9:H13	2.28	0.68
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.68
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.75	0.68
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.68
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:93:HIS:NE2	19:a:27:HIS:ND1	2.40	0.68
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.74	0.68
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.68
17:X:50:GLU:HG3	17:X:56:CYS:SG	2.33	0.68
2:B:94:THR:HB	2:B:104:MET:HE1	1.74	0.68
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.68
7:G:226:CYS:SG	25:G:802:SF4:FE1	1.82	0.68
8:H:33:LEU:HD23	22:r:25:GLN:HG2	1.76	0.68
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.23	0.68
14:T:138:LEU:HD13	14:T:144:ILE:CG1	2.22	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.74	0.68
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.76	0.68
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.05	0.68
7:G:126:LEU:HD11	12:R:89:PRO:HB2	1.75	0.68
4:D:97:LEU:HD22	4:D:99:LEU:HD21	1.75	0.68
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.68
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.68
10:P:192:ARG:NH2	10:P:200:ILE:HD11	2.09	0.68
1:A:105:GLU:CG	1:A:111:LEU:HG	2.25	0.67
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.67
1:A:3:LEU:HD23	24:A:401:3PE:H251	1.75	0.67
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.67
11:Q:160:TYR:CE2	11:Q:164:PHE:CZ	2.80	0.67
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.67
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.67
13:S:16:LEU:HB3	13:S:69:TYR:HD1	1.58	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.67
9:I:188:GLU:OE2	12:R:56:ASN:HB2	1.94	0.67
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.57	0.67
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.09	0.67
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.58	0.67
10:P:192:ARG:HH22	10:P:198:ALA:CB	2.07	0.67
10:P:197:GLU:HB3	10:P:259:VAL:CG2	2.24	0.67
10:P:302:GLY:HA2	10:P:314:THR:HG23	1.77	0.67
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.28	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
4:D:338:ARG:HH12	18:Z:23:ARG:HA	1.58	0.67
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.67
8:H:93:HIS:CE1	19:a:24:ALA:HA	2.30	0.67
10:P:94:LEU:HA	10:P:97:MET:HE3	1.77	0.67
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.67
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.67
9:I:188:GLU:CD	12:R:56:ASN:HB2	2.19	0.67
1:A:8:PHE:HE1	24:A:401:3PE:H2C1	1.60	0.67
5:E:139:CYS:SG	26:E:301:FES:FE1	1.87	0.67
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.76	0.67
8:H:23:VAL:HG11	19:a:9:LEU:HD21	1.77	0.67
14:T:130:ILE:HG23	14:T:131:PRO:HD2	1.77	0.67
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.66
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.66
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.66
16:W:121:PHE:HA	16:W:124:LYS:HE2	1.76	0.66
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.77	0.66
6:F:300:ILE:HD13	6:F:307:VAL:HG23	1.77	0.66
9:I:80:GLU:OE2	22:r:26:LEU:CD1	2.44	0.66
9:I:93:LEU:O	21:q:93:MET:HG2	1.94	0.66
13:S:24:CYS:SG	13:S:61:VAL:O	2.53	0.66
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.77	0.66
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.77	0.66
6:F:41:ILE:HG23	6:F:253:THR:HG21	1.76	0.66
6:F:228:PRO:HG3	11:Q:160:TYR:HD2	1.59	0.66
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.66
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.66
9:I:35:THR:CG2	22:r:107:SER:HA	2.26	0.66
14:T:83:VAL:HG22	14:T:126:PHE:CZ	2.31	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.31	0.66
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.66
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.25	0.66
10:P:199:ILE:HD11	10:P:258:ALA:O	1.96	0.66
14:T:87:LEU:CD2	14:T:104:PHE:CZ	2.78	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
6:F:297:LYS:HB2	6:F:333:GLU:HA	1.76	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.66
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.66
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.66
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.66
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.74	0.66
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.66
15:V:44:TYR:CE1	15:V:48:THR:HG23	2.30	0.66
10:P:59:PHE:HB2	10:P:130:ILE:HD11	1.79	0.65
12:R:42:ASP:HB3	12:R:44:ARG:HH11	1.61	0.65
16:W:42:TRP:CH2	16:W:93:LEU:HA	2.31	0.65
2:B:93:MET:HE1	2:B:131:MET:HE2	1.78	0.65
3:C:141:ARG:NH1	4:D:410:TYR:HE1	1.93	0.65
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.65
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.79	0.65
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.77	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.65
2:B:173:TYR:O	3:C:203:LEU:HD22	1.97	0.65
6:F:33:GLY:HA2	6:F:291:GLU:CB	2.16	0.65
8:H:283:ASP:OD1	8:H:284:GLN:N	2.29	0.65
3:C:79:CYS:O	3:C:80:LEU:HB2	1.96	0.65
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.28	0.65
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.65
10:P:169:HIS:H	10:P:184:LYS:CE	2.09	0.65
13:S:16:LEU:HB3	13:S:69:TYR:CD1	2.32	0.65
18:Z:69:ILE:HG23	20:b:54:PRO:CD	2.27	0.65
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.74	0.65
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
9:I:79:ARG:HG2	22:r:12:ARG:HH21	1.62	0.65
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.65
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.77	0.65
2:B:91:TRP:CH2	28:H:400:UQ9:H1M	2.31	0.65
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.65
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.65
18:Z:62:ILE:HG12	20:b:49:THR:HA	1.78	0.65
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.26	0.65
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.65
7:G:179:CYS:SG	25:G:802:SF4:FE3	1.88	0.65
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.65
8:H:33:LEU:CD2	22:r:25:GLN:HG2	2.26	0.65
8:H:249:ILE:CD1	17:X:99:HIS:CG	2.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.65
10:P:236:VAL:CG1	10:P:270:ARG:HH21	2.10	0.65
10:P:284:THR:HG23	10:P:356:HIS:HB2	1.79	0.65
17:X:65:GLY:HA2	17:X:68:LEU:HD12	1.78	0.65
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.62	0.64
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.64
14:T:87:LEU:HD21	14:T:104:PHE:CZ	2.32	0.64
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.64
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.64
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.78	0.64
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.79	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.63	0.64
4:D:166:ARG:NH2	18:Z:10:MET:HG2	2.11	0.64
6:F:425:CYS:SG	25:F:502:SF4:FE1	1.78	0.64
14:T:118:ILE:HG23	14:T:122:MET:HE3	1.78	0.64
18:Z:69:ILE:CG2	20:b:54:PRO:HD3	2.27	0.64
18:Z:86:ILE:HA	18:Z:128:ARG:HH21	1.62	0.64
2:B:92:PRO:HD2	2:B:120:VAL:HG12	1.80	0.64
3:C:98:PHE:CA	15:V:90:LEU:HD11	2.19	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
13:S:58:CYS:HB2	13:S:61:VAL:HG12	1.78	0.64
14:T:83:VAL:HG23	14:T:126:PHE:HZ	1.63	0.64
4:D:338:ARG:NH1	18:Z:23:ARG:CA	2.60	0.64
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.64
10:P:226:VAL:HG21	10:P:281:PHE:CZ	2.32	0.64
12:R:89:PRO:HG2	12:R:106:TYR:CZ	2.33	0.64
5:E:79:LEU:HB2	5:E:80:PRO:HD3	1.78	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.32	0.64
2:B:94:THR:CB	2:B:104:MET:HE1	2.27	0.64
2:B:146:ARG:O	2:B:147:LYS:C	2.39	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	0.64
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.64
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.64
10:P:88:VAL:HG12	10:P:92:MET:HE2	1.80	0.64
10:P:191:VAL:HG13	10:P:192:ARG:NH2	2.12	0.64
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.64
6:F:228:PRO:HG3	11:Q:160:TYR:CD2	2.33	0.64
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.64
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:163:ASN:OD1	11:Q:164:PHE:N	2.31	0.64
12:R:32:THR:HG22	12:R:36:GLN:N	2.10	0.64
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.64
13:S:16:LEU:HD12	13:S:16:LEU:C	2.22	0.64
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.64
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	0.64
17:X:37:ASP:OD1	17:X:38:LYS:N	2.31	0.64
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.64
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.64
8:H:42:PRO:HD2	8:H:45:ILE:CG1	2.28	0.64
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.64
16:W:101:LYS:NZ	16:W:109:PHE:HE2	1.94	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.63
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.63
1:A:52:SER:HB2	1:A:54:LYS:HG2	1.79	0.63
4:D:238:LEU:HA	18:Z:9:ASP:HB2	1.80	0.63
10:P:180:SER:O	10:P:184:LYS:HG3	1.98	0.63
18:Z:65:LEU:O	18:Z:68:ARG:HG2	1.98	0.63
4:D:85:GLY:HA2	4:D:89:PRO:HG3	1.80	0.63
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.33	0.63
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.63
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.80	0.63
14:T:79:ILE:CB	14:T:145:VAL:HG13	2.28	0.63
4:D:142:VAL:HG13	4:D:207:ARG:NH1	2.14	0.63
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
21:q:6:VAL:HA	21:q:9:ARG:HG2	1.79	0.63
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.64	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
10:P:93:HIS:NE2	10:P:94:LEU:HD11	2.14	0.63
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.61	0.63
2:B:136:THR:CG2	2:B:177:VAL:HG22	2.29	0.63
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.63
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.63
9:I:54:THR:HG21	18:Z:33:TYR:CE2	2.34	0.63
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.63
14:T:93:ILE:CG2	14:T:110:LEU:HD13	2.28	0.63
22:r:109:ASP:O	22:r:110:GLN:HG2	1.99	0.63
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.63
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.63
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ARG:HG3	2:B:73:TYR:H	1.63	0.63
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.63
12:R:98:GLU:CD	12:R:98:GLU:H	2.07	0.63
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.81	0.62
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.81	0.62
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.81	0.62
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.62
8:H:195:ARG:O	8:H:199:ASP:HB2	1.99	0.62
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.62
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.48	0.62
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.80	0.62
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.98	0.62
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.29	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.65	0.62
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.79	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.28	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.28	0.62
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.82	0.62
13:S:16:LEU:HA	13:S:69:TYR:HA	1.79	0.62
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.34	0.62
16:W:83:ASP:O	16:W:86:VAL:HG22	1.99	0.62
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.34	0.62
21:q:3:LEU:HD12	21:q:6:VAL:HG21	1.81	0.62
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.62
5:E:230:LEU:HD11	6:F:48:ARG:HE	1.64	0.62
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.81	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
7:G:617:ARG:NH1	16:W:129:HIS:HA	2.14	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
13:S:15:GLY:HA3	13:S:17:ARG:HH22	1.63	0.62
16:W:55:LEU:CB	16:W:107:MET:HE2	2.30	0.62
17:X:37:ASP:OD2	20:b:70:PRO:HD3	2.00	0.62
21:q:71:LYS:O	21:q:72:ASN:CG	2.43	0.62
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.30	0.62
18:Z:28:ARG:HG3	18:Z:28:ARG:O	1.99	0.62
18:Z:135:ASN:HD21	19:a:52:ARG:NH1	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:166:ARG:HH22	18:Z:10:MET:CG	2.11	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.62
20:b:11:ASN:O	20:b:15:LYS:N	2.31	0.62
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.35	0.62
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.62
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.62
7:G:82:ILE:CG2	7:G:100:TRP:HB3	2.30	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
10:P:169:HIS:HD2	10:P:181:LEU:HD11	1.65	0.62
2:B:125:PRO:HG3	4:D:88:HIS:CE1	2.35	0.62
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
7:G:399:VAL:CG2	7:G:462:PHE:HZ	2.12	0.62
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.62
22:r:20:LEU:HD12	22:r:21:GLN:N	2.14	0.62
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.26	0.61
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.63	0.61
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.61
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.61
21:q:34:ARG:NE	21:q:58:ARG:NH2	2.48	0.61
7:G:651:PRO:CD	13:S:56:ARG:HB3	2.30	0.61
8:H:25:ARG:HD2	28:H:400:UQ9:H10A	1.81	0.61
10:P:240:VAL:HB	10:P:266:THR:O	2.00	0.61
14:T:83:VAL:CG2	14:T:126:PHE:CZ	2.83	0.61
14:T:103:HIS:ND1	14:T:140:CYS:SG	2.73	0.61
17:X:69:ASN:O	17:X:73:GLN:HG3	2.00	0.61
2:B:194:CYS:O	25:B:301:SF4:S2	2.58	0.61
4:D:202:TRP:CZ3	4:D:261:MET:HG3	2.36	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.61
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.36	0.61
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.35	0.61
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.61
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.61
5:E:182:ALA:O	5:E:183:PRO:C	2.42	0.61
7:G:421:SER:CB	7:G:427:LEU:CD1	2.78	0.61
10:P:263:PHE:HD2	10:P:333:PRO:O	1.83	0.61
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
8:H:292:ASN:O	20:b:18:VAL:HG11	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:142:TYR:HA	18:Z:115:ARG:HD3	1.82	0.61
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.83	0.61
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
2:B:97:LEU:CD2	2:B:141:MET:HG2	2.30	0.61
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.36	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
10:P:299:SER:HB3	10:P:316:LYS:HE3	1.83	0.61
7:G:117:MET:HE3	7:G:143:SER:CA	2.30	0.61
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.61
2:B:93:MET:HB2	2:B:128:ALA:CB	2.30	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
6:F:416:SER:O	6:F:419:ILE:HG22	2.01	0.61
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.61
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.61
9:I:80:GLU:OE2	22:r:26:LEU:HD11	2.01	0.61
10:P:262:THR:N	10:P:332:LEU:HD12	2.12	0.61
16:W:42:TRP:CZ2	16:W:93:LEU:CB	2.83	0.61
16:W:55:LEU:CB	16:W:107:MET:CE	2.75	0.61
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.61
8:H:249:ILE:CD1	17:X:99:HIS:ND1	2.64	0.61
10:P:192:ARG:HA	10:P:192:ARG:CZ	2.31	0.61
11:Q:167:ASN:O	11:Q:168:LYS:CG	2.48	0.61
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.60
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.60
21:q:3:LEU:O	21:q:6:VAL:HG22	2.01	0.60
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.82	0.60
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.60
10:P:333:PRO:HB2	10:P:337:ASP:CB	2.25	0.60
14:T:138:LEU:O	14:T:138:LEU:CD1	2.40	0.60
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.60
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.60
14:T:138:LEU:HD12	14:T:138:LEU:C	2.24	0.60
16:W:97:ILE:HG23	16:W:98:LYS:HG3	1.83	0.60
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.60
13:S:19:ILE:HG13	13:S:95:LEU:CD1	2.31	0.60
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.02	0.60
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.60
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.60
10:P:318:LYS:O	10:P:322:ILE:HG13	2.02	0.60
12:R:89:PRO:CG	12:R:106:TYR:CE1	2.83	0.60
13:S:16:LEU:CB	13:S:69:TYR:HD1	2.14	0.60
18:Z:69:ILE:CG2	20:b:54:PRO:CD	2.80	0.60
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.60
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.81	0.60
12:R:32:THR:HA	12:R:55:VAL:HG23	1.83	0.60
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.65	0.60
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	0.60
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.60
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.31	0.60
10:P:315:THR:O	10:P:316:LYS:C	2.45	0.60
12:R:42:ASP:HB3	12:R:44:ARG:NH1	2.17	0.60
5:E:71:GLU:HB2	23:s:59:GLN:HB3	1.82	0.60
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.60
7:G:304:GLU:OE2	10:P:41:ILE:HG12	2.01	0.60
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.67	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
14:T:103:HIS:HB2	14:T:106:LYS:HB2	1.83	0.60
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.60
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.60
17:X:20:VAL:HG12	17:X:25:LEU:HD21	1.84	0.60
17:X:37:ASP:HA	17:X:40:ASN:HB2	1.84	0.60
18:Z:143:TYR:O	18:Z:144:THR:C	2.45	0.60
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.60
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.67	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.60
4:D:202:TRP:CH2	4:D:261:MET:HG3	2.37	0.59
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.82	0.59
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.84	0.59
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.59
10:P:136:THR:CG2	10:P:139:PHE:HB2	2.31	0.59
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.37	0.59
16:W:53:MET:SD	16:W:106:VAL:HG21	2.42	0.59
4:D:92:HIS:ND1	4:D:458:PHE:HD2	1.99	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.37	0.59
10:P:66:GLY:O	10:P:67:ARG:C	2.42	0.59
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.59
3:C:70:LYS:O	15:V:103:LEU:HD12	2.02	0.59
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.67	0.59
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.59
8:H:19:PHE:HB3	19:a:12:MET:HG3	1.83	0.59
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.59
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.59
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.59
4:D:86:PRO:CD	4:D:87:GLN:OE1	2.43	0.59
6:F:44:ASN:HB3	6:F:134:ASP:HB2	1.85	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.59
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.85	0.59
21:q:51:ASP:O	21:q:59:HIS:HB2	2.02	0.59
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.59
10:P:178:SER:O	10:P:182:ARG:HG2	2.02	0.59
12:R:37:VAL:O	12:R:38:TYR:C	2.44	0.59
23:s:57:LEU:HG	23:s:58:PRO:HD2	1.84	0.59
2:B:91:TRP:CH2	28:H:400:UQ9:C1M	2.86	0.59
2:B:144:ALA:O	2:B:145:LEU:C	2.45	0.59
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.37	0.59
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.84	0.59
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
17:X:134:ASP:O	17:X:135:ARG:C	2.45	0.59
2:B:126:ARG:NH1	8:H:61:MET:SD	2.76	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.84	0.59
8:H:93:HIS:HE1	19:a:24:ALA:HA	1.66	0.59
8:H:180:PRO:HD3	18:Z:43:LEU:HD21	1.83	0.59
17:X:78:CYS:SG	17:X:110:CYS:HB3	2.42	0.59
6:F:119:GLU:HB3	6:F:124:THR:CG2	2.32	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
10:P:357:ARG:HD3	10:P:361:TRP:O	2.03	0.59
20:b:6:SER:O	20:b:9:LEU:HB3	2.03	0.59
20:b:8:PHE:HA	20:b:11:ASN:ND2	2.18	0.59
7:G:126:LEU:HD12	12:R:89:PRO:HB2	1.84	0.59
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.85	0.58
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.85	0.58
8:H:142:TYR:CG	8:H:289:LEU:HD12	2.37	0.58
10:P:96:LEU:HD12	10:P:96:LEU:C	2.28	0.58
1:A:68:GLU:CD	1:A:98:LEU:HG	2.28	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	2.01	0.58
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.83	0.58
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.58
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.58
12:R:40:GLU:HA	12:R:45:ARG:CZ	2.32	0.58
13:S:23:LEU:O	13:S:23:LEU:CD1	2.41	0.58
14:T:123:GLU:OE1	16:W:44:ARG:NH1	2.36	0.58
17:X:123:GLY:HA2	18:Z:66:GLU:CD	2.27	0.58
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.58
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.17	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.85	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
8:H:302:MET:SD	20:b:26:TRP:CD1	2.97	0.58
10:P:122:HIS:CB	12:R:46:VAL:HG12	2.33	0.58
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.58
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.33	0.58
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.84	0.58
2:B:110:PRO:HB3	8:H:33:LEU:O	2.03	0.58
4:D:128:THR:H	4:D:131:GLN:NE2	2.00	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.32	0.58
12:R:88:HIS:O	12:R:89:PRO:C	2.45	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.58
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.39	0.58
13:S:47:ALA:O	13:S:49:PRO:HD3	2.03	0.58
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.58
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.02	0.58
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.58
2:B:115:ASP:HA	2:B:119:VAL:O	2.04	0.58
4:D:388:GLY:HA3	4:D:417:SER:OG	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:57:THR:HG23	10:P:123:SER:HB2	1.86	0.58
10:P:191:VAL:HG13	10:P:192:ARG:HH21	1.66	0.58
13:S:16:LEU:O	13:S:16:LEU:CD1	2.51	0.58
18:Z:98:MET:HB2	18:Z:104:TRP:NE1	2.18	0.58
18:Z:105:LYS:O	18:Z:106:VAL:C	2.46	0.58
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.04	0.58
4:D:375:MET:HE1	7:G:126:LEU:CA	2.33	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.58
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.86	0.58
21:q:129:THR:O	21:q:129:THR:HG22	2.03	0.58
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.58
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.37	0.58
6:F:382:CYS:SG	25:F:502:SF4:S1	3.02	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.58
10:P:57:THR:HG23	10:P:123:SER:CB	2.33	0.58
10:P:220:TYR:HA	10:P:223:PHE:HD2	1.67	0.58
14:T:90:TYR:CE2	14:T:92:LYS:CB	2.87	0.58
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.04	0.58
2:B:153:PRO:HB2	2:B:155:PRO:HD2	1.85	0.58
2:B:164:CYS:SG	25:B:301:SF4:S4	3.02	0.58
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.58
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.58
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.84	0.58
9:I:62:MET:SD	18:Z:35:MET:HG2	2.43	0.58
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.58
8:H:85:LEU:CD2	8:H:108:THR:HB	2.34	0.58
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.62	0.58
10:P:192:ARG:CZ	10:P:198:ALA:HB3	2.34	0.58
18:Z:58:ARG:CZ	20:b:49:THR:HG21	2.33	0.58
1:A:60:ILE:O	1:A:61:THR:C	2.46	0.57
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.36	0.57
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.57
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.86	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.04	0.57
18:Z:129:THR:HB	18:Z:132:GLU:HG3	1.86	0.57
3:C:186:ILE:HG13	3:C:187:LEU:N	2.17	0.57
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.57
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.29	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.57
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.57
16:W:83:ASP:O	16:W:87:ILE:HG12	2.04	0.57
18:Z:65:LEU:HB3	20:b:50:PRO:O	2.03	0.57
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.68	0.57
6:F:293:SER:N	6:F:338:ASP:OD1	2.37	0.57
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.86	0.57
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.57
10:P:245:VAL:O	10:P:249:ILE:HG13	2.04	0.57
14:T:90:TYR:CE2	14:T:92:LYS:HB3	2.39	0.57
17:X:52:ASP:OD2	17:X:55:ARG:HG3	2.03	0.57
2:B:170:TYR:OH	4:D:131:GLN:O	2.22	0.57
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
16:W:42:TRP:CZ2	31:W:201:EHZ:O1	2.58	0.57
21:q:13:GLN:HB3	21:q:33:ILE:HG22	1.86	0.57
21:q:68:MET:SD	21:q:81:MET:HB3	2.44	0.57
2:B:69:SER:O	2:B:70:ARG:C	2.48	0.57
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.05	0.57
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.39	0.57
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.57
5:E:164:PRO:C	5:E:166:LYS:H	2.11	0.57
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.57
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.86	0.57
6:F:48:ARG:NH1	6:F:48:ARG:HA	2.19	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.57
18:Z:122:GLY:O	18:Z:126:GLY:N	2.34	0.57
1:A:105:GLU:HG2	1:A:111:LEU:HG	1.87	0.57
4:D:80:MET:SD	4:D:101:LEU:HB2	2.45	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.85	0.57
14:T:130:ILE:HD11	14:T:148:ILE:HD11	1.86	0.57
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.66	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.57
17:X:130:LYS:HG2	20:b:67:PRO:HA	1.86	0.57
17:X:141:PRO:O	17:X:142:TYR:HB2	2.04	0.57
4:D:338:ARG:CZ	18:Z:23:ARG:HB3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
8:H:179:TRP:CD1	18:Z:43:LEU:HD21	2.40	0.57
23:s:35:LEU:HB3	23:s:38:HIS:HB2	1.85	0.57
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.56
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.56
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.56
20:b:69:HIS:CD2	20:b:70:PRO:HD2	2.37	0.56
1:A:113:TRP:HH2	8:H:287:HIS:CD2	2.23	0.56
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.40	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.56
8:H:69:SER:C	8:H:71:PHE:N	2.61	0.56
8:H:142:TYR:CE1	8:H:289:LEU:HD12	2.39	0.56
2:B:93:MET:HE1	2:B:95:PHE:CE2	2.40	0.56
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.56
6:F:39:ASP:HA	6:F:261:TRP:HZ2	1.70	0.56
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.41	0.56
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
8:H:51:ASP:OD2	28:H:400:UQ9:H12	2.06	0.56
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.88	0.56
10:P:188:GLU:O	10:P:192:ARG:HG2	2.05	0.56
12:R:59:PHE:O	12:R:63:LEU:HG	2.06	0.56
16:W:23:ILE:HG13	16:W:80:ARG:HG2	1.87	0.56
18:Z:140:PHE:CE1	19:a:45:TRP:HB2	2.40	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.56
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.06	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.41	0.56
10:P:320:GLU:O	10:P:324:ILE:HG12	2.05	0.56
17:X:5:VAL:HG13	17:X:7:LEU:HG	1.87	0.56
18:Z:7:LYS:HB2	18:Z:7:LYS:NZ	2.20	0.56
1:A:22:PHE:O	1:A:25:PRO:HD2	2.05	0.56
6:F:213:ILE:HG23	6:F:235:VAL:HA	1.86	0.56
6:F:293:SER:HB3	6:F:338:ASP:OD2	2.06	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
11:Q:165:SER:HB3	11:Q:168:LYS:O	2.06	0.56
14:T:134:ASP:OD1	14:T:134:ASP:O	2.23	0.56
21:q:65:THR:HG22	21:q:66:THR:N	2.20	0.56
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
12:R:62:ASP:O	12:R:66:GLN:HG3	2.06	0.56
17:X:137:LEU:HD23	17:X:138:PRO:O	2.05	0.56
4:D:266:ARG:NH1	9:I:60:ILE:HA	2.20	0.56
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.56
9:I:89:GLU:HG3	21:q:61:TRP:HB3	1.87	0.56
11:Q:167:ASN:O	11:Q:168:LYS:HG2	2.04	0.56
16:W:25:SER:HB3	16:W:30:GLU:HB3	1.88	0.56
17:X:39:THR:HG23	17:X:40:ASN:N	2.20	0.56
18:Z:92:GLU:O	18:Z:96:ILE:HG13	2.05	0.56
2:B:95:PHE:CE2	2:B:131:MET:SD	2.99	0.56
2:B:97:LEU:HD21	2:B:141:MET:HG2	1.88	0.56
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.58	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56
10:P:64:PHE:HE1	10:P:209:ARG:O	1.88	0.56
11:Q:110:PRO:HB3	12:R:43:TYR:OH	2.06	0.56
16:W:104:THR:O	16:W:108:ARG:HG3	2.05	0.56
3:C:184:ARG:HA	16:W:91:MET:SD	2.46	0.56
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.56
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.56
8:H:69:SER:C	8:H:71:PHE:H	2.12	0.56
16:W:42:TRP:CE2	16:W:93:LEU:HB2	2.41	0.56
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.87	0.56
4:D:279:THR:HA	15:V:12:VAL:HG13	1.87	0.56
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.36	0.56
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.56
13:S:16:LEU:HD11	13:S:51:LEU:CD1	2.29	0.56
17:X:124:GLN:C	17:X:125:LEU:HD12	2.31	0.56
5:E:139:CYS:CB	5:E:144:SER:HB3	2.35	0.55
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.87	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.55
2:B:194:CYS:HB2	9:I:153:ILE:O	2.06	0.55
3:C:80:LEU:HD21	4:D:157:LYS:O	2.05	0.55
4:D:266:ARG:NH2	9:I:59:ARG:O	2.38	0.55
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.07	0.55
5:E:233:LEU:HD11	6:F:289:GLU:OE2	2.07	0.55
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.55
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.41	0.55
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.55
8:H:310:PHE:HB3	20:b:33:PRO:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.88	0.55
10:P:145:PHE:O	10:P:149:PRO:HG2	2.05	0.55
1:A:102:LEU:CD1	1:A:111:LEU:HD11	2.37	0.55
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.55
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.55
7:G:401:LEU:HD11	7:G:462:PHE:HE2	1.71	0.55
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.46	0.55
10:P:140:ASP:OD1	10:P:142:GLU:HB2	2.06	0.55
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.49	0.55
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.55
14:T:90:TYR:HE2	14:T:92:LYS:CB	2.19	0.55
19:a:31:ASN:HD21	19:a:36:LYS:HB2	1.71	0.55
20:b:8:PHE:CG	20:b:9:LEU:N	2.74	0.55
2:B:174:SER:HA	3:C:203:LEU:CD2	2.37	0.55
7:G:35:PHE:O	7:G:101:ASN:HA	2.07	0.55
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
8:H:171:HIS:CE1	18:Z:53:TRP:CE3	2.95	0.55
8:H:183:MET:SD	24:I:301:3PE:H341	2.47	0.55
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.70	0.55
11:Q:160:TYR:OH	11:Q:164:PHE:HZ	1.89	0.55
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.87	0.55
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.55
22:r:9:GLN:O	22:r:12:ARG:HB2	2.06	0.55
2:B:99:CYS:C	2:B:101:ALA:N	2.59	0.55
7:G:382:ARG:HD2	13:S:56:ARG:CD	2.37	0.55
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.21	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55
9:I:75:SER:O	22:r:12:ARG:HG2	2.07	0.55
14:T:128:PHE:CE2	14:T:130:ILE:HG13	2.42	0.55
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.35	0.55
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.55
4:D:98:VAL:HG12	4:D:110:ASP:O	2.07	0.55
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.07	0.55
6:F:300:ILE:HD11	6:F:311:TRP:HD1	1.72	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.55
10:P:71:ASN:HA	10:P:97:MET:SD	2.47	0.55
17:X:33:GLY:HA3	18:Z:70:ALA:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.32	0.55
4:D:232:VAL:HG23	4:D:356:ILE:HD13	1.88	0.55
4:D:256:ASP:OD1	18:Z:23:ARG:HA	2.07	0.55
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.55
16:W:42:TRP:CZ2	16:W:93:LEU:CA	2.89	0.55
22:r:7:VAL:O	22:r:11:LEU:HG	2.06	0.55
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.87	0.55
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.55
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.37	0.55
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.55
16:W:35:VAL:HG21	31:W:201:EHZ:N2	2.22	0.55
16:W:53:MET:HB2	16:W:55:LEU:HG	1.89	0.55
17:X:53:PRO:HD2	18:Z:116:TRP:NE1	2.22	0.55
3:C:100:ARG:HH12	15:V:86:LYS:HZ1	1.55	0.55
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.55
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.14	0.55
6:F:48:ARG:HA	6:F:48:ARG:HH11	1.72	0.55
6:F:119:GLU:HG3	6:F:127:ASP:OD2	2.07	0.55
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.55
10:P:376:ASN:OD1	10:P:376:ASN:C	2.50	0.55
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.71	0.55
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.30	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
6:F:170:GLN:HB3	23:s:48:LEU:HD22	1.89	0.55
10:P:98:GLY:HA3	10:P:103:LEU:HG	1.87	0.55
10:P:122:HIS:HB2	12:R:46:VAL:HG12	1.88	0.55
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.71	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
14:T:118:ILE:HG23	14:T:122:MET:CE	2.37	0.54
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.06	0.54
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.88	0.54
2:B:126:ARG:HG3	8:H:213:VAL:O	2.07	0.54
4:D:145:MET:HA	4:D:148:GLU:HG3	1.88	0.54
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.54
5:E:162:THR:HG22	5:E:166:LYS:HA	1.88	0.54
7:G:617:ARG:HH12	16:W:128:GLY:C	2.16	0.54
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.54
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
10:P:300:TRP:O	10:P:304:LEU:HG	2.08	0.54
14:T:97:LYS:HG3	14:T:97:LYS:O	2.08	0.54
15:V:50:GLN:HE22	22:r:94:ALA:H	1.56	0.54
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.43	0.54
4:D:87:GLN:O	4:D:88:HIS:C	2.49	0.54
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.07	0.54
8:H:133:LEU:O	8:H:136:VAL:HG12	2.08	0.54
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.54
14:T:87:LEU:HD22	14:T:104:PHE:CZ	2.41	0.54
19:a:58:ASN:HB2	19:a:61:TYR:CD2	2.43	0.54
1:A:106:TRP:HH2	20:b:19:LEU:HD11	1.73	0.54
6:F:235:VAL:HG22	6:F:236:PHE:HD2	1.68	0.54
6:F:382:CYS:SG	25:F:502:SF4:S4	3.05	0.54
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.54
8:H:43:TYR:CE2	21:q:27:PHE:HZ	2.25	0.54
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.54
18:Z:56:GLU:HA	18:Z:59:ARG:HH11	1.72	0.54
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.54
21:q:17:HIS:NE2	21:q:33:ILE:HG23	2.23	0.54
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.23	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
5:E:164:PRO:C	5:E:166:LYS:N	2.64	0.54
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.37	0.54
6:F:67:GLU:O	6:F:71:LYS:HG2	2.06	0.54
6:F:299:LEU:CD1	6:F:300:ILE:HG23	2.37	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.73	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.07	0.54
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.54
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.54
10:P:207:PHE:CE1	10:P:214:LEU:HD22	2.43	0.54
1:A:106:TRP:CZ3	20:b:19:LEU:HD21	2.42	0.54
4:D:82:LEU:HG	4:D:84:PHE:HB2	1.88	0.54
4:D:91:ALA:HA	4:D:193:ASP:OD2	2.08	0.54
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.46	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:80:GLU:CB	22:r:26:LEU:HD11	2.38	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
10:P:236:VAL:HG13	10:P:270:ARG:HH21	1.71	0.54
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.90	0.54
10:P:316:LYS:O	10:P:320:GLU:HG2	2.08	0.54
4:D:98:VAL:CG1	4:D:110:ASP:HB3	2.38	0.54
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.85	0.54
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.54
9:I:123:CYS:SG	25:I:302:SF4:S3	3.06	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.54
4:D:98:VAL:HG13	4:D:110:ASP:HB3	1.89	0.54
6:F:339:PHE:HA	6:F:349:LEU:HB2	1.90	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.54
20:b:8:PHE:O	20:b:9:LEU:C	2.50	0.54
3:C:100:ARG:HH12	15:V:86:LYS:NZ	2.06	0.54
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.54
6:F:294:VAL:HG12	6:F:337:MET:HB2	1.90	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:170:LYS:O	7:G:231:LEU:HA	2.08	0.54
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
17:X:64:ASN:O	17:X:68:LEU:HG	2.07	0.54
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.54
4:D:259:GLU:CB	18:Z:25:LEU:HD11	2.35	0.54
5:E:39:VAL:HG21	7:G:163:LYS:HZ2	1.73	0.54
5:E:199:ASP:O	5:E:203:ILE:HG13	2.08	0.54
6:F:235:VAL:HG12	6:F:240:THR:OG1	2.08	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
9:I:80:GLU:HB3	22:r:26:LEU:HD11	1.90	0.54
10:P:370:LYS:HG3	10:P:370:LYS:O	2.07	0.54
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.54
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.90	0.54
21:q:6:VAL:HG23	21:q:7:LEU:N	2.21	0.54
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:139:CYS:C	5:E:144:SER:HB3	2.33	0.53
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.53
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.53
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.53
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.53
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.53
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.53
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.23	0.53
20:b:59:ASP:HA	20:b:63:MET:HE2	1.89	0.53
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.53
1:A:112:GLU:C	1:A:113:TRP:CG	2.86	0.53
3:C:217:ARG:HH12	16:W:112:GLU:CB	2.19	0.53
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.88	0.53
5:E:180:VAL:CG1	5:E:224:CYS:SG	2.96	0.53
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.53
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.90	0.53
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.53
6:F:329:LYS:HA	6:F:332:CYS:SG	2.49	0.53
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.53
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.37	0.53
10:P:142:GLU:HA	10:P:146:VAL:HG12	1.90	0.53
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.44	0.53
6:F:85:LEU:HD13	6:F:262:PHE:CE2	2.44	0.53
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.91	0.53
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.53
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.90	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.52	0.53
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.90	0.53
9:I:80:GLU:OE2	22:r:26:LEU:HD13	2.08	0.53
1:A:110:GLY:O	1:A:111:LEU:HB2	2.08	0.53
2:B:81:LEU:CG	8:H:53:MET:HE1	2.34	0.53
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.53
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.53
7:G:617:ARG:NH1	16:W:128:GLY:C	2.66	0.53
14:T:83:VAL:HG22	14:T:126:PHE:HZ	1.66	0.53
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.53
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.90	0.53
6:F:259:GLY:O	6:F:263:ALA:N	2.40	0.53
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.53
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:58:VAL:O	10:P:83:PRO:HD2	2.09	0.53
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.39	0.53
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.33	0.53
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.43	0.53
7:G:364:ASP:C	7:G:364:ASP:OD1	2.52	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.09	0.53
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.39	0.53
13:S:16:LEU:HD13	13:S:19:ILE:CD1	2.38	0.53
2:B:92:PRO:HD3	2:B:119:VAL:HG13	1.91	0.53
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.23	0.53
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.53
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.53
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.53
9:I:109:GLY:O	12:R:63:LEU:HD12	2.08	0.53
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.53
19:a:42:GLN:O	19:a:43:TYR:C	2.51	0.53
2:B:154:GLU:O	10:P:89:TYR:OH	2.21	0.53
3:C:80:LEU:HD22	4:D:157:LYS:HB3	1.90	0.53
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.53
4:D:84:PHE:C	4:D:86:PRO:HD3	2.34	0.53
4:D:248:SER:HB2	18:Z:19:ILE:HD13	1.90	0.53
6:F:80:MET:HE2	6:F:95:THR:HG21	1.89	0.53
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.53
10:P:85:ARG:HE	29:P:401:NDP:C2A	2.21	0.53
10:P:172:ALA:H	10:P:202:ARG:NH2	2.06	0.53
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.53
13:S:30:SER:O	13:S:31:GLN:C	2.49	0.53
14:T:100:VAL:O	14:T:141:PRO:HD2	2.09	0.53
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.42	0.53
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.27	0.53
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.22	0.53
4:D:368:ARG:HA	4:D:371:MET:HG2	1.90	0.53
5:E:65:ILE:HA	5:E:68:ASN:ND2	2.24	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53
7:G:372:PHE:H	7:G:532:PRO:HB2	1.74	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.53
18:Z:69:ILE:O	20:b:53:TYR:HE1	1.92	0.53
1:A:102:LEU:HD11	1:A:111:LEU:HD11	1.91	0.53
4:D:210:MET:O	4:D:211:PHE:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:338:ARG:NH1	18:Z:23:ARG:N	2.56	0.53
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.89	0.53
5:E:39:VAL:HG11	7:G:163:LYS:HZ3	1.73	0.53
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.53
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.53
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
12:R:98:GLU:HA	12:R:113:GLN:CD	2.34	0.53
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.53
18:Z:58:ARG:NH2	20:b:49:THR:CG2	2.69	0.53
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.07	0.52
4:D:93:GLY:O	4:D:94:VAL:C	2.52	0.52
5:E:77:ALA:C	5:E:80:PRO:HD2	2.33	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.45	0.52
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.91	0.52
14:T:87:LEU:HD23	14:T:122:MET:HE1	1.91	0.52
17:X:80:GLU:HB3	17:X:81:PRO:HD3	1.91	0.52
2:B:105:MET:CE	4:D:200:PHE:CE2	2.80	0.52
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.75	0.52
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.91	0.52
5:E:177:GLY:O	26:E:301:FES:S1	2.68	0.52
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.74	0.52
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.52
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.52
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.90	0.52
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.52
4:D:253:LEU:HD11	22:r:18:GLN:HG3	1.90	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.52
7:G:617:ARG:HH12	16:W:129:HIS:N	2.07	0.52
8:H:222:LEU:O	8:H:223:PHE:C	2.51	0.52
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.52
12:R:69:VAL:HG12	12:R:112:LYS:N	2.24	0.52
21:q:9:ARG:HA	21:q:12:GLN:CG	2.37	0.52
21:q:29:ARG:HD3	21:q:74:PHE:CE1	2.44	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.10	0.52
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.90	0.52
7:G:399:VAL:HG21	7:G:462:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.52
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.52
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52
20:b:66:VAL:HG11	20:b:70:PRO:HA	1.92	0.52
4:D:381:HIS:HE1	9:I:161:ALA:O	1.93	0.52
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.52
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.52
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.91	0.52
10:P:265:PHE:HD1	10:P:334:GLY:HA3	1.74	0.52
14:T:130:ILE:CG2	14:T:131:PRO:HD2	2.40	0.52
3:C:73:GLN:NE2	15:V:112:TRP:HE1	2.07	0.52
6:F:126:LYS:HG3	6:F:275:LEU:CB	2.39	0.52
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
17:X:77:HIS:HD2	17:X:115:LEU:HD21	1.74	0.52
21:q:55:PHE:CG	22:r:26:LEU:HD22	2.43	0.52
21:q:56:PHE:HD1	21:q:59:HIS:NE2	2.06	0.52
21:q:73:THR:HA	21:q:76:ASP:OD1	2.09	0.52
1:A:3:LEU:HA	8:H:96:ILE:CD1	2.40	0.52
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.91	0.52
2:B:136:THR:HG21	4:D:118:ARG:HG2	1.90	0.52
3:C:104:ASN:O	22:r:97:PRO:HD3	2.10	0.52
3:C:170:TRP:CZ2	16:W:91:MET:HE1	2.44	0.52
4:D:97:LEU:HD22	4:D:99:LEU:CD2	2.39	0.52
4:D:101:LEU:HG	4:D:106:VAL:HA	1.91	0.52
4:D:256:ASP:O	18:Z:25:LEU:HD21	2.10	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.52
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.52
10:P:236:VAL:HG11	10:P:270:ARG:HH21	1.75	0.52
10:P:283:MET:HE2	10:P:366:ILE:HG22	1.92	0.52
10:P:305:PHE:CG	10:P:314:THR:HG22	2.44	0.52
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.52
21:q:65:THR:CG2	21:q:66:THR:N	2.72	0.52
1:A:113:TRP:CH2	8:H:287:HIS:HD2	2.27	0.52
2:B:127:GLN:H	2:B:127:GLN:CD	2.18	0.52
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.92	0.52
5:E:39:VAL:HG21	7:G:163:LYS:NZ	2.25	0.52
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.40	0.52
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.52
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.52
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.52
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.52
8:H:200:LEU:C	8:H:200:LEU:HD12	2.35	0.52
14:T:79:ILE:CG2	14:T:145:VAL:HG13	2.40	0.52
18:Z:139:GLY:O	19:a:45:TRP:CZ2	2.63	0.52
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.52
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.91	0.52
1:A:73:LEU:O	8:H:160:TYR:OH	2.25	0.52
4:D:145:MET:O	4:D:148:GLU:N	2.42	0.52
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.45	0.52
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.52
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.44	0.52
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.91	0.52
10:P:353:LEU:HA	10:P:356:HIS:HD2	1.74	0.52
1:A:21:ALA:HB2	8:H:218:GLY:HA3	1.90	0.52
1:A:113:TRP:CH2	8:H:287:HIS:CD2	2.98	0.52
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.43	0.52
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.52
6:F:411:SER:HA	6:F:414:GLU:CD	2.34	0.52
7:G:179:CYS:HG	25:G:802:SF4:FE3	1.26	0.52
7:G:541:PRO:HB2	7:G:561:PRO:HD3	1.91	0.52
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.44	0.52
10:P:157:LYS:O	10:P:158:GLU:C	2.53	0.52
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.52
20:b:48:ALA:O	20:b:49:THR:C	2.53	0.52
21:q:29:ARG:HD3	21:q:74:PHE:CD1	2.44	0.52
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.75	0.52
4:D:299:GLN:HB3	22:r:104:TRP:CE3	2.45	0.51
8:H:142:TYR:CA	8:H:289:LEU:CD1	2.74	0.51
8:H:172:MET:HE1	18:Z:46:GLY:HA3	1.91	0.51
16:W:97:ILE:C	16:W:99:VAL:H	2.18	0.51
21:q:125:VAL:HG23	21:q:125:VAL:O	2.08	0.51
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.45	0.51
3:C:241:PHE:H	7:G:146:PHE:HE1	1.58	0.51
4:D:218:SER:CB	4:D:224:ALA:HB1	2.41	0.51
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.25	0.51
4:D:304:LYS:HE2	9:I:35:THR:N	2.24	0.51
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.51
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.51
7:G:639:LEU:HD23	7:G:639:LEU:C	2.36	0.51
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.92	0.51
1:A:105:GLU:HG3	1:A:111:LEU:HG	1.91	0.51
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.45	0.51
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	2.98	0.51
5:E:196:THR:O	5:E:197:PRO:C	2.54	0.51
6:F:331:VAL:O	6:F:335:VAL:HG23	2.10	0.51
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.99	0.51
10:P:192:ARG:NH1	10:P:198:ALA:HB3	2.25	0.51
18:Z:61:LEU:O	18:Z:64:ASP:OD1	2.29	0.51
4:D:260:GLU:HG3	18:Z:25:LEU:CD2	2.40	0.51
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.75	0.51
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.11	0.51
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.51
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.92	0.51
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.51
8:H:93:HIS:CD2	19:a:27:HIS:ND1	2.63	0.51
9:I:68:ARG:NH2	18:Z:26:PRO:O	2.43	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.45	0.51
10:P:336:GLU:CG	10:P:342:PRO:HD3	2.38	0.51
14:T:87:LEU:HD23	14:T:122:MET:CE	2.41	0.51
16:W:94:GLN:HA	16:W:97:ILE:HG22	1.92	0.51
17:X:137:LEU:HG	17:X:138:PRO:HD2	1.92	0.51
1:A:106:TRP:CD1	1:A:111:LEU:HD12	2.45	0.51
4:D:338:ARG:HB3	18:Z:21:TYR:O	2.11	0.51
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.51
9:I:71:GLY:O	22:r:15:ALA:HB1	2.11	0.51
9:I:155:CYS:SG	25:I:302:SF4:S2	3.08	0.51
10:P:207:PHE:HE1	10:P:214:LEU:HD22	1.76	0.51
16:W:65:LYS:HE3	16:W:69:MET:HE2	1.92	0.51
17:X:29:ALA:CB	18:Z:71:LEU:CD1	2.88	0.51
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:ARG:HB3	6:F:289:GLU:CD	2.36	0.51
6:F:225:LEU:HB2	11:Q:160:TYR:CZ	2.45	0.51
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.41	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
9:I:68:ARG:HH21	18:Z:26:PRO:HD2	1.76	0.51
10:P:65:LEU:HD23	10:P:129:LEU:HD22	1.93	0.51
1:A:11:ILE:CD1	24:A:401:3PE:H2D1	2.41	0.51
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.51
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.51
10:P:135:GLU:CG	10:P:140:ASP:HA	2.41	0.51
17:X:128:VAL:HG23	20:b:55:VAL:O	2.11	0.51
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.93	0.51
3:C:124:ARG:HD2	11:Q:140:LYS:HZ1	1.76	0.51
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.69	0.51
6:F:217:GLU:CD	11:Q:166:TRP:HE1	2.18	0.51
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.51
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.51
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.51
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.51
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.51
14:T:130:ILE:HG23	14:T:131:PRO:CD	2.40	0.51
2:B:171:TYR:CE1	4:D:120:THR:HG22	2.46	0.51
4:D:166:ARG:NH1	18:Z:9:ASP:O	2.22	0.51
4:D:348:LEU:HB3	18:Z:16:TYR:CD2	2.46	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:310:PHE:O	20:b:38:TYR:HB2	2.11	0.51
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.51
10:P:209:ARG:N	10:P:352:VAL:HG22	2.26	0.51
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.51
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.51
19:a:3:PHE:O	19:a:6:LEU:HG	2.11	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
2:B:125:PRO:HB3	2:B:148:VAL:HG13	1.93	0.50
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.24	0.50
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.50
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.50
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:172:ALA:H	10:P:202:ARG:HH21	1.59	0.50
10:P:305:PHE:HB2	10:P:314:THR:HG22	1.92	0.50
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.64	0.50
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.50
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.50
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.50
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.50
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.50
8:H:200:LEU:HD22	8:H:282:TYR:HD1	1.76	0.50
11:Q:167:ASN:C	11:Q:168:LYS:HG2	2.36	0.50
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.50
16:W:120:ASP:HB3	16:W:123:SER:HG	1.76	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
17:X:25:LEU:O	17:X:29:ALA:N	2.44	0.50
4:D:80:MET:HB3	4:D:101:LEU:H	1.76	0.50
4:D:259:GLU:C	4:D:261:MET:N	2.68	0.50
4:D:260:GLU:CG	18:Z:25:LEU:HD22	2.40	0.50
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.50
5:E:134:CYS:SG	5:E:139:CYS:SG	3.06	0.50
5:E:188:ASN:O	5:E:189:ASP:HB3	2.10	0.50
7:G:126:LEU:HD11	12:R:89:PRO:CB	2.41	0.50
10:P:234:LYS:HG2	10:P:234:LYS:O	2.10	0.50
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.50
14:T:105:MET:HB2	14:T:139:MET:SD	2.51	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.50
4:D:359:ASP:O	7:G:150:ARG:NH2	2.44	0.50
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.93	0.50
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.50
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.50
7:G:651:PRO:HD2	13:S:56:ARG:HD2	1.93	0.50
4:D:145:MET:O	4:D:146:CYS:C	2.54	0.50
4:D:259:GLU:C	4:D:261:MET:H	2.18	0.50
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.50
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.50
6:F:185:ASN:HA	6:F:189:SER:O	2.11	0.50
10:P:108:TRP:CZ2	29:P:401:NDP:H2A	2.46	0.50
17:X:29:ALA:HB2	18:Z:71:LEU:CD1	2.36	0.50
17:X:49:GLU:HB3	17:X:138:PRO:HG3	1.93	0.50
18:Z:66:GLU:HA	18:Z:69:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:135:ASN:ND2	19:a:52:ARG:NH1	2.59	0.50
1:A:19:LEU:O	1:A:20:VAL:C	2.50	0.50
2:B:84:TRP:HA	2:B:87:ARG:HG2	1.93	0.50
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.50
10:P:212:ARG:O	10:P:213:PHE:C	2.55	0.50
10:P:238:GLN:HB2	10:P:270:ARG:HG2	1.94	0.50
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.11	0.50
12:R:55:VAL:HG22	12:R:56:ASN:H	1.77	0.50
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.50
14:T:103:HIS:HD1	14:T:140:CYS:HG	1.50	0.50
15:V:44:TYR:CD1	15:V:48:THR:HG23	2.46	0.50
20:b:11:ASN:OD1	20:b:12:ALA:N	2.44	0.50
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.73	0.50
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.50
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.50
18:Z:129:THR:HG22	18:Z:131:GLU:H	1.77	0.50
1:A:54:LYS:O	1:A:58:VAL:HG23	2.12	0.50
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.50
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.50
5:E:245:GLN:HB3	6:F:256:ARG:O	2.11	0.50
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.50
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
6:F:383:THR:O	6:F:384:PRO:C	2.55	0.50
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.50
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.50
10:P:367:GLU:HG2	10:P:368:GLU:N	2.26	0.50
10:P:374:THR:HG23	10:P:374:THR:O	2.11	0.50
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.50
19:a:4:GLU:O	19:a:7:PRO:HD2	2.11	0.50
2:B:99:CYS:O	2:B:101:ALA:N	2.44	0.50
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.50
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.50
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.50
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.50
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.50
14:T:140:CYS:HB2	14:T:143:GLU:CG	2.40	0.50
14:T:140:CYS:O	14:T:144:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.50
17:X:38:LYS:O	17:X:42:GLU:HG3	2.11	0.50
2:B:171:TYR:HE1	4:D:120:THR:HG22	1.76	0.49
3:C:79:CYS:O	3:C:80:LEU:CB	2.60	0.49
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.49
13:S:36:PHE:CZ	13:S:44:LEU:HD11	2.37	0.49
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.46	0.49
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.30	0.49
4:D:99:LEU:HD22	4:D:109:CYS:SG	2.52	0.49
5:E:70:PRO:HB3	23:s:60:PRO:HG3	1.92	0.49
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.42	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.12	0.49
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.49
13:S:24:CYS:N	13:S:58:CYS:SG	2.85	0.49
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.49
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.49
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.94	0.49
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.49
6:F:342:LEU:HD12	6:F:349:LEU:CA	2.42	0.49
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.92	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.94	0.49
10:P:192:ARG:CZ	10:P:200:ILE:HD11	2.42	0.49
10:P:205:ASP:OD1	10:P:205:ASP:O	2.30	0.49
15:V:56:LEU:HA	15:V:59:VAL:HB	1.94	0.49
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.93	0.49
16:W:32:LYS:CD	31:W:201:EHZ:C19	2.90	0.49
2:B:127:GLN:NE2	8:H:215:TYR:O	2.46	0.49
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.13	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.48	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
8:H:249:ILE:HD11	17:X:99:HIS:HB3	1.93	0.49
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.49
14:T:88:LYS:NZ	14:T:96:GLU:H	2.11	0.49
1:A:18:ILE:O	1:A:21:ALA:HB3	2.13	0.49
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.42	0.49
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:ASP:OD1	4:D:148:GLU:HG2	2.12	0.49
4:D:460:GLU:O	4:D:463:ARG:HG2	2.11	0.49
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.49
6:F:49:HIS:O	6:F:50:ASP:C	2.54	0.49
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.49
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.49
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.49
8:H:311:THR:HB	18:Z:51:MET:SD	2.52	0.49
10:P:59:PHE:CB	10:P:130:ILE:HD11	2.42	0.49
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.49
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.94	0.49
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
8:H:19:PHE:CE1	19:a:11:ILE:HD12	2.47	0.49
8:H:155:LEU:O	8:H:315:PRO:HG3	2.12	0.49
9:I:106:TYR:O	9:I:107:PRO:C	2.55	0.49
10:P:70:VAL:HG12	10:P:97:MET:SD	2.52	0.49
17:X:73:GLN:OE1	17:X:117:TRP:HZ2	1.96	0.49
17:X:112:LEU:HD13	17:X:118:VAL:HG22	1.95	0.49
17:X:126:SER:HB2	18:Z:66:GLU:HG2	1.94	0.49
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.95	0.49
3:C:224:GLU:OE2	10:P:45:LYS:HB3	2.13	0.49
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49
4:D:142:VAL:CG2	4:D:185:MET:CE	2.90	0.49
6:F:427:LEU:HB2	27:F:501:FMN:C7M	2.43	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:34:VAL:HG11	7:G:96:VAL:HG22	1.94	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
9:I:154:TYR:CD1	9:I:154:TYR:N	2.81	0.49
10:P:150:ARG:O	10:P:151:ALA:C	2.55	0.49
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.43	0.49
12:R:67:GLN:HG2	12:R:109:LEU:HD21	1.95	0.49
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.49
1:A:11:ILE:HD11	24:A:401:3PE:H2D1	1.95	0.49
4:D:289:SER:N	4:D:293:LEU:HG	2.27	0.49
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.49
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.24	0.49
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.30	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:49:ASP:O	9:I:50:MET:C	2.55	0.49
10:P:315:THR:H	10:P:318:LYS:HB3	1.76	0.49
17:X:38:LYS:HD2	17:X:38:LYS:HA	1.67	0.49
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.49
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.49
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.27	0.49
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.49
6:F:343:VAL:O	6:F:344:GLN:C	2.54	0.49
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.95	0.49
14:T:87:LEU:CD2	14:T:104:PHE:HZ	2.12	0.49
17:X:69:ASN:O	17:X:70:PHE:C	2.56	0.49
6:F:126:LYS:HG3	6:F:275:LEU:HB3	1.94	0.49
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.49
8:H:17:MET:CE	8:H:225:MET:HB3	2.41	0.49
14:T:90:TYR:HE2	14:T:92:LYS:HB3	1.78	0.49
2:B:117:PHE:HA	8:H:39:ILE:HG21	1.95	0.48
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.48
6:F:379:CYS:SG	25:F:502:SF4:S1	3.11	0.48
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.48
7:G:272:ARG:HH11	7:G:274:LEU:HD23	1.77	0.48
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.48
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.48
9:I:50:MET:HB3	18:Z:33:TYR:OH	2.13	0.48
13:S:42:VAL:O	13:S:46:LYS:HG3	2.12	0.48
16:W:42:TRP:CE2	16:W:93:LEU:HD12	2.47	0.48
17:X:115:LEU:HD13	17:X:117:TRP:CZ3	2.48	0.48
2:B:99:CYS:C	2:B:101:ALA:H	2.19	0.48
3:C:73:GLN:HE21	15:V:112:TRP:HE1	1.60	0.48
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.26	0.48
5:E:142:ARG:O	5:E:143:ASP:HB2	2.13	0.48
5:E:222:PHE:O	5:E:223:CYS:C	2.56	0.48
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.48
7:G:33:GLU:OE2	7:G:40:SER:HA	2.14	0.48
9:I:55:ASP:OD1	18:Z:32:GLY:N	2.44	0.48
10:P:64:PHE:CZ	10:P:211:ASP:HB3	2.48	0.48
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.48
19:a:2:TRP:O	19:a:3:PHE:C	2.53	0.48
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.48
3:C:176:PHE:CE1	16:W:87:ILE:HG21	2.48	0.48
4:D:94:VAL:HG13	4:D:458:PHE:CD2	2.48	0.48
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.48
9:I:53:ALA:O	9:I:54:THR:C	2.56	0.48
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.48
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.48
17:X:80:GLU:O	17:X:81:PRO:C	2.56	0.48
18:Z:143:TYR:HE2	19:a:36:LYS:NZ	2.11	0.48
19:a:37:ARG:CB	19:a:48:MET:HE2	2.43	0.48
1:A:109:LYS:HD2	1:A:112:GLU:OE2	2.14	0.48
2:B:174:SER:HB2	4:D:123:LEU:HD21	1.96	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
4:D:142:VAL:HG13	4:D:207:ARG:HH12	1.78	0.48
4:D:148:GLU:O	4:D:149:GLN:C	2.56	0.48
4:D:250:ASN:O	4:D:251:PHE:C	2.54	0.48
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.41	0.48
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.95	0.48
14:T:119:ILE:HG13	14:T:135:ALA:HB1	1.95	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
3:C:234:LEU:O	4:D:387:GLU:HG3	2.13	0.48
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.48
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.49	0.48
4:D:279:THR:HA	15:V:12:VAL:CG1	2.43	0.48
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.48
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.48
5:E:143:ASP:O	5:E:144:SER:C	2.55	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.48
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.48
10:P:191:VAL:CG1	10:P:192:ARG:HH21	2.26	0.48
11:Q:64:LEU:HD12	16:W:85:LEU:HD21	1.96	0.48
14:T:138:LEU:HD13	14:T:144:ILE:CD1	2.42	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48
4:D:338:ARG:NH2	18:Z:23:ARG:CB	2.77	0.48
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.49	0.48
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.48
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
8:H:224:PHE:CZ	28:H:400:UQ9:H11	2.49	0.48
9:I:49:ASP:O	9:I:53:ALA:N	2.41	0.48
13:S:50:ASN:O	13:S:51:LEU:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.95	0.48
16:W:46:VAL:N	16:W:47:PRO:HD2	2.29	0.48
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.93	0.48
18:Z:86:ILE:CG2	18:Z:128:ARG:HE	2.16	0.48
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.49	0.48
3:C:151:PRO:HG2	16:W:23:ILE:HG23	1.96	0.48
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.48
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.79	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.44	0.48
10:P:170:LEU:HG	10:P:171:ASN:N	2.28	0.48
10:P:304:LEU:O	10:P:307:LEU:HB3	2.14	0.48
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.48
2:B:224:ARG:HG3	10:P:85:ARG:HH22	1.79	0.48
4:D:81:THR:H	4:D:100:GLU:HA	1.79	0.48
4:D:97:LEU:O	4:D:99:LEU:HG	2.13	0.48
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.48
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.96	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.48
12:R:89:PRO:HG2	12:R:106:TYR:CE2	2.49	0.48
4:D:202:TRP:CH2	9:I:72:MET:HG2	2.48	0.48
4:D:248:SER:CB	18:Z:19:ILE:HD13	2.44	0.48
7:G:82:ILE:HG21	7:G:100:TRP:HB3	1.96	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
8:H:200:LEU:HD22	8:H:282:TYR:CD1	2.49	0.48
10:P:79:GLN:NE2	10:P:102:GLN:O	2.47	0.48
11:Q:160:TYR:CE1	11:Q:164:PHE:HZ	2.25	0.48
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.48
23:s:55:PHE:O	23:s:56:ARG:C	2.57	0.48
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.48
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.44	0.48
4:D:338:ARG:NH2	18:Z:23:ARG:HB3	2.29	0.48
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.48
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48
6:F:270:ASN:ND2	6:F:338:ASP:HB3	2.29	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.49	0.48
8:H:249:ILE:CD1	17:X:99:HIS:HB3	2.44	0.48
9:I:114:ILE:HD13	12:R:106:TYR:CD1	2.48	0.48
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.13	0.48
11:Q:160:TYR:CD2	11:Q:164:PHE:CE2	2.91	0.48
14:T:104:PHE:CZ	14:T:118:ILE:HG21	2.48	0.48
1:A:102:LEU:HG	1:A:106:TRP:HE1	1.79	0.47
2:B:100:CYS:HG	25:B:301:SF4:FE4	1.27	0.47
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.47
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.47
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.47
16:W:120:ASP:OD1	16:W:121:PHE:N	2.46	0.47
18:Z:62:ILE:HG23	20:b:50:PRO:CD	2.44	0.47
18:Z:85:GLN:O	18:Z:89:GLU:HG3	2.14	0.47
20:b:68:SER:O	20:b:69:HIS:C	2.56	0.47
21:q:55:PHE:CD1	22:r:26:LEU:CD2	2.95	0.47
22:r:109:ASP:O	22:r:110:GLN:OE1	2.32	0.47
1:A:113:TRP:CH2	8:H:287:HIS:HB2	2.49	0.47
6:F:425:CYS:SG	25:F:502:SF4:S4	3.13	0.47
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.48	0.47
8:H:66:THR:HA	8:H:124:ASN:OD1	2.13	0.47
10:P:360:ARG:HD3	10:P:360:ARG:O	2.15	0.47
3:C:70:LYS:HB2	15:V:99:PRO:O	2.14	0.47
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.47
4:D:299:GLN:OE1	22:r:104:TRP:HB2	2.14	0.47
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:82:ILE:HG23	7:G:100:TRP:HB3	1.96	0.47
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.96	0.47
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.47
10:P:55:VAL:HG12	10:P:123:SER:HA	1.96	0.47
10:P:197:GLU:HB3	10:P:259:VAL:HG23	1.93	0.47
10:P:228:LEU:HD11	10:P:288:PHE:HZ	1.78	0.47
17:X:4:ILE:CG2	17:X:5:VAL:N	2.50	0.47
1:A:72:LEU:HB3	8:H:151:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ASP:O	2:B:116:ARG:C	2.55	0.47
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.47
5:E:221:ARG:HH21	5:E:227:ALA:HB2	1.79	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.47
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.47
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.47
7:G:541:PRO:HB2	7:G:561:PRO:CG	2.44	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
10:P:235:THR:O	10:P:236:VAL:C	2.56	0.47
10:P:311:GLU:O	10:P:312:PRO:C	2.57	0.47
15:V:56:LEU:HD12	15:V:57:ASP:CA	2.44	0.47
17:X:17:GLU:HB3	17:X:19:LYS:HG3	1.96	0.47
17:X:130:LYS:HE2	20:b:67:PRO:HB3	1.92	0.47
24:A:401:3PE:O14	24:A:401:3PE:N	2.38	0.47
5:E:45:GLU:H	5:E:45:GLU:CD	2.21	0.47
6:F:110:PRO:O	6:F:238:CYS:HB3	2.15	0.47
6:F:213:ILE:CG2	6:F:224:ARG:HH21	2.27	0.47
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.97	0.47
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.93	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
9:I:188:GLU:OE1	12:R:56:ASN:CB	2.63	0.47
10:P:294:PRO:HB3	10:P:296:PHE:HD1	1.79	0.47
16:W:46:VAL:O	16:W:50:VAL:HG23	2.14	0.47
1:A:92:PHE:CD2	20:b:30:ILE:HD12	2.48	0.47
1:A:108:GLN:C	1:A:110:GLY:N	2.72	0.47
4:D:264:ASN:O	9:I:65:GLU:OE1	2.32	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.47
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.47
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.14	0.47
7:G:496:MET:O	7:G:500:ILE:HG13	2.14	0.47
8:H:179:TRP:CD1	18:Z:43:LEU:CD2	2.96	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.47
10:P:76:MET:HE1	10:P:254:LYS:CE	2.45	0.47
10:P:276:LEU:O	10:P:280:ILE:HG13	2.15	0.47
10:P:335:LEU:O	10:P:336:GLU:HB2	2.15	0.47
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.47
17:X:139:GLU:O	17:X:140:ASN:C	2.57	0.47
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.47
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:301:SF4:S4	4:D:138:ARG:HD3	2.55	0.47
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.47
3:C:209:LEU:HD21	16:W:108:ARG:NH1	2.29	0.47
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.47
4:D:142:VAL:HG21	4:D:185:MET:CE	2.41	0.47
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.45	0.47
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.47
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.50	0.47
6:F:299:LEU:HD11	6:F:300:ILE:HG23	1.95	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	0.47
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
10:P:209:ARG:O	10:P:210:GLU:HB2	2.15	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
12:R:32:THR:CG2	12:R:36:GLN:H	2.18	0.47
12:R:88:HIS:HE1	12:R:91:VAL:HG22	1.80	0.47
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.44	0.47
20:b:69:HIS:HD2	20:b:70:PRO:CD	2.26	0.47
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.50	0.47
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.47
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.47
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.47
8:H:140:ILE:HG13	8:H:141:SER:N	2.30	0.47
9:I:123:CYS:SG	25:I:302:SF4:S4	3.13	0.47
9:I:209:TYR:CG	12:R:86:LEU:HD21	2.50	0.47
10:P:287:THR:HG23	10:P:289:ILE:HD11	1.97	0.47
13:S:58:CYS:HB2	13:S:61:VAL:CG1	2.43	0.47
16:W:32:LYS:O	16:W:36:ARG:HG3	2.15	0.47
17:X:90:ASP:OD2	19:a:62:VAL:HG11	2.15	0.47
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.29	0.47
6:F:39:ASP:CA	6:F:261:TRP:HZ2	2.28	0.47
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
8:H:134:ARG:HH21	8:H:200:LEU:HD13	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
9:I:35:THR:HG22	22:r:107:SER:HA	1.97	0.47
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.96	0.47
10:P:207:PHE:CD2	10:P:241:TYR:HD1	2.33	0.47
15:V:116:ILE:O	15:V:116:ILE:CG2	2.61	0.47
17:X:39:THR:CG2	17:X:40:ASN:N	2.77	0.47
20:b:69:HIS:CD2	20:b:71:GLN:H	2.33	0.47
21:q:14:VAL:HA	21:q:23:LEU:HD13	1.97	0.47
2:B:136:THR:HG21	2:B:177:VAL:CG2	2.44	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.48	0.47
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.14	0.47
7:G:275:PRO:HB3	7:G:286:ILE:HG23	1.96	0.47
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.47
8:H:307:LEU:O	8:H:311:THR:OG1	2.28	0.47
17:X:7:LEU:HD13	18:Z:87:LEU:C	2.40	0.47
21:q:48:TYR:OH	21:q:83:PRO:HD2	2.15	0.47
2:B:93:MET:HB2	2:B:128:ALA:HB2	1.97	0.46
3:C:134:LEU:H	3:C:134:LEU:HD12	1.81	0.46
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.98	0.46
6:F:281:HIS:HB3	6:F:358:ASP:CG	2.40	0.46
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	0.46
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.97	0.46
2:B:99:CYS:O	2:B:102:VAL:N	2.45	0.46
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.49	0.46
4:D:280:ALA:CB	15:V:11:LEU:CG	2.90	0.46
6:F:51:TRP:HZ2	23:s:36:GLN:HG3	1.80	0.46
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.46
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.46
9:I:171:PRO:HB3	21:q:93:MET:CE	2.38	0.46
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.97	0.46
17:X:115:LEU:HD13	17:X:117:TRP:CZ2	2.51	0.46
18:Z:28:ARG:O	18:Z:28:ARG:CG	2.64	0.46
18:Z:87:LEU:HD21	18:Z:119:PRO:HG3	1.97	0.46
2:B:99:CYS:O	2:B:100:CYS:C	2.57	0.46
3:C:55:LYS:HB3	3:C:55:LYS:HE2	1.84	0.46
3:C:141:ARG:NH1	4:D:410:TYR:CE1	2.80	0.46
4:D:351:MET:O	18:Z:10:MET:HE3	2.15	0.46
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.98	0.46
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.03	0.46
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.46
12:R:33:HIS:HE1	12:R:56:ASN:HD22	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.39	0.46
17:X:41:LYS:O	17:X:42:GLU:C	2.59	0.46
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.28	0.46
21:q:8:LYS:HG2	21:q:12:GLN:HE21	1.79	0.46
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.46
2:B:116:ARG:HA	8:H:37:PRO:HA	1.97	0.46
2:B:140:LYS:O	2:B:143:PRO:HD2	2.14	0.46
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.39	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
6:F:299:LEU:CD1	6:F:300:ILE:N	2.68	0.46
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.46
8:H:306:SER:OG	20:b:33:PRO:HG3	2.16	0.46
9:I:64:THR:HG21	18:Z:35:MET:HE1	1.98	0.46
12:R:38:TYR:CD1	12:R:44:ARG:HB2	2.51	0.46
16:W:71:MET:C	16:W:73:ASN:N	2.70	0.46
16:W:99:VAL:HG13	16:W:99:VAL:O	2.15	0.46
17:X:91:TYR:OH	19:a:28:LYS:HE2	2.15	0.46
19:a:22:SER:O	19:a:23:THR:C	2.57	0.46
19:a:49:GLU:CD	19:a:52:ARG:HH11	2.22	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
4:D:92:HIS:CD2	4:D:457:VAL:HA	2.50	0.46
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.46
5:E:184:MET:HG3	5:E:192:TYR:O	2.16	0.46
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.51	0.46
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.46
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.46
20:b:28:LEU:O	20:b:32:MET:HG2	2.16	0.46
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.46
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.46
4:D:279:THR:HG23	15:V:13:GLY:CA	2.23	0.46
5:E:143:ASP:O	5:E:146:SER:N	2.49	0.46
6:F:251:SER:N	6:F:252:PRO:HD2	2.30	0.46
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.46
10:P:245:VAL:HA	10:P:265:PHE:CD2	2.49	0.46
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.46
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.46
14:T:114:ASP:OD1	16:W:67:ARG:NH1	2.48	0.46
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.50	0.46
16:W:50:VAL:HA	16:W:55:LEU:HD12	1.97	0.46
23:s:52:LEU:HB3	23:s:56:ARG:HH11	1.81	0.46
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.97	0.46
4:D:80:MET:CE	4:D:101:LEU:HB2	2.46	0.46
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.46
4:D:348:LEU:HB3	18:Z:16:TYR:CE2	2.51	0.46
4:D:368:ARG:NH2	9:I:165:ASP:HB2	2.31	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
8:H:288:LEU:HD11	24:I:301:3PE:H222	1.98	0.46
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.46
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.46
6:F:44:ASN:ND2	6:F:133:HIS:O	2.48	0.46
6:F:51:TRP:CB	6:F:133:HIS:O	2.64	0.46
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.46
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.46
10:P:131:GLY:HA3	29:P:401:NDP:O3D	2.15	0.46
10:P:285:HIS:CE1	10:P:364:SER:HB3	2.51	0.46
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.46
15:V:56:LEU:HD13	15:V:60:LYS:HE2	1.98	0.46
17:X:5:VAL:CG1	17:X:7:LEU:HG	2.46	0.46
17:X:35:GLN:HG3	17:X:70:PHE:HE1	1.80	0.46
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
5:E:145:ASP:O	5:E:146:SER:C	2.56	0.46
7:G:163:LYS:HE2	12:R:97:LYS:NZ	2.31	0.46
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.46
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.46
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.46
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.46
10:P:66:GLY:O	10:P:69:VAL:N	2.48	0.46
10:P:157:LYS:O	10:P:160:GLY:N	2.49	0.46
10:P:261:LYS:HB2	10:P:263:PHE:CE1	2.51	0.46
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.48	0.46
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.46
17:X:20:VAL:CG2	17:X:24:VAL:HG21	2.40	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.59	0.46
1:A:25:PRO:HG3	8:H:60:PRO:CD	2.42	0.46
24:A:401:3PE:H352	24:A:401:3PE:H262	1.98	0.46
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.16	0.46
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.97	0.46
4:D:271:ARG:CD	8:H:279:ARG:O	2.62	0.46
5:E:163:THR:O	5:E:166:LYS:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:235:THR:HG22	10:P:323:HIS:O	2.15	0.46
12:R:32:THR:HA	12:R:55:VAL:CG2	2.45	0.46
15:V:22:GLU:O	15:V:26:ILE:HG12	2.16	0.46
17:X:41:LYS:HD2	20:b:56:PRO:HG3	1.97	0.46
21:q:71:LYS:HB2	21:q:73:THR:HG23	1.98	0.46
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.45
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.45
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.44	0.45
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.45
6:F:35:LEU:HG	6:F:39:ASP:HB2	1.97	0.45
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.45
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.96	0.45
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.45
10:P:310:PHE:O	10:P:311:GLU:C	2.60	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
14:T:87:LEU:CD2	14:T:122:MET:HE1	2.46	0.45
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.45
16:W:32:LYS:CE	31:W:201:EHZ:C19	2.90	0.45
17:X:133:THR:HG23	20:b:58:ARG:HH12	1.81	0.45
19:a:58:ASN:HB2	19:a:61:TYR:CE2	2.50	0.45
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.45
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.99	0.45
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.97	0.45
5:E:45:GLU:O	5:E:50:THR:HG21	2.15	0.45
6:F:137:LYS:HG2	6:F:249:ALA:HB1	1.98	0.45
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.45
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.45
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.45
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	0.45
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.45
10:P:259:VAL:H	10:P:261:LYS:HG2	1.82	0.45
14:T:117:GLU:HG2	16:W:43:TYR:CZ	2.51	0.45
18:Z:140:PHE:O	18:Z:141:THR:C	2.56	0.45
20:b:45:ILE:N	20:b:80:TRP:HH2	2.14	0.45
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.98	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.45
8:H:25:ARG:NH1	28:H:400:UQ9:H10A	2.32	0.45
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.45
10:P:170:LEU:HD12	10:P:171:ASN:H	1.81	0.45
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.32	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
3:C:243:ALA:C	7:G:105:ASN:ND2	2.75	0.45
4:D:198:THR:HA	8:H:32:GLN:HG2	1.98	0.45
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.45
6:F:227:PRO:HB2	6:F:228:PRO:HD3	1.99	0.45
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.45
7:G:283:GLU:O	7:G:283:GLU:CG	2.51	0.45
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.45
10:P:156:SER:HB2	10:P:161:VAL:CG2	2.46	0.45
12:R:39:ASP:CG	12:R:40:GLU:N	2.74	0.45
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.45
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.45
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.45
15:V:56:LEU:HD11	15:V:57:ASP:OD1	2.17	0.45
4:D:87:GLN:OE1	4:D:87:GLN:N	2.49	0.45
4:D:239:GLY:H	18:Z:9:ASP:CG	2.25	0.45
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.45
4:D:266:ARG:HD3	24:I:301:3PE:O14	2.16	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
4:D:446:ASP:O	4:D:450:ILE:HG13	2.17	0.45
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.45
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.45
8:H:179:TRP:HE1	18:Z:43:LEU:HG	1.82	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
9:I:90:LYS:HG2	21:q:90:LEU:HD21	1.97	0.45
13:S:42:VAL:HB	13:S:46:LYS:HE3	1.97	0.45
14:T:83:VAL:HG21	14:T:145:VAL:HG22	1.99	0.45
18:Z:66:GLU:HA	18:Z:69:ILE:CG1	2.46	0.45
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.51	0.45
3:C:98:PHE:HB2	15:V:94:MET:CE	2.47	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.45
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.45
7:G:97:MET:HB2	7:G:100:TRP:NE1	2.30	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:382:ARG:HD2	13:S:56:ARG:HD3	1.99	0.45
7:G:401:LEU:HD11	7:G:462:PHE:CE2	2.51	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:23:VAL:HG11	19:a:9:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:63:TRP:CZ2	24:I:301:3PE:H322	2.52	0.45
9:I:92:PRO:HB3	21:q:92:CYS:HB2	1.98	0.45
10:P:315:THR:HB	10:P:318:LYS:HB2	1.98	0.45
17:X:7:LEU:O	18:Z:88:ARG:CZ	2.64	0.45
3:C:75:VAL:HG23	3:C:83:LEU:HD11	1.98	0.45
5:E:163:THR:HG23	5:E:168:PHE:O	2.17	0.45
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.46	0.45
6:F:249:ALA:O	6:F:252:PRO:HD2	2.16	0.45
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.45
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.45
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.45
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.45
7:G:362:ASP:HB2	13:S:71:PHE:CD1	2.52	0.45
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.80	0.45
8:H:224:PHE:CZ	28:H:400:UQ9:C13	2.94	0.45
10:P:192:ARG:HH12	10:P:198:ALA:HB3	1.80	0.45
12:R:32:THR:HG21	21:q:129:THR:HG23	1.98	0.45
14:T:130:ILE:CG2	14:T:131:PRO:CD	2.95	0.45
17:X:40:ASN:O	17:X:41:LYS:C	2.58	0.45
18:Z:140:PHE:CD1	19:a:45:TRP:HB2	2.52	0.45
1:A:109:LYS:HA	1:A:112:GLU:CD	2.42	0.45
2:B:147:LYS:HA	2:B:147:LYS:HD2	1.74	0.45
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.45
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.45
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.74	0.45
5:E:52:PHE:O	5:E:99:LYS:HG3	2.17	0.45
6:F:224:ARG:HG2	11:Q:164:PHE:CZ	2.52	0.45
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.45
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.45
7:G:341:ILE:HD12	7:G:555:ILE:CG1	2.47	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.31	0.45
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.45
10:P:218:ALA:HB2	10:P:280:ILE:CG2	2.47	0.45
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.32	0.45
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.45
12:R:47:ARG:HG3	12:R:48:PHE:N	2.32	0.45
13:S:19:ILE:HD12	13:S:94:VAL:CG1	2.44	0.45
14:T:133:ILE:HG23	14:T:134:ASP:N	2.32	0.45
17:X:46:CYS:SG	17:X:135:ARG:NH1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:68:ARG:O	18:Z:69:ILE:C	2.60	0.45
3:C:73:GLN:NE2	15:V:107:PRO:HB3	2.31	0.45
4:D:92:HIS:O	4:D:94:VAL:HG12	2.16	0.45
5:E:222:PHE:H	5:E:225:GLU:CD	2.25	0.45
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.45
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.45
14:T:90:TYR:O	14:T:91:ASP:HB2	2.17	0.45
16:W:45:GLU:O	16:W:46:VAL:C	2.58	0.45
21:q:21:ARG:O	21:q:25:ARG:HG3	2.17	0.45
2:B:80:ASP:O	2:B:81:LEU:C	2.59	0.44
2:B:94:THR:HB	2:B:104:MET:CE	2.45	0.44
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.44
5:E:59:TYR:O	5:E:62:ILE:HB	2.17	0.44
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.44
6:F:398:ARG:HH12	6:F:408:GLU:CD	2.25	0.44
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.44
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.44
8:H:303:TRP:CZ3	20:b:28:LEU:HG	2.52	0.44
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.44
13:S:24:CYS:SG	13:S:61:VAL:HG12	2.58	0.44
20:b:38:TYR:O	20:b:39:THR:C	2.59	0.44
22:r:109:ASP:O	22:r:110:GLN:CG	2.64	0.44
23:s:52:LEU:O	23:s:56:ARG:HG2	2.17	0.44
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.32	0.44
4:D:258:VAL:O	4:D:261:MET:HB2	2.17	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
7:G:176:CYS:SG	25:G:802:SF4:S1	3.14	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.44
10:P:245:VAL:HA	10:P:265:PHE:HD2	1.82	0.44
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.44
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.44
18:Z:98:MET:HB2	18:Z:104:TRP:CE2	2.52	0.44
24:A:401:3PE:H112	18:Z:141:THR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:GLY:CA	2:B:101:ALA:HB2	2.40	0.44
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.44
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.44
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.17	0.44
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.83	0.44
5:E:162:THR:CG2	5:E:166:LYS:HA	2.46	0.44
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.44
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.83	0.44
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.44
7:G:450:LYS:HG3	7:G:450:LYS:O	2.17	0.44
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.80	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.44
14:T:79:ILE:O	14:T:83:VAL:HG23	2.17	0.44
14:T:118:ILE:CG2	14:T:122:MET:HE3	2.47	0.44
2:B:93:MET:CE	2:B:95:PHE:CE2	3.00	0.44
2:B:126:ARG:C	2:B:128:ALA:H	2.24	0.44
2:B:146:ARG:NH2	3:C:211:TYR:CZ	2.86	0.44
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.99	0.44
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.44
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.44
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.48	0.44
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.48	0.44
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.44
16:W:20:VAL:HG21	16:W:80:ARG:CZ	2.48	0.44
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.44
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.44
2:B:99:CYS:HB3	4:D:141:TYR:CD2	2.52	0.44
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.23	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.44
6:F:257:ARG:CG	6:F:261:TRP:CD2	2.93	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.57	0.44
7:G:607:LYS:HG2	11:Q:78:ARG:HH11	1.82	0.44
9:I:78:PHE:HB2	22:r:12:ARG:CG	2.48	0.44
9:I:79:ARG:HG2	22:r:12:ARG:NH2	2.29	0.44
9:I:188:GLU:OE1	12:R:56:ASN:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:130:ILE:N	10:P:130:ILE:HD12	2.33	0.44
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.44
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.44
11:Q:160:TYR:CE1	11:Q:164:PHE:CZ	3.02	0.44
12:R:79:CYS:O	12:R:88:HIS:CE1	2.71	0.44
14:T:119:ILE:CD1	14:T:138:LEU:HD11	2.43	0.44
19:a:37:ARG:HB2	19:a:48:MET:HE2	1.99	0.44
2:B:124:SER:HB3	2:B:125:PRO:HD2	2.00	0.44
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.44
3:C:170:TRP:CE2	16:W:91:MET:HE1	2.52	0.44
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
6:F:119:GLU:HB3	6:F:124:THR:HG22	2.00	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.44
6:F:427:LEU:HB2	27:F:501:FMN:HM73	2.00	0.44
8:H:176:LEU:O	18:Z:43:LEU:HD23	2.18	0.44
10:P:220:TYR:HA	10:P:223:PHE:CD2	2.51	0.44
10:P:305:PHE:CB	10:P:314:THR:HG22	2.47	0.44
14:T:82:ARG:NH2	14:T:126:PHE:HD1	2.15	0.44
14:T:92:LYS:O	14:T:92:LYS:HG2	2.16	0.44
18:Z:144:THR:OG1	19:a:48:MET:HE1	2.18	0.44
3:C:93:ILE:HD11	3:C:153:ASP:HB3	1.99	0.44
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.44
5:E:48:PRO:C	5:E:50:THR:N	2.74	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.52	0.44
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.97	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.44
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
8:H:171:HIS:HE1	18:Z:53:TRP:CE3	2.36	0.44
9:I:197:TRP:CZ3	21:q:84:PRO:HA	2.53	0.44
10:P:55:VAL:HA	10:P:79:GLN:O	2.18	0.44
10:P:168:SER:O	10:P:202:ARG:HA	2.17	0.44
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.44
13:S:16:LEU:CB	13:S:69:TYR:CD1	2.97	0.44
14:T:133:ILE:O	14:T:136:GLU:N	2.46	0.44
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.44
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.52	0.44
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.44
5:E:195:LEU:HD21	5:E:218:ARG:HG2	1.99	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	2.00	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.52	0.44
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.44
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.44
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.44
10:P:209:ARG:CA	10:P:352:VAL:HG22	2.47	0.44
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
14:T:117:GLU:HA	14:T:120:MET:CE	2.41	0.44
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.52	0.44
21:q:3:LEU:O	21:q:6:VAL:CG2	2.66	0.44
1:A:63:LEU:O	1:A:64:LEU:C	2.60	0.44
2:B:71:ALA:O	2:B:75:VAL:N	2.47	0.44
2:B:90:LEU:O	2:B:119:VAL:HA	2.18	0.44
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.81	0.44
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.98	0.44
4:D:92:HIS:ND1	4:D:92:HIS:O	2.47	0.44
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.44
6:F:225:LEU:N	11:Q:160:TYR:OH	2.39	0.44
6:F:292:MET:O	6:F:293:SER:OG	2.33	0.44
6:F:382:CYS:HA	7:G:74:ASN:O	2.17	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.44
7:G:466:LEU:O	7:G:467:LYS:C	2.61	0.44
8:H:63:PRO:HD2	8:H:66:THR:HG21	2.00	0.44
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44
12:R:39:ASP:H	12:R:42:ASP:CG	2.21	0.44
12:R:44:ARG:C	12:R:46:VAL:N	2.73	0.44
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.44
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.44
16:W:71:MET:O	16:W:72:LYS:C	2.59	0.44
1:A:112:GLU:O	1:A:113:TRP:C	2.58	0.43
5:E:81:VAL:O	5:E:82:LEU:C	2.60	0.43
5:E:90:GLY:HA3	5:E:126:VAL:HG12	1.99	0.43
6:F:294:VAL:CG1	6:F:337:MET:HG3	2.48	0.43
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.18	0.43
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.17	0.43
10:P:64:PHE:CE1	10:P:209:ARG:O	2.69	0.43
10:P:122:HIS:HB3	12:R:46:VAL:HG12	1.98	0.43
21:q:14:VAL:HG13	21:q:23:LEU:CD2	2.43	0.43
3:C:221:GLU:OE1	16:W:114:GLU:HB2	2.18	0.43
4:D:85:GLY:N	4:D:86:PRO:CD	2.80	0.43
4:D:232:VAL:CG2	4:D:356:ILE:HB	2.48	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
5:E:183:PRO:HB2	5:E:195:LEU:N	2.33	0.43
5:E:192:TYR:OH	5:E:213:PRO:HD2	2.18	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:126:LYS:O	6:F:129:GLU:HG2	2.18	0.43
8:H:89:LEU:HD12	8:H:89:LEU:HA	1.87	0.43
8:H:123:SER:HB3	8:H:214:GLU:HG3	2.00	0.43
10:P:76:MET:HE1	10:P:254:LYS:HE2	2.01	0.43
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.43
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.43
16:W:97:ILE:C	16:W:99:VAL:N	2.73	0.43
20:b:15:LYS:O	20:b:15:LYS:HG3	2.18	0.43
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.49	0.43
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.43
7:G:36:VAL:O	7:G:39:GLN:HG2	2.19	0.43
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.99	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.43
8:H:43:TYR:CE2	21:q:27:PHE:CZ	3.06	0.43
9:I:50:MET:O	9:I:51:LYS:C	2.60	0.43
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.43
13:S:51:LEU:HA	13:S:52:PRO:HD3	1.86	0.43
14:T:113:LEU:O	14:T:116:VAL:HB	2.17	0.43
18:Z:69:ILE:O	20:b:53:TYR:CE1	2.72	0.43
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.43
24:A:401:3PE:H2E1	24:A:401:3PE:H2H2	1.84	0.43
3:C:102:HIS:CE1	15:V:48:THR:CG2	2.89	0.43
3:C:136:PHE:O	3:C:137:ASN:C	2.60	0.43
4:D:144:MET:HE2	4:D:214:TYR:CE2	2.54	0.43
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:356:ASP:OD2	7:G:645:ARG:NE	2.51	0.43
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.77	0.43
9:I:78:PHE:HB2	22:r:12:ARG:HG2	2.00	0.43
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.43
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.83	0.43
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.43
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.43
12:R:45:ARG:HA	12:R:48:PHE:HE1	1.83	0.43
13:S:23:LEU:HB3	13:S:33:VAL:HG12	2.00	0.43
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.98	0.43
2:B:126:ARG:O	2:B:128:ALA:N	2.50	0.43
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.43
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.43
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.43
7:G:466:LEU:HD13	7:G:500:ILE:HD13	2.00	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
10:P:354:ARG:HG3	10:P:362:LEU:CD2	2.48	0.43
13:S:30:SER:O	13:S:33:VAL:N	2.51	0.43
14:T:109:GLY:O	14:T:110:LEU:C	2.61	0.43
1:A:23:TRP:O	1:A:26:GLN:HG3	2.19	0.43
2:B:70:ARG:HG3	2:B:70:ARG:O	2.18	0.43
2:B:117:PHE:HA	8:H:39:ILE:CG2	2.49	0.43
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.83	0.43
3:C:101:ASP:OD1	15:V:86:LYS:HE3	2.19	0.43
5:E:124:LYS:HB3	5:E:125:PRO:HD2	2.00	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
6:F:333:GLU:HG2	6:F:334:THR:N	2.34	0.43
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.43
7:G:117:MET:SD	7:G:143:SER:HB2	2.59	0.43
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.73	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
28:H:400:UQ9:H20B	28:H:400:UQ9:H22	1.87	0.43
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.83	0.43
12:R:91:VAL:HG11	12:R:106:TYR:HE2	1.82	0.43
21:q:79:GLY:O	21:q:82:VAL:HG22	2.19	0.43
1:A:73:LEU:O	1:A:76:PRO:HD2	2.18	0.43
1:A:87:MET:HE3	1:A:87:MET:HB3	1.84	0.43
24:A:401:3PE:HN2	24:A:401:3PE:P	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:LYS:O	15:V:103:LEU:HA	2.18	0.43
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.43
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.43
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.43
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:279:GLU:HG3	11:Q:154:LYS:HG3	2.00	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.43
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.28	0.43
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.96	0.43
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.43
9:I:90:LYS:HG3	21:q:90:LEU:CD2	2.48	0.43
10:P:170:LEU:O	10:P:171:ASN:CG	2.61	0.43
14:T:93:ILE:HD11	14:T:118:ILE:HD11	2.00	0.43
17:X:126:SER:O	20:b:54:PRO:CG	2.67	0.43
18:Z:108:GLU:O	18:Z:109:SER:C	2.61	0.43
1:A:106:TRP:CH2	20:b:19:LEU:HD21	2.53	0.43
3:C:124:ARG:HH12	3:C:125:PHE:HZ	1.56	0.43
4:D:94:VAL:O	4:D:94:VAL:HG22	2.18	0.43
5:E:140:MET:HE1	6:F:366:ALA:HA	2.01	0.43
6:F:340:ASP:O	6:F:343:VAL:HB	2.19	0.43
7:G:617:ARG:NH1	16:W:129:HIS:N	2.66	0.43
8:H:33:LEU:HD21	22:r:25:GLN:HG2	2.01	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
10:P:306:GLY:HA2	10:P:312:PRO:HB3	2.01	0.43
15:V:56:LEU:CD1	15:V:57:ASP:OD1	2.67	0.43
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.34	0.43
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.43
6:F:166:ALA:HB1	23:s:45:PHE:HD2	1.84	0.43
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.43
7:G:450:LYS:CD	7:G:453:GLN:HG3	2.32	0.43
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.43
9:I:162:CYS:SG	25:I:303:SF4:S2	3.17	0.43
12:R:88:HIS:ND1	12:R:89:PRO:O	2.50	0.43
17:X:123:GLY:HA2	18:Z:66:GLU:OE1	2.19	0.43
21:q:22:GLY:O	21:q:26:VAL:HG23	2.18	0.43
4:D:82:LEU:HB2	8:H:126:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.43
5:E:81:VAL:HB	5:E:104:LEU:HD11	2.00	0.43
5:E:138:PRO:CG	6:F:122:PRO:HB3	2.47	0.43
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.43
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.43
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.43
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.43
8:H:90:PRO:O	8:H:91:MET:C	2.60	0.43
8:H:138:GLN:HG3	8:H:139:THR:N	2.34	0.43
8:H:311:THR:O	18:Z:51:MET:HG3	2.17	0.43
10:P:376:ASN:O	10:P:377:TYR:C	2.61	0.43
17:X:7:LEU:CD1	18:Z:87:LEU:HB3	2.49	0.43
18:Z:129:THR:HG22	18:Z:131:GLU:N	2.33	0.43
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.43
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
2:B:94:THR:CB	2:B:104:MET:CE	2.97	0.42
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.42
4:D:198:THR:HG23	8:H:275:ALA:O	2.18	0.42
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.42
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.42
6:F:224:ARG:HD3	11:Q:164:PHE:CD1	2.54	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.42
6:F:392:MET:HE2	6:F:416:SER:HA	1.93	0.42
7:G:82:ILE:HG22	7:G:100:TRP:HE3	1.83	0.42
7:G:496:MET:HG2	7:G:500:ILE:HD11	2.01	0.42
8:H:14:LEU:HD23	8:H:14:LEU:HA	1.86	0.42
8:H:17:MET:HE1	8:H:225:MET:HE3	2.01	0.42
10:P:237:LYS:HE3	10:P:322:ILE:O	2.19	0.42
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.42
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.42
12:R:48:PHE:CD2	21:q:125:VAL:HG21	2.54	0.42
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.42
17:X:32:TYR:OH	18:Z:74:LEU:HB2	2.19	0.42
18:Z:74:LEU:O	18:Z:78:GLU:HG3	2.19	0.42
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.42
19:a:12:MET:HE2	19:a:12:MET:HB3	1.90	0.42
19:a:55:SER:O	19:a:56:GLY:C	2.61	0.42
21:q:4:VAL:HG23	21:q:5:GLU:N	2.33	0.42
21:q:5:GLU:HG3	21:q:9:ARG:HE	1.84	0.42
2:B:91:TRP:CE3	28:H:400:UQ9:H1M	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.42
5:E:165:ASP:O	5:E:166:LYS:C	2.62	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
6:F:413:TRP:CH2	6:F:436:GLN:HG2	2.53	0.42
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.42
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.42
8:H:257:THR:O	8:H:260:MET:HB3	2.19	0.42
10:P:259:VAL:N	10:P:261:LYS:HG2	2.33	0.42
11:Q:55:VAL:HG21	16:W:78:ASP:OD1	2.19	0.42
16:W:38:LEU:HG	16:W:70:PHE:HZ	1.84	0.42
16:W:120:ASP:OD1	16:W:120:ASP:C	2.61	0.42
18:Z:72:MET:O	18:Z:73:PRO:C	2.59	0.42
19:a:17:VAL:O	19:a:18:ILE:C	2.62	0.42
22:r:12:ARG:HB3	22:r:20:LEU:CD2	2.49	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.19	0.42
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
6:F:299:LEU:HD12	6:F:300:ILE:HG23	2.01	0.42
8:H:19:PHE:CB	19:a:12:MET:HG3	2.47	0.42
8:H:68:MET:HG3	8:H:68:MET:O	2.19	0.42
9:I:53:ALA:HB1	20:b:14:ALA:HB2	2.00	0.42
11:Q:85:ASN:C	11:Q:87:MET:N	2.76	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.54	0.42
17:X:10:LEU:H	17:X:10:LEU:HD12	1.84	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.42
4:D:345:GLU:HB2	18:Z:19:ILE:HD12	2.01	0.42
6:F:38:GLU:HG3	6:F:39:ASP:N	2.34	0.42
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.42
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
7:G:404:GLY:HA2	7:G:684:LEU:HD11	2.00	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
8:H:310:PHE:HA	20:b:39:THR:HA	2.01	0.42
9:I:63:TRP:NE1	24:I:301:3PE:O21	2.53	0.42
9:I:152:CYS:SG	25:I:302:SF4:S1	3.17	0.42
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	2.00	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
16:W:120:ASP:HB3	16:W:123:SER:OG	2.19	0.42
17:X:26:LYS:HD3	17:X:95:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:70:PHE:CE1	17:X:117:TRP:CZ3	3.08	0.42
17:X:130:LYS:HG2	20:b:67:PRO:CA	2.49	0.42
22:r:10:LYS:O	22:r:11:LEU:C	2.62	0.42
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.42
4:D:339:GLN:HE21	9:I:37:LYS:NZ	2.17	0.42
5:E:94:ILE:HD13	7:G:209:TYR:CE2	2.53	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
5:E:137:THR:HG22	6:F:370:LEU:HD21	2.02	0.42
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.42
6:F:126:LYS:HE2	6:F:274:LYS:HZ3	1.85	0.42
6:F:261:TRP:CE2	6:F:265:PHE:CZ	3.08	0.42
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.42
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.42
7:G:664:TYR:OH	13:S:23:LEU:HD11	2.20	0.42
8:H:8:THR:O	8:H:9:LEU:CB	2.68	0.42
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.42
8:H:114:TYR:O	8:H:115:SER:C	2.60	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.00	0.42
13:S:16:LEU:HD13	13:S:19:ILE:HD11	2.02	0.42
13:S:20:ARG:HG3	13:S:54:LEU:CB	2.43	0.42
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.84	0.42
4:D:99:LEU:HB3	4:D:101:LEU:CD1	2.49	0.42
4:D:140:ASP:O	4:D:147:ASN:ND2	2.53	0.42
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42
5:E:221:ARG:HB2	5:E:225:GLU:HG2	2.00	0.42
6:F:50:ASP:O	6:F:55:GLY:HA3	2.19	0.42
6:F:398:ARG:NH1	6:F:408:GLU:CD	2.78	0.42
6:F:416:SER:O	6:F:419:ILE:CG2	2.65	0.42
6:F:419:ILE:HG23	6:F:432:ALA:HB2	2.01	0.42
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
10:P:207:PHE:O	10:P:241:TYR:HA	2.19	0.42
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.42
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.42
16:W:55:LEU:CB	16:W:107:MET:HE1	2.38	0.42
23:s:53:SER:HA	23:s:56:ARG:HG2	2.02	0.42
3:C:64:VAL:HG11	3:C:85:ILE:HD13	2.02	0.42
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.42
6:F:47:GLY:C	6:F:49:HIS:H	2.27	0.42
6:F:410:ASP:OD1	6:F:411:SER:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
17:X:26:LYS:HE2	17:X:26:LYS:HB3	1.85	0.42
17:X:52:ASP:O	17:X:53:PRO:C	2.61	0.42
18:Z:10:MET:HE2	18:Z:10:MET:HB3	1.72	0.42
20:b:15:LYS:O	20:b:16:GLU:HB2	2.20	0.42
22:r:113:LEU:HA	22:r:113:LEU:HD12	1.76	0.42
2:B:125:PRO:HG3	4:D:88:HIS:HE1	1.84	0.42
4:D:83:ASN:OD1	4:D:83:ASN:N	2.47	0.42
5:E:133:VAL:HG22	5:E:185:VAL:CG1	2.45	0.42
5:E:136:THR:HB	26:E:301:FES:S2	2.60	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.42
6:F:291:GLU:OE2	6:F:292:MET:N	2.53	0.42
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.42
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.62	0.42
15:V:56:LEU:C	15:V:56:LEU:CD1	2.85	0.42
16:W:28:LEU:O	16:W:32:LYS:HG3	2.20	0.42
20:b:11:ASN:O	20:b:15:LYS:HG2	2.20	0.42
21:q:25:ARG:O	21:q:26:VAL:C	2.62	0.42
1:A:18:ILE:HG12	8:H:222:LEU:CD2	2.48	0.42
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
8:H:42:PRO:HD2	8:H:45:ILE:CD1	2.49	0.42
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.42
9:I:61:LEU:O	24:I:301:3PE:H342	2.19	0.42
9:I:63:TRP:CE2	24:I:301:3PE:H221	2.55	0.42
9:I:152:CYS:SG	25:I:302:SF4:S3	3.17	0.42
10:P:197:GLU:HB3	10:P:259:VAL:HG22	1.99	0.42
10:P:243:ALA:O	10:P:244:ASP:C	2.62	0.42
10:P:300:TRP:NE1	10:P:304:LEU:HD21	2.35	0.42
14:T:87:LEU:CD2	14:T:122:MET:CE	2.98	0.42
14:T:90:TYR:CD2	14:T:92:LYS:HB3	2.54	0.42
16:W:76:VAL:HG13	16:W:82:VAL:HG22	2.02	0.42
17:X:75:LYS:O	17:X:79:ALA:HB2	2.19	0.42
18:Z:62:ILE:CG1	20:b:49:THR:HG22	2.50	0.42
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.55	0.42
21:q:64:TYR:CD1	21:q:77:VAL:HG11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:85:GLU:HG2	21:q:98:PRO:HB3	2.01	0.42
22:r:18:GLN:OE1	22:r:18:GLN:N	2.53	0.42
1:A:73:LEU:N	1:A:74:PRO:HD2	2.35	0.42
1:A:112:GLU:O	1:A:113:TRP:CD1	2.73	0.42
2:B:78:LEU:HD23	2:B:78:LEU:HA	1.91	0.42
3:C:72:VAL:HG23	3:C:72:VAL:O	2.20	0.42
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.81	0.42
5:E:203:ILE:HG12	5:E:218:ARG:NH1	2.35	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.52	0.42
10:P:220:TYR:CG	10:P:226:VAL:HG13	2.55	0.42
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.42
16:W:83:ASP:O	16:W:86:VAL:CG2	2.66	0.42
16:W:93:LEU:HD23	16:W:93:LEU:C	2.45	0.42
18:Z:44:ILE:HD13	18:Z:44:ILE:HA	1.85	0.42
20:b:59:ASP:HA	20:b:63:MET:CE	2.50	0.42
1:A:24:LEU:HD13	1:A:24:LEU:O	2.20	0.41
2:B:111:ARG:CZ	4:D:208:GLU:HG2	2.50	0.41
2:B:111:ARG:NE	4:D:208:GLU:HG2	2.35	0.41
3:C:48:PRO:HD3	4:D:162:GLN:OE1	2.20	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
6:F:47:GLY:N	6:F:133:HIS:ND1	2.68	0.41
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.41
7:G:32:ILE:CG2	7:G:98:LYS:HA	2.50	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.41
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.41
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
9:I:130:ILE:HD11	9:I:145:TYR:HE1	1.85	0.41
10:P:231:LEU:HD11	10:P:290:PRO:HB2	2.02	0.41
10:P:265:PHE:CD1	10:P:334:GLY:HA3	2.55	0.41
10:P:331:ASP:CG	10:P:332:LEU:H	2.28	0.41
18:Z:144:THR:HA	19:a:45:TRP:HZ3	1.84	0.41
19:a:49:GLU:OE2	19:a:49:GLU:HA	2.20	0.41
21:q:50:GLU:HA	21:q:59:HIS:O	2.20	0.41
23:s:35:LEU:HA	23:s:37:HIS:CE1	2.55	0.41
1:A:93:ILE:HD13	1:A:93:ILE:HA	1.90	0.41
2:B:95:PHE:HE2	2:B:131:MET:CE	2.33	0.41
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.41
4:D:259:GLU:O	4:D:261:MET:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:VAL:HG11	7:G:163:LYS:HZ2	1.83	0.41
5:E:134:CYS:SG	5:E:175:CYS:HA	2.60	0.41
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.41
6:F:119:GLU:CD	27:F:501:FMN:HN3	2.28	0.41
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.41
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.55	0.41
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.52	0.41
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.41
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.41
14:T:87:LEU:CD2	14:T:104:PHE:CE1	2.94	0.41
20:b:61:GLY:O	20:b:63:MET:HG3	2.20	0.41
21:q:56:PHE:CD1	21:q:59:HIS:NE2	2.77	0.41
2:B:146:ARG:NH2	3:C:211:TYR:CE2	2.89	0.41
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.41
4:D:339:GLN:NE2	9:I:37:LYS:HZ2	2.18	0.41
4:D:384:LEU:HD23	4:D:384:LEU:HA	1.89	0.41
5:E:69:TYR:HB3	5:E:70:PRO:CD	2.50	0.41
6:F:70:LEU:O	6:F:71:LYS:C	2.63	0.41
6:F:126:LYS:HG3	6:F:275:LEU:HB2	2.01	0.41
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	0.41
7:G:62:ARG:HD2	7:G:65:TYR:CD2	2.29	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.85	0.41
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.41
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.41
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.41
10:P:242:VAL:HG13	10:P:243:ALA:N	2.35	0.41
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.41
10:P:316:LYS:C	10:P:316:LYS:HD3	2.46	0.41
12:R:81:GLY:HA3	12:R:88:HIS:CD2	2.55	0.41
2:B:91:TRP:CZ2	28:H:400:UQ9:C1M	3.03	0.41
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.20	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
4:D:198:THR:N	4:D:199:PRO:CD	2.84	0.41
4:D:201:PHE:HB2	8:H:32:GLN:HB3	2.03	0.41
4:D:240:LEU:O	4:D:241:LEU:C	2.62	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.41
6:F:299:LEU:C	6:F:299:LEU:CD1	2.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.41
8:H:42:PRO:HD2	8:H:45:ILE:HD11	2.02	0.41
8:H:196:ALA:C	8:H:198:PHE:N	2.77	0.41
28:H:400:UQ9:H15B	28:H:400:UQ9:H17	1.80	0.41
12:R:64:ILE:HD12	12:R:64:ILE:HA	1.95	0.41
14:T:80:LYS:O	14:T:84:LEU:HG	2.20	0.41
1:A:52:SER:O	1:A:53:MET:C	2.61	0.41
24:A:401:3PE:H362	8:H:104:PHE:CE2	2.55	0.41
2:B:163:SER:HB2	9:I:150:THR:O	2.20	0.41
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.41
3:C:243:ALA:C	7:G:105:ASN:HD21	2.27	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.41
4:D:338:ARG:CZ	18:Z:23:ARG:CB	2.99	0.41
4:D:376:GLU:HG2	7:G:121:LEU:CD1	2.51	0.41
5:E:48:PRO:HD3	5:E:94:ILE:CG2	2.51	0.41
5:E:179:CYS:C	5:E:181:ASN:N	2.78	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41
6:F:311:TRP:CH2	6:F:333:GLU:HB3	2.55	0.41
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.41
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.42	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
8:H:249:ILE:HD13	17:X:99:HIS:CE1	2.51	0.41
8:H:316:PRO:HA	18:Z:58:ARG:NH1	2.32	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
10:P:230:SER:O	10:P:231:LEU:C	2.64	0.41
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.21	0.41
12:R:60:ALA:O	12:R:61:ILE:C	2.63	0.41
18:Z:102:PRO:O	18:Z:103:ASN:C	2.62	0.41
3:C:241:PHE:O	3:C:242:PRO:C	2.62	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
5:E:225:GLU:O	5:E:226:PRO:C	2.60	0.41
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.41
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.41
8:H:25:ARG:HD2	28:H:400:UQ9:C10	2.48	0.41
8:H:300:LEU:HD23	20:b:25:VAL:HG11	2.02	0.41
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.55	0.41
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.85	0.41
13:S:85:ASP:O	13:S:89:ARG:N	2.41	0.41
17:X:128:VAL:CG2	20:b:56:PRO:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
1:A:102:LEU:O	1:A:106:TRP:HD1	2.04	0.41
2:B:94:THR:OG1	2:B:104:MET:HE1	2.20	0.41
2:B:138:THR:HG21	4:D:116:LEU:HA	2.02	0.41
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.41
4:D:265:ASN:C	4:D:267:ILE:H	2.29	0.41
5:E:62:ILE:HG21	5:E:103:VAL:HG11	2.02	0.41
5:E:192:TYR:CD2	5:E:203:ILE:HD13	2.56	0.41
6:F:94:PRO:CG	6:F:97:LEU:HD12	2.45	0.41
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.41
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.41
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
8:H:202:GLU:OE2	28:H:400:UQ9:H4M	2.20	0.41
9:I:50:MET:O	9:I:54:THR:N	2.37	0.41
12:R:31:ILE:HG22	12:R:55:VAL:HG21	2.02	0.41
14:T:99:SER:HB2	14:T:102:SER:HB2	2.03	0.41
18:Z:120:LEU:HD12	18:Z:121:ILE:H	1.85	0.41
18:Z:140:PHE:C	18:Z:142:TRP:N	2.77	0.41
20:b:11:ASN:CG	20:b:15:LYS:HE3	2.45	0.41
20:b:16:GLU:N	20:b:17:PRO:HD3	2.35	0.41
20:b:25:VAL:O	20:b:26:TRP:C	2.64	0.41
4:D:99:LEU:HB3	4:D:101:LEU:HD11	2.03	0.41
5:E:60:LYS:O	5:E:61:ARG:C	2.62	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
6:F:61:ASP:O	6:F:256:ARG:NH2	2.54	0.41
7:G:272:ARG:HH11	7:G:274:LEU:CD2	2.33	0.41
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.41
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.41
10:P:265:PHE:CD1	10:P:265:PHE:N	2.87	0.41
14:T:118:ILE:HD13	14:T:118:ILE:HA	1.82	0.41
14:T:120:MET:O	14:T:121:ALA:C	2.63	0.41
16:W:71:MET:O	16:W:74:ALA:N	2.39	0.41
18:Z:90:ASN:O	18:Z:94:GLU:HB2	2.21	0.41
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.95	0.41
2:B:137:LEU:HD11	2:B:142:ALA:HA	2.03	0.41
3:C:70:LYS:HD3	3:C:71:TYR:CZ	2.56	0.41
4:D:80:MET:HB3	4:D:101:LEU:N	2.35	0.41
4:D:163:PRO:HG2	4:D:168:GLN:HG3	2.03	0.41
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.54	0.41
4:D:264:ASN:O	4:D:265:ASN:C	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:266:ARG:CA	9:I:65:GLU:OE2	2.68	0.41
4:D:310:VAL:C	4:D:312:ASP:H	2.29	0.41
5:E:61:ARG:O	5:E:65:ILE:HG13	2.21	0.41
5:E:109:MET:HE2	7:G:196:GLY:CA	2.51	0.41
6:F:337:MET:O	6:F:338:ASP:OD1	2.38	0.41
27:F:501:FMN:HM73	27:F:501:FMN:HM81	1.92	0.41
7:G:49:VAL:HB	7:G:91:ALA:HA	2.03	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:160:VAL:CG1	7:G:161:GLU:N	2.83	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
8:H:23:VAL:O	8:H:23:VAL:CG1	2.69	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
9:I:42:LYS:HA	9:I:42:LYS:HD3	1.85	0.41
10:P:73:LEU:HD23	10:P:73:LEU:HA	1.89	0.41
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.41
10:P:288:PHE:CZ	10:P:290:PRO:HB3	2.56	0.41
13:S:19:ILE:O	13:S:53:ILE:HD12	2.20	0.41
13:S:20:ARG:HD2	13:S:22:HIS:NE2	2.35	0.41
13:S:22:HIS:CD2	13:S:66:TRP:HD1	2.38	0.41
15:V:98:LYS:HG2	15:V:100:TRP:CZ2	2.55	0.41
17:X:70:PHE:O	17:X:74:ILE:HG13	2.20	0.41
18:Z:143:TYR:HE2	19:a:36:LYS:HZ2	1.68	0.41
19:a:49:GLU:O	19:a:50:ARG:C	2.62	0.41
20:b:60:ASP:OD1	20:b:60:ASP:C	2.60	0.41
21:q:64:TYR:CE2	21:q:81:MET:HB2	2.56	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
1:A:20:VAL:O	1:A:21:ALA:C	2.63	0.41
3:C:139:ARG:NH1	4:D:306:GLN:OE1	2.49	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.02	0.41
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.41
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.41
4:D:261:MET:HE3	4:D:261:MET:HB3	1.90	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
5:E:167:LEU:HD23	5:E:168:PHE:HE1	1.86	0.41
6:F:280:GLY:O	6:F:356:VAL:HB	2.20	0.41
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.54	0.41
7:G:277:MET:HE1	11:Q:153:PRO:HD3	2.03	0.41
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.56	0.41
8:H:235:ASN:ND2	8:H:270:PHE:CD2	2.73	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
9:I:162:CYS:HB3	9:I:165:ASP:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:96:LEU:C	10:P:96:LEU:CD1	2.94	0.41
10:P:228:LEU:HD11	10:P:288:PHE:CZ	2.54	0.41
10:P:293:LEU:HD12	10:P:294:PRO:HD2	2.01	0.41
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.41
17:X:132:LYS:HE2	17:X:132:LYS:HB3	1.84	0.41
18:Z:19:ILE:HG22	18:Z:20:ASP:N	2.36	0.41
18:Z:62:ILE:HG23	20:b:50:PRO:HD3	2.02	0.41
19:a:9:LEU:O	19:a:10:ALA:C	2.64	0.41
21:q:129:THR:O	21:q:129:THR:CG2	2.67	0.41
2:B:201:LEU:HD12	2:B:201:LEU:HA	1.83	0.40
4:D:119:GLY:O	4:D:123:LEU:HD23	2.21	0.40
4:D:202:TRP:HZ2	9:I:73:THR:HG22	1.86	0.40
5:E:190:ASN:HD22	5:E:192:TYR:HE1	1.69	0.40
6:F:119:GLU:CD	6:F:127:ASP:OD2	2.65	0.40
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.40
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.40
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.40
7:G:302:LEU:N	7:G:571:HIS:O	2.45	0.40
9:I:89:GLU:CG	21:q:61:TRP:HB3	2.50	0.40
9:I:93:LEU:O	21:q:93:MET:CG	2.65	0.40
10:P:190:GLU:O	10:P:193:SER:N	2.54	0.40
10:P:362:LEU:HA	10:P:362:LEU:HD23	1.88	0.40
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.40
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.35	0.40
17:X:37:ASP:OD1	17:X:37:ASP:C	2.62	0.40
17:X:135:ARG:HE	17:X:135:ARG:HB3	1.72	0.40
18:Z:65:LEU:CB	20:b:50:PRO:O	2.68	0.40
18:Z:140:PHE:HE1	19:a:45:TRP:HB2	1.84	0.40
2:B:81:LEU:HD12	2:B:81:LEU:HA	1.90	0.40
2:B:145:LEU:O	2:B:146:ARG:C	2.64	0.40
2:B:170:TYR:CB	9:I:153:ILE:HG21	2.43	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
3:C:128:VAL:HG22	3:C:143:LYS:HB3	2.03	0.40
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.40
4:D:304:LYS:HD2	4:D:318:VAL:HG23	2.04	0.40
5:E:238:LYS:HB3	5:E:242:PHE:CG	2.56	0.40
6:F:61:ASP:O	6:F:140:GLU:OE1	2.40	0.40
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.40
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.40
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.40
8:H:87:VAL:HB	8:H:88:PRO:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:105:PHE:C	10:P:106:LEU:HD12	2.47	0.40
10:P:231:LEU:CD1	10:P:290:PRO:HB2	2.51	0.40
11:Q:158:LYS:HE3	11:Q:158:LYS:HB3	1.91	0.40
16:W:122:LEU:HG	16:W:126:TYR:CE2	2.56	0.40
17:X:16:GLU:CD	17:X:68:LEU:HD13	2.46	0.40
21:q:68:MET:HE1	21:q:81:MET:O	2.21	0.40
1:A:16:THR:O	1:A:20:VAL:HG23	2.22	0.40
1:A:107:THR:OG1	1:A:108:GLN:N	2.55	0.40
3:C:93:ILE:HB	3:C:94:PRO:CD	2.48	0.40
3:C:224:GLU:OE1	10:P:50:SER:OG	2.40	0.40
4:D:90:ALA:O	4:D:91:ALA:C	2.62	0.40
4:D:259:GLU:HB2	18:Z:25:LEU:HD21	2.02	0.40
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.40
6:F:114:VAL:CG1	6:F:212:LEU:HD23	2.51	0.40
6:F:169:LEU:O	6:F:173:ILE:N	2.49	0.40
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.40
8:H:224:PHE:CD2	28:H:400:UQ9:H13	2.50	0.40
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.40
9:I:201:ILE:O	9:I:205:ILE:HG12	2.21	0.40
10:P:192:ARG:HH21	10:P:200:ILE:HD11	1.83	0.40
10:P:336:GLU:N	10:P:340:VAL:O	2.55	0.40
21:q:7:LEU:O	21:q:11:VAL:HG23	2.21	0.40
1:A:65:PHE:CZ	8:H:294:LEU:HD21	2.56	0.40
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.40
3:C:47:ARG:HG3	4:D:160:ASN:HA	2.04	0.40
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.85	0.40
4:D:116:LEU:O	4:D:118:ARG:HG3	2.22	0.40
4:D:139:LEU:HD13	4:D:424:ILE:HG12	2.03	0.40
4:D:142:VAL:CG1	4:D:185:MET:SD	3.10	0.40
4:D:339:GLN:HE21	9:I:37:LYS:HZ2	1.68	0.40
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.37	0.40
5:E:145:ASP:OD1	5:E:145:ASP:N	2.54	0.40
6:F:257:ARG:HG2	6:F:261:TRP:CE3	2.55	0.40
6:F:300:ILE:CD1	6:F:307:VAL:HG23	2.49	0.40
6:F:379:CYS:SG	25:F:502:SF4:S3	3.20	0.40
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.40
9:I:50:MET:O	9:I:54:THR:HG23	2.22	0.40
9:I:63:TRP:CZ2	24:I:301:3PE:H221	2.57	0.40
9:I:149:MET:HE2	9:I:185:TYR:HD2	1.87	0.40
10:P:56:ALA:HA	10:P:125:VAL:O	2.20	0.40
10:P:146:VAL:HG13	10:P:147:ASN:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.40
11:Q:57:GLU:O	11:Q:58:LYS:C	2.65	0.40
12:R:55:VAL:HG22	12:R:56:ASN:N	2.35	0.40
14:T:123:GLU:HG2	14:T:130:ILE:HD12	2.02	0.40
17:X:121:ASP:OD1	17:X:122:LEU:N	2.54	0.40
20:b:43:SER:O	20:b:47:LYS:HB2	2.22	0.40
1:A:69:ILE:O	1:A:72:LEU:N	2.55	0.40
3:C:160:ILE:HB	4:D:286:TYR:CE1	2.57	0.40
4:D:87:GLN:C	4:D:88:HIS:CG	2.99	0.40
4:D:197:MET:HG3	8:H:32:GLN:NE2	2.36	0.40
5:E:190:ASN:HB3	5:E:215:PRO:HB3	2.04	0.40
6:F:102:MET:HE2	6:F:149:MET:HB2	2.03	0.40
6:F:337:MET:HA	6:F:337:MET:HE2	2.02	0.40
6:F:383:THR:HG21	7:G:120:LEU:HD23	2.00	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:32:ILE:HG22	7:G:33:GLU:N	2.36	0.40
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.40
7:G:379:THR:HG22	7:G:379:THR:O	2.22	0.40
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.40
8:H:114:TYR:O	8:H:117:LEU:N	2.55	0.40
8:H:174:LEU:HD23	8:H:174:LEU:HA	1.81	0.40
9:I:94:SER:HB2	9:I:95:PRO:CD	2.34	0.40
10:P:138:ASN:OD1	10:P:138:ASN:N	2.55	0.40
10:P:315:THR:HB	10:P:318:LYS:H	1.86	0.40
17:X:36:CYS:O	17:X:40:ASN:CG	2.65	0.40
17:X:117:TRP:CD1	17:X:117:TRP:N	2.87	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	89/115 (77%)	82 (92%)	7 (8%)	0	100	100
2	B	154/224 (69%)	142 (92%)	10 (6%)	2 (1%)	9	39
3	C	196/263 (74%)	187 (95%)	9 (5%)	0	100	100
4	D	382/463 (82%)	351 (92%)	31 (8%)	0	100	100
5	E	208/248 (84%)	190 (91%)	18 (9%)	0	100	100
6	F	424/464 (91%)	405 (96%)	19 (4%)	0	100	100
7	G	685/727 (94%)	630 (92%)	55 (8%)	0	100	100
8	H	306/318 (96%)	288 (94%)	17 (6%)	1 (0%)	36	65
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	P	338/377 (90%)	312 (92%)	26 (8%)	0	100	100
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	76 (94%)	5 (6%)	0	100	100
13	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
14	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
15	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
16	W	112/131 (86%)	110 (98%)	2 (2%)	0	100	100
17	X	140/172 (81%)	130 (93%)	10 (7%)	0	100	100
18	Z	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
19	a	64/70 (91%)	60 (94%)	4 (6%)	0	100	100
20	b	77/84 (92%)	71 (92%)	6 (8%)	0	100	100
21	q	116/145 (80%)	113 (97%)	3 (3%)	0	100	100
22	r	46/113 (41%)	44 (96%)	2 (4%)	0	100	100
23	s	24/104 (23%)	24 (100%)	0	0	100	100
All	All	4129/5036 (82%)	3886 (94%)	240 (6%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	127	GLN
8	H	92	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	85/104 (82%)	85 (100%)	0	100	100
2	B	132/185 (71%)	132 (100%)	0	100	100
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	331/395 (84%)	331 (100%)	0	100	100
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	80
6	F	341/370 (92%)	340 (100%)	1 (0%)	86	83
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	274/280 (98%)	274 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	P	297/325 (91%)	295 (99%)	2 (1%)	76	78
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68	75
12	R	70/96 (73%)	69 (99%)	1 (1%)	59	71
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	71
14	T	69/135 (51%)	68 (99%)	1 (1%)	59	71
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	129 (100%)	0	100	100
18	Z	120/123 (98%)	119 (99%)	1 (1%)	73	77
19	a	56/60 (93%)	56 (100%)	0	100	100
20	b	70/73 (96%)	70 (100%)	0	100	100
21	q	108/131 (82%)	108 (100%)	0	100	100
22	r	44/96 (46%)	44 (100%)	0	100	100
23	s	26/95 (27%)	26 (100%)	0	100	100
All	All	3628/4292 (84%)	3618 (100%)	10 (0%)	84	83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	244	VAL
6	F	337	MET
7	G	271	MET
10	P	192	ARG
10	P	242	VAL
11	Q	96	LYS
12	R	64	ILE
13	S	68	ARG
14	T	103	HIS
18	Z	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	54	HIS
3	C	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	112	HIS
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	339	GLN
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	44	ASN
6	F	49	HIS

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Mol	Chain	Res	Type
6	F	168	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	277	ASN
6	F	346	GLN
6	F	393	ASN
6	F	436	GLN
7	G	59	GLN
7	G	74	ASN
7	G	105	ASN
7	G	140	GLN
7	G	164	ASN
7	G	205	GLN
7	G	406	ASN
7	G	495	ASN
7	G	498	GLN
7	G	569	GLN
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	97	ASN
8	H	169	GLN
8	H	171	HIS
8	H	258	ASN
8	H	287	HIS
10	P	43	HIS
10	P	71	ASN
10	P	79	GLN
10	P	154	GLN
10	P	166	HIS
10	P	216	HIS
10	P	251	ASN
10	P	269	ASN
10	P	275	HIS
10	P	323	HIS
10	P	341	GLN

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Mol	Chain	Res	Type
10	P	356	HIS
11	Q	51	GLN
11	Q	88	GLN
12	R	33	HIS
13	S	81	ASN
15	V	41	HIS
15	V	50	GLN
16	W	54	GLN
17	X	30	HIS
17	X	77	HIS
18	Z	135	ASN
19	a	31	ASN
20	b	69	HIS
20	b	83	ASN
21	q	12	GLN
21	q	31	ASN
21	q	52	ASN
21	q	54	GLN
21	q	87	HIS
21	q	91	HIS
22	r	9	GLN
22	r	21	GLN
22	r	110	GLN
23	s	59	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	3PE	A	401	-	45,45,50	1.13	5 (11%)	48,50,55	1.20	3 (6%)
31	EHZ	W	201	-	29,31,37	1.80	7 (24%)	37,41,47	1.93	12 (32%)
29	NDP	P	401	-	51,52,52	1.17	6 (11%)	71,80,80	1.54	11 (15%)
28	UQ9	H	400	-	35,35,58	0.84	2 (5%)	43,45,73	0.60	1 (2%)
25	SF4	G	802	7	0,12,12	-	-	-	-	-
24	3PE	I	301	-	28,28,50	1.22	2 (7%)	31,33,55	1.23	4 (12%)
25	SF4	I	302	9	0,12,12	-	-	-	-	-
25	SF4	F	502	6	0,12,12	-	-	-	-	-
26	FES	E	301	5	0,4,4	-	-	-	-	-
26	FES	G	803	7	0,4,4	-	-	-	-	-
25	SF4	G	801	7	0,12,12	-	-	-	-	-
25	SF4	B	301	2	0,12,12	-	-	-	-	-
25	SF4	I	303	9	0,12,12	-	-	-	-	-
27	FMN	F	501	-	33,33,33	1.42	4 (12%)	48,50,50	1.21	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	3PE	A	401	-	-	18/49/49/54	-
31	EHZ	W	201	-	-	21/39/39/45	-
29	NDP	P	401	-	-	3/34/77/77	0/5/5/5
28	UQ9	H	400	-	-	14/30/54/81	0/1/1/1
25	SF4	G	802	7	-	-	0/6/5/5
24	3PE	I	301	-	-	7/32/32/54	-
25	SF4	I	302	9	-	-	0/6/5/5
25	SF4	F	502	6	-	-	0/6/5/5
26	FES	E	301	5	-	-	0/1/1/1
26	FES	G	803	7	-	-	0/1/1/1
25	SF4	G	801	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SF4	B	301	2	-	-	0/6/5/5
25	SF4	I	303	9	-	-	0/6/5/5
27	FMN	F	501	-	-	3/18/18/18	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	501	FMN	C9A-C5A	5.03	1.49	1.41
31	W	201	EHZ	C15-N2	5.01	1.45	1.33
31	W	201	EHZ	C12-N1	4.94	1.45	1.33
29	P	401	NDP	C5A-C4A	4.38	1.46	1.39
24	I	301	3PE	O31-C31	4.18	1.45	1.33
24	I	301	3PE	O21-C21	4.09	1.45	1.34
27	F	501	FMN	C8-C7	3.19	1.48	1.40
24	A	401	3PE	O21-C21	3.15	1.43	1.34
24	A	401	3PE	O31-C31	3.04	1.42	1.33
28	H	400	UQ9	C3-C2	-2.77	1.40	1.48
31	W	201	EHZ	P1-O7	2.66	1.64	1.54
27	F	501	FMN	C4-N3	-2.65	1.33	1.38
31	W	201	EHZ	O4-C15	-2.61	1.18	1.23
29	P	401	NDP	C5A-N7A	-2.53	1.34	1.39
29	P	401	NDP	C5A-C6A	2.51	1.48	1.41
28	H	400	UQ9	C4-C5	-2.48	1.41	1.48
31	W	201	EHZ	O3-C12	-2.45	1.18	1.23
31	W	201	EHZ	C9-S1	2.43	1.82	1.76
27	F	501	FMN	C5A-N5	-2.40	1.35	1.39
31	W	201	EHZ	P1-OP3	-2.33	1.46	1.54
29	P	401	NDP	C8A-N7A	2.31	1.36	1.31
24	A	401	3PE	O21-C2	-2.28	1.41	1.46
24	A	401	3PE	O31-C3	-2.20	1.40	1.45
24	A	401	3PE	P-O12	-2.15	1.45	1.55
29	P	401	NDP	C4A-N9A	-2.05	1.33	1.37
29	P	401	NDP	C6N-C5N	2.03	1.39	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	W	201	EHZ	C8-C9-S1	6.22	121.41	113.56
29	P	401	NDP	C5A-C4A-N3A	-5.75	118.81	126.72
29	P	401	NDP	N3A-C4A-N9A	4.55	134.90	127.17
24	A	401	3PE	O21-C21-C22	4.23	120.62	111.48
24	I	301	3PE	O21-C21-C22	3.87	119.84	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	401	NDP	C2A-N3A-C4A	3.74	120.95	111.83
29	P	401	NDP	C4A-C5A-N7A	-3.38	106.72	110.58
29	P	401	NDP	N3A-C2A-N1A	-3.34	123.52	128.58
31	W	201	EHZ	O2-C9-C8	-3.19	118.72	123.74
31	W	201	EHZ	C14-C13-C12	-3.04	107.32	112.39
31	W	201	EHZ	OP3-P1-O9	-2.94	99.36	110.83
31	W	201	EHZ	C7-C8-C9	-2.90	107.38	113.86
31	W	201	EHZ	C13-C12-N1	2.87	121.57	116.34
29	P	401	NDP	C4A-N9A-C8A	2.76	108.63	105.74
24	A	401	3PE	O31-C31-C32	2.61	119.78	111.83
24	I	301	3PE	O31-C31-C32	2.57	119.67	111.83
29	P	401	NDP	C5A-N7A-C8A	2.50	107.38	103.45
27	F	501	FMN	C4-C4A-N5	2.50	121.66	118.21
31	W	201	EHZ	C5-C6-C7	-2.41	108.05	114.68
27	F	501	FMN	O4-C4-C4A	-2.39	120.21	126.53
31	W	201	EHZ	C10-S1-C9	2.38	108.88	101.84
27	F	501	FMN	C4A-C10-N1	-2.36	118.79	124.59
24	I	301	3PE	C2-O21-C21	-2.36	112.14	117.80
24	A	401	3PE	O12-P-O14	-2.24	102.04	112.44
31	W	201	EHZ	O2-C9-S1	-2.22	119.86	122.68
27	F	501	FMN	O2-C2-N1	-2.22	118.12	121.80
31	W	201	EHZ	O6-P1-O9	2.21	112.41	106.44
27	F	501	FMN	C4A-C10-N10	2.21	119.64	116.48
29	P	401	NDP	C3D-C2D-C1D	2.18	105.58	101.46
31	W	201	EHZ	C11-N1-C12	-2.16	118.80	122.82
29	P	401	NDP	N9A-C8A-N7A	-2.09	110.97	113.94
29	P	401	NDP	C6A-C5A-N7A	2.09	136.11	132.09
24	I	301	3PE	O21-C21-O22	-2.06	118.89	123.70
31	W	201	EHZ	O3-C12-N1	-2.03	119.04	123.03
29	P	401	NDP	C6N-N1N-C2N	2.02	121.48	119.32
28	H	400	UQ9	C7-C6-C1	-2.01	121.45	124.89

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	401	3PE	C11-O13-P-O11
24	A	401	3PE	C11-O13-P-O12
24	A	401	3PE	C11-O13-P-O14
24	A	401	3PE	C12-C11-O13-P
24	A	401	3PE	O32-C31-O31-C3
24	A	401	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
24	I	301	3PE	O22-C21-O21-C2
27	F	501	FMN	C5'-O5'-P-O2P
27	F	501	FMN	C5'-O5'-P-O3P
28	H	400	UQ9	C20-C19-C21-C22
28	H	400	UQ9	C18-C19-C21-C22
28	H	400	UQ9	C17-C18-C19-C21
28	H	400	UQ9	C17-C18-C19-C20
28	H	400	UQ9	C12-C13-C14-C16
28	H	400	UQ9	C12-C13-C14-C15
31	W	201	EHZ	O1-C7-C8-C9
31	W	201	EHZ	C6-C7-C8-C9
31	W	201	EHZ	S1-C10-C11-N1
31	W	201	EHZ	C16-C17-C20-O6
31	W	201	EHZ	C20-O6-P1-O7
31	W	201	EHZ	C20-O6-P1-O9
31	W	201	EHZ	C20-O6-P1-OP3
24	I	301	3PE	C22-C21-O21-C2
28	H	400	UQ9	C15-C14-C16-C17
28	H	400	UQ9	C24-C26-C27-C28
28	H	400	UQ9	C22-C23-C24-C25
28	H	400	UQ9	C22-C23-C24-C26
24	A	401	3PE	C22-C21-O21-C2
28	H	400	UQ9	C19-C21-C22-C23
28	H	400	UQ9	C9-C11-C12-C13
24	A	401	3PE	O22-C21-O21-C2
28	H	400	UQ9	C13-C14-C16-C17
28	H	400	UQ9	C14-C16-C17-C18
24	I	301	3PE	C32-C31-O31-C3
24	I	301	3PE	O32-C31-O31-C3
24	A	401	3PE	C37-C38-C39-C3A
27	F	501	FMN	C5'-O5'-P-O1P
24	A	401	3PE	C3-C2-O21-C21
31	W	201	EHZ	N2-C15-C16-C17
24	I	301	3PE	O11-C1-C2-O21
31	W	201	EHZ	C3-C4-C5-C6
24	I	301	3PE	O11-C1-C2-C3
24	A	401	3PE	C2A-C2B-C2C-C2D
31	W	201	EHZ	O4-C15-C16-O5
31	W	201	EHZ	C18-C17-C20-O6
31	W	201	EHZ	C19-C17-C20-O6
24	A	401	3PE	C2-C1-O11-P
31	W	201	EHZ	C11-C10-S1-C9

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Mol	Chain	Res	Type	Atoms
29	P	401	NDP	O4D-C1D-N1N-C6N
24	I	301	3PE	C2-C1-O11-P
31	W	201	EHZ	C5-C6-C7-O1
29	P	401	NDP	PN-O3-PA-O2A
29	P	401	NDP	C2B-O2B-P2B-O2X
31	W	201	EHZ	C2-C3-C4-C5
24	A	401	3PE	C2B-C2C-C2D-C2E
24	A	401	3PE	C28-C29-C2A-C2B
31	W	201	EHZ	N2-C15-C16-O5
24	A	401	3PE	O11-C1-C2-O21
31	W	201	EHZ	O2-C9-S1-C10
24	A	401	3PE	C25-C26-C27-C28
31	W	201	EHZ	C15-C16-C17-C18
24	A	401	3PE	C33-C34-C35-C36
24	A	401	3PE	O11-C1-C2-C3
31	W	201	EHZ	O5-C16-C17-C18
31	W	201	EHZ	O4-C15-C16-C17
31	W	201	EHZ	C15-C16-C17-C20

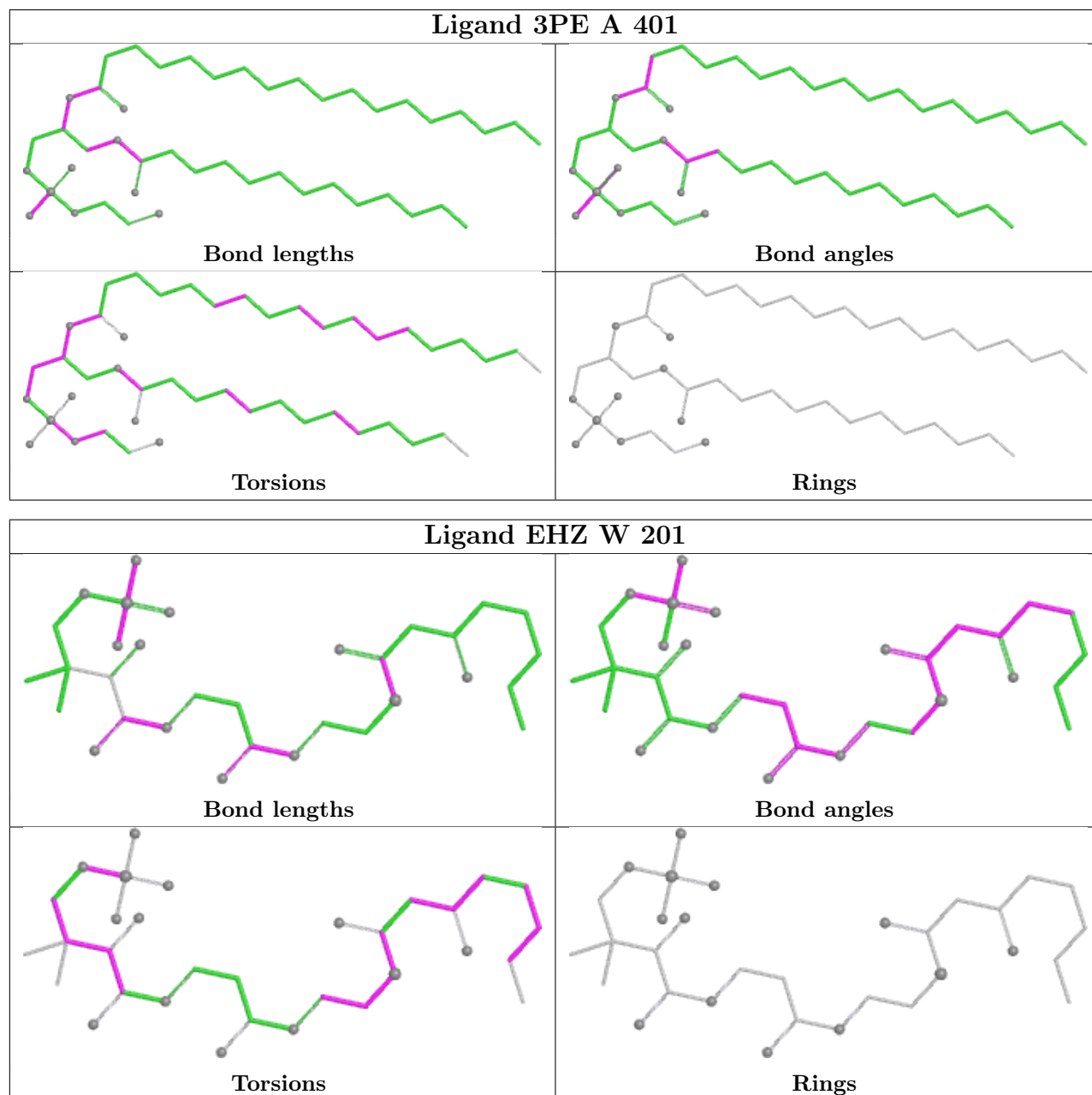
There are no ring outliers.

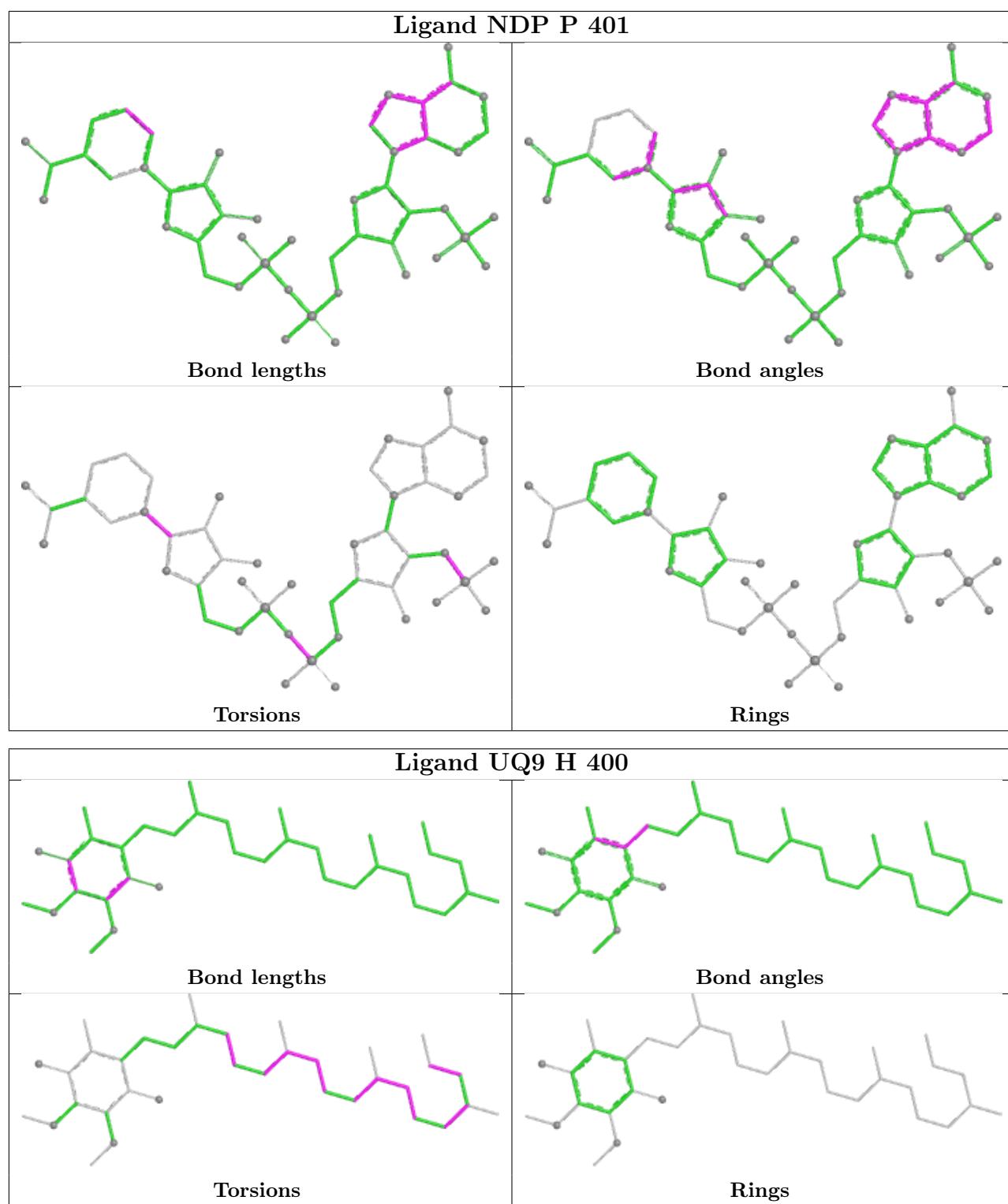
13 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	401	3PE	11	0
31	W	201	EHZ	7	0
29	P	401	NDP	4	0
28	H	400	UQ9	18	0
25	G	802	SF4	7	0
24	I	301	3PE	8	0
25	I	302	SF4	11	0
25	F	502	SF4	11	0
26	E	301	FES	5	0
26	G	803	FES	5	0
25	B	301	SF4	5	0
25	I	303	SF4	5	0
27	F	501	FMN	4	0

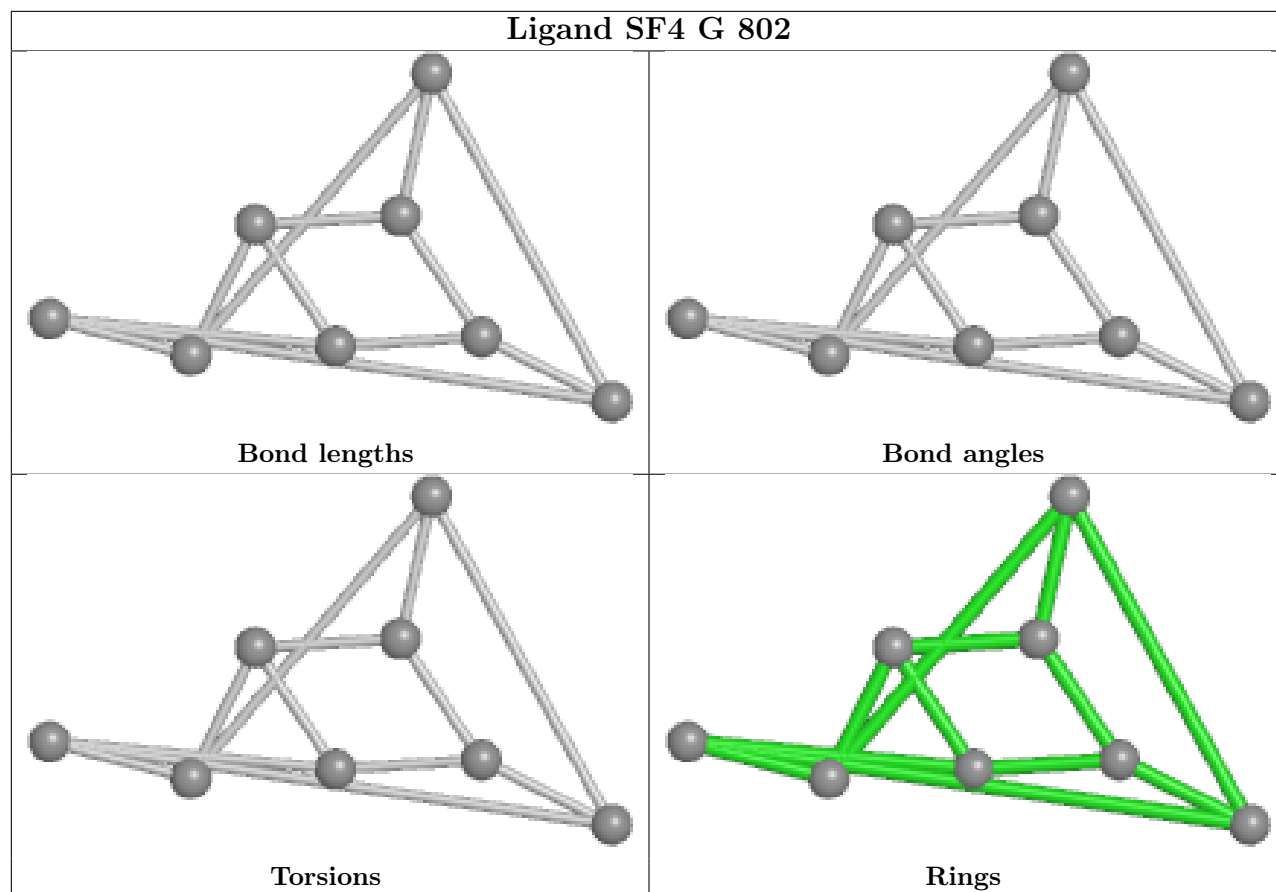
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

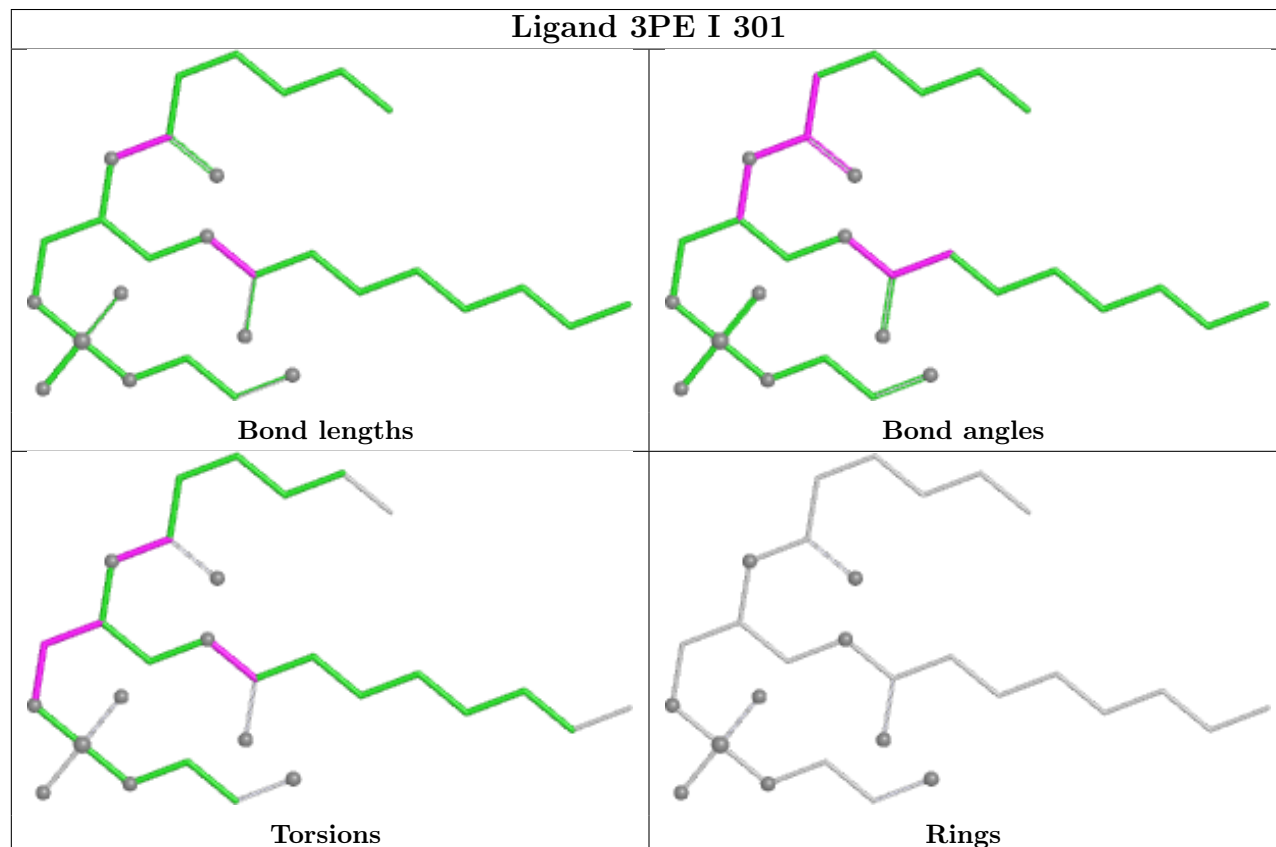




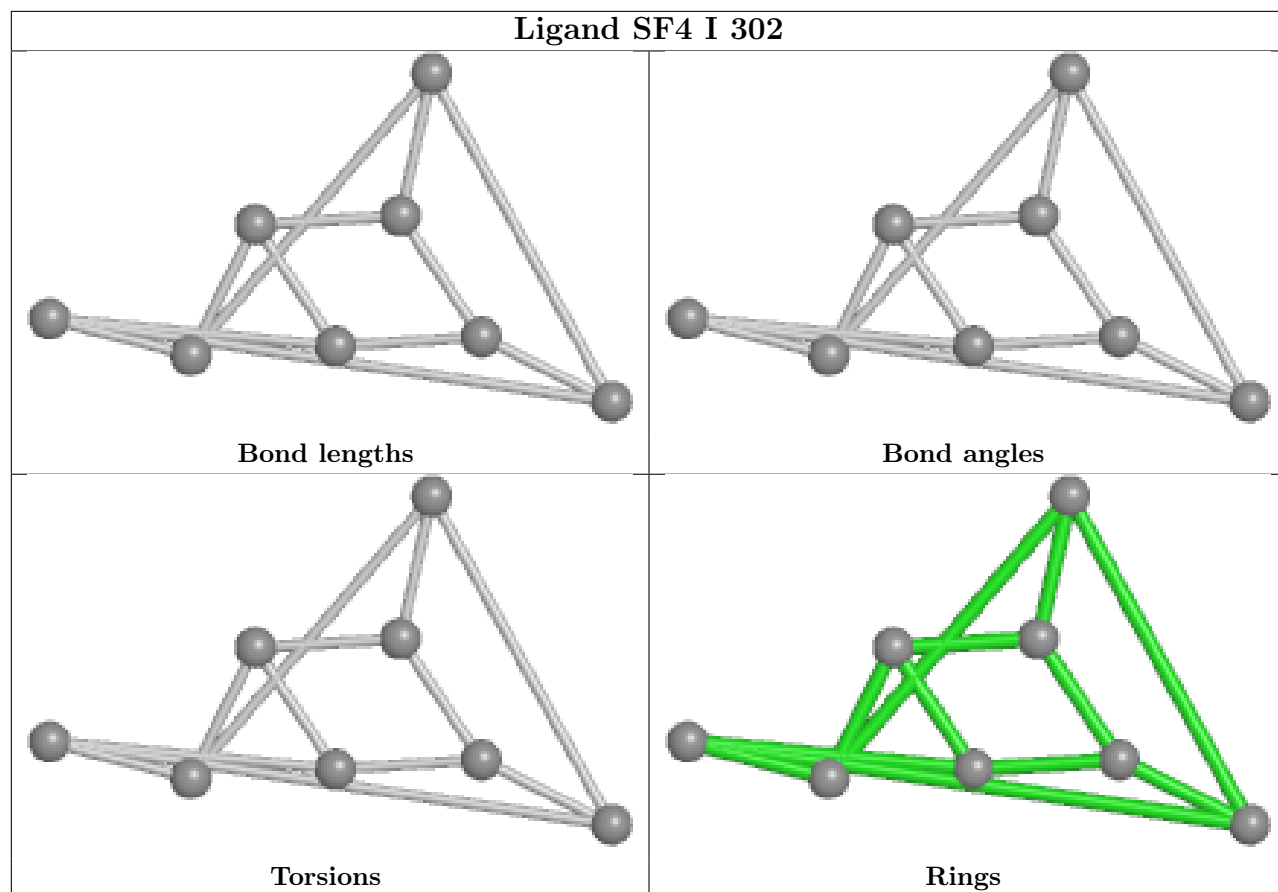
Ligand SF4 G 802



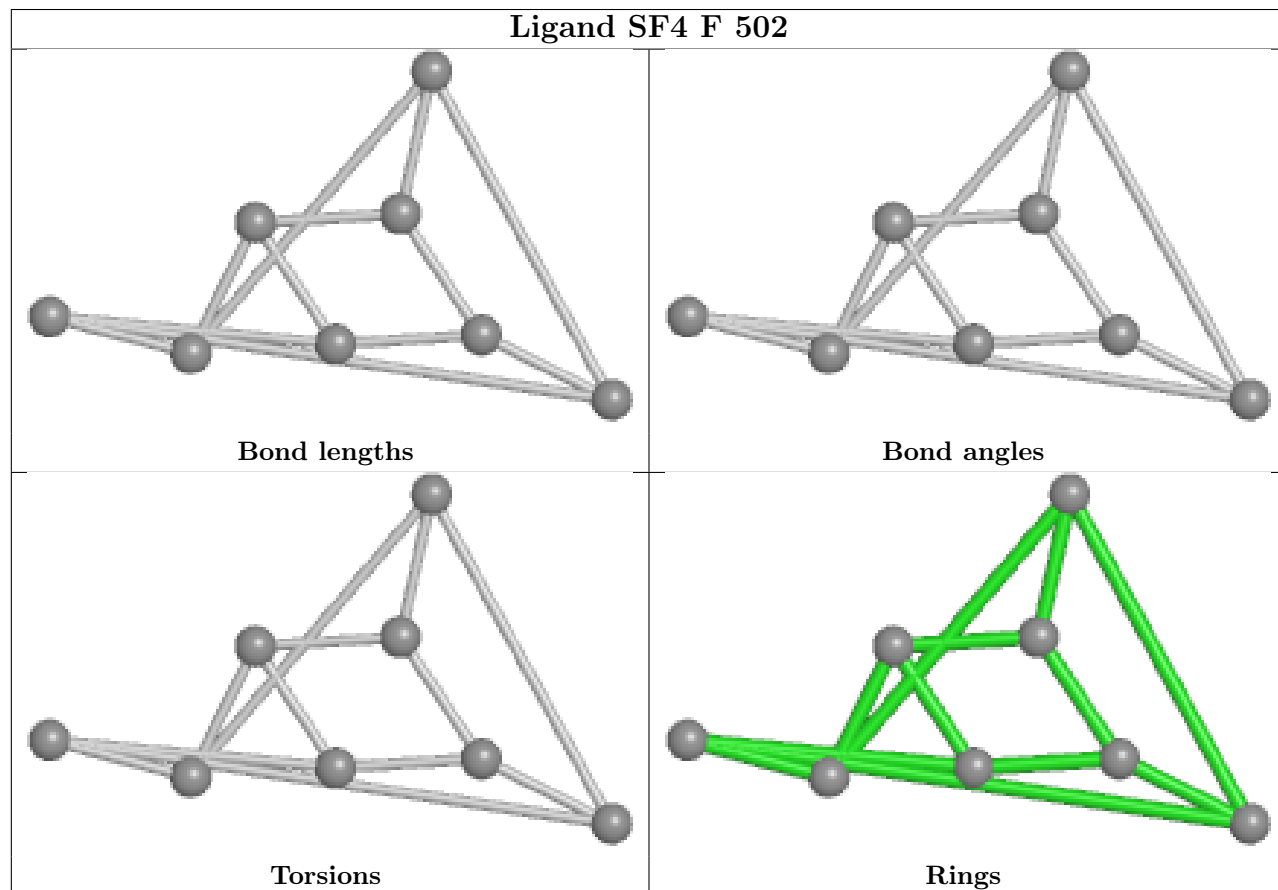
Ligand 3PE I 301

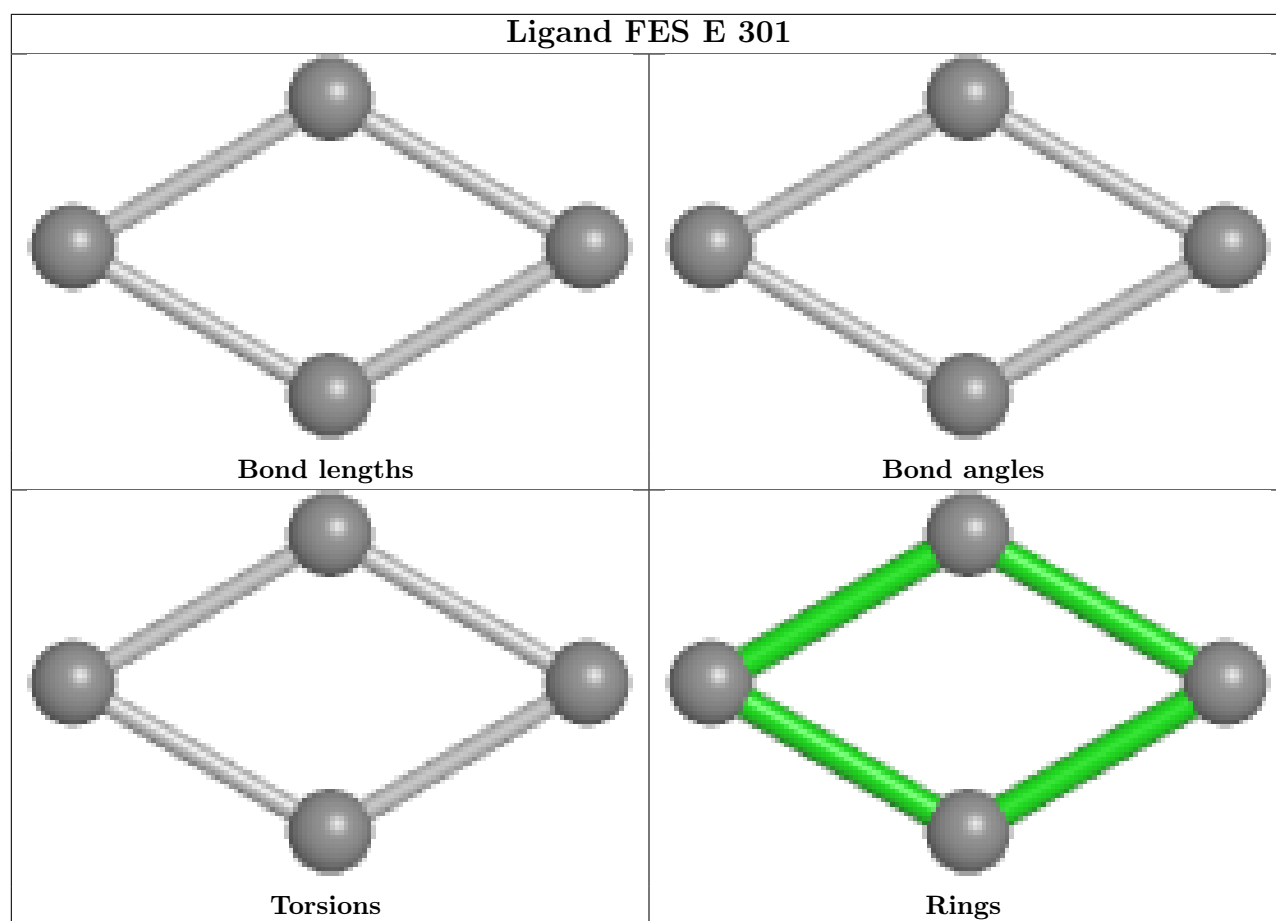


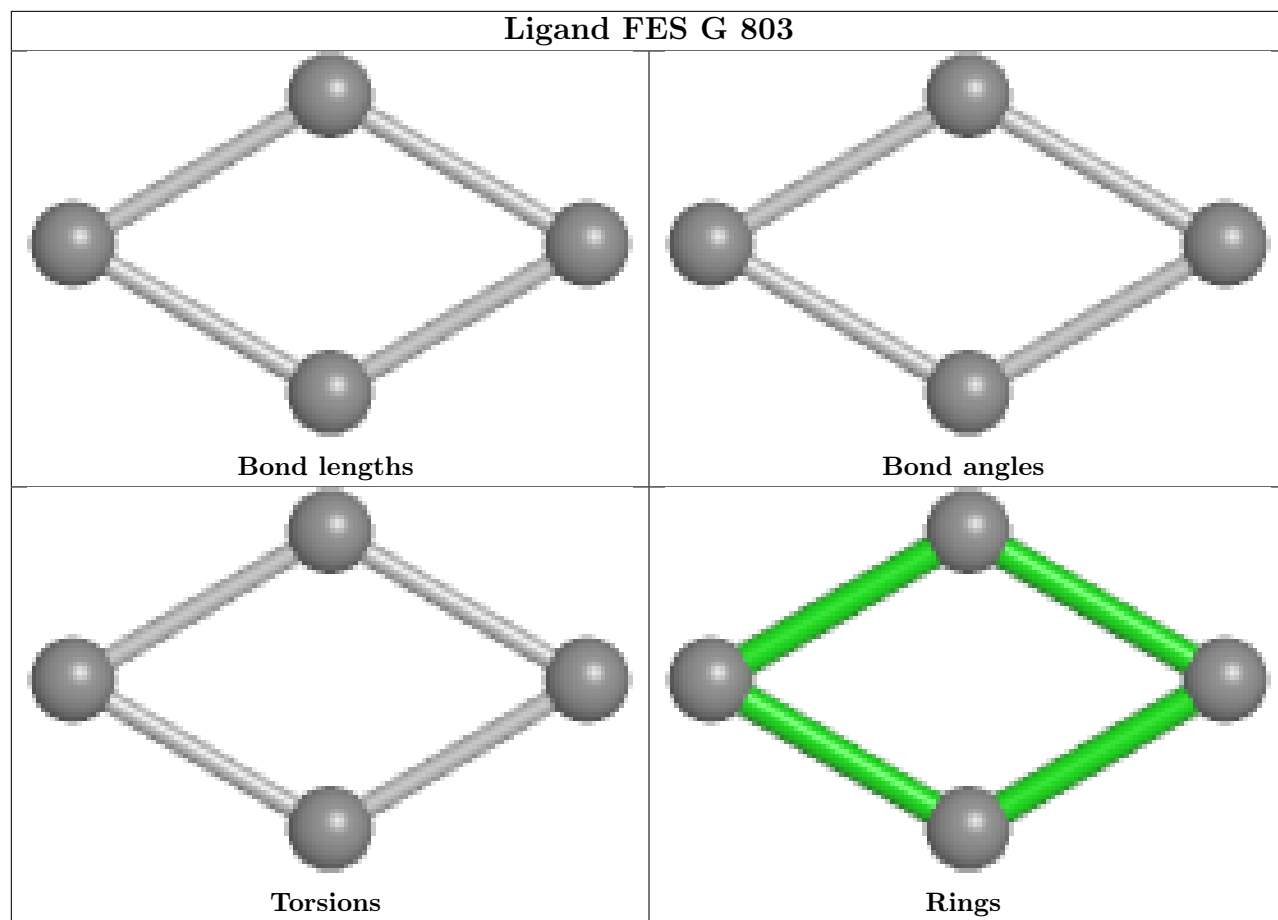
Ligand SF4 I 302

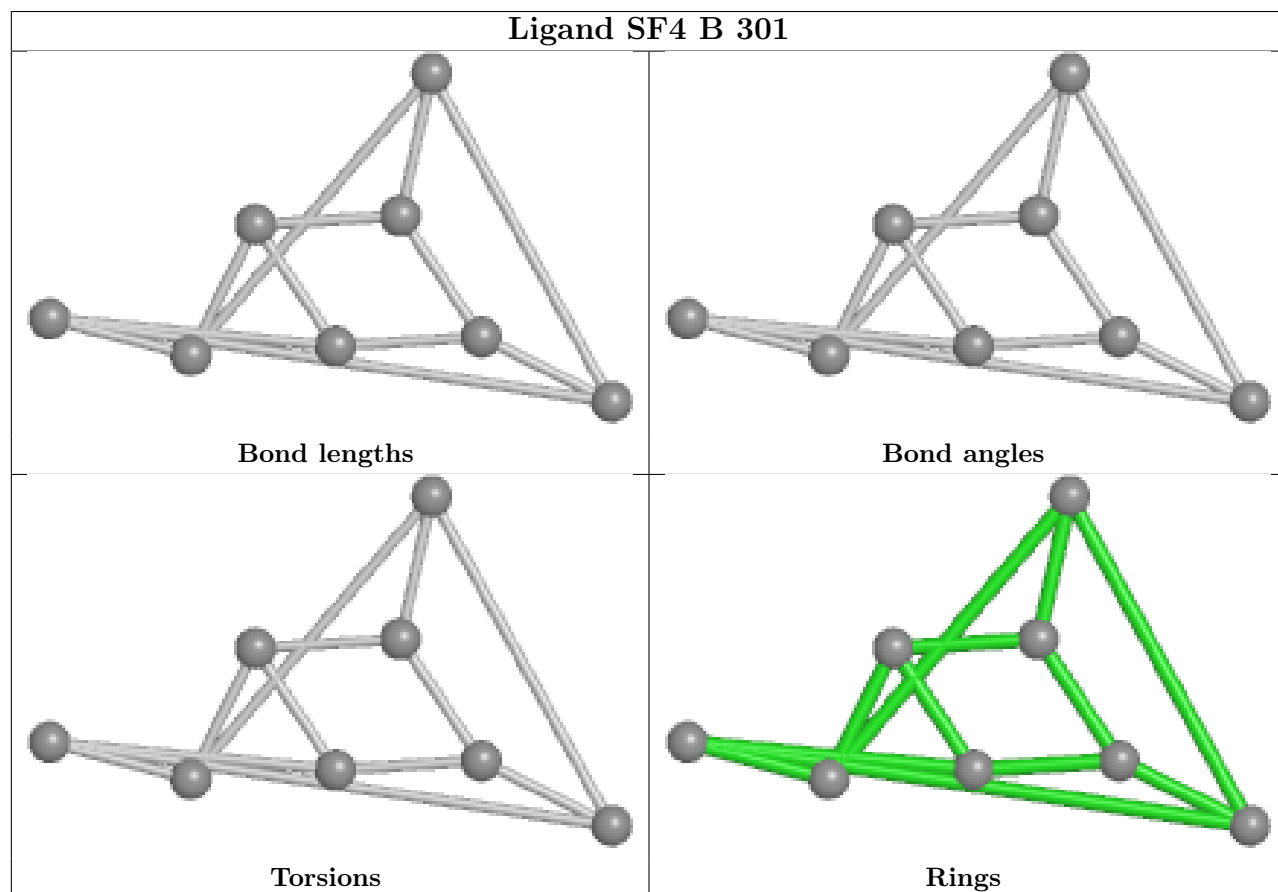
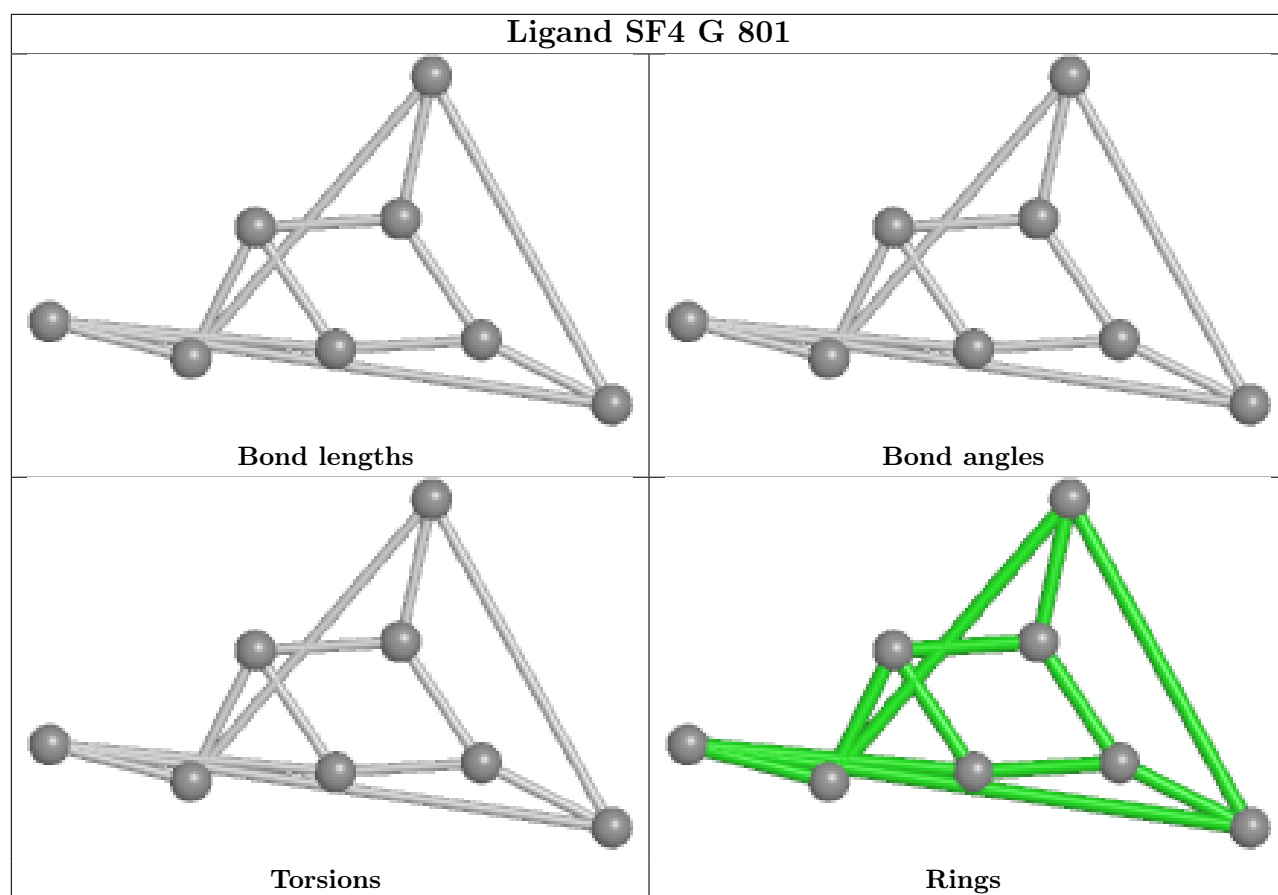


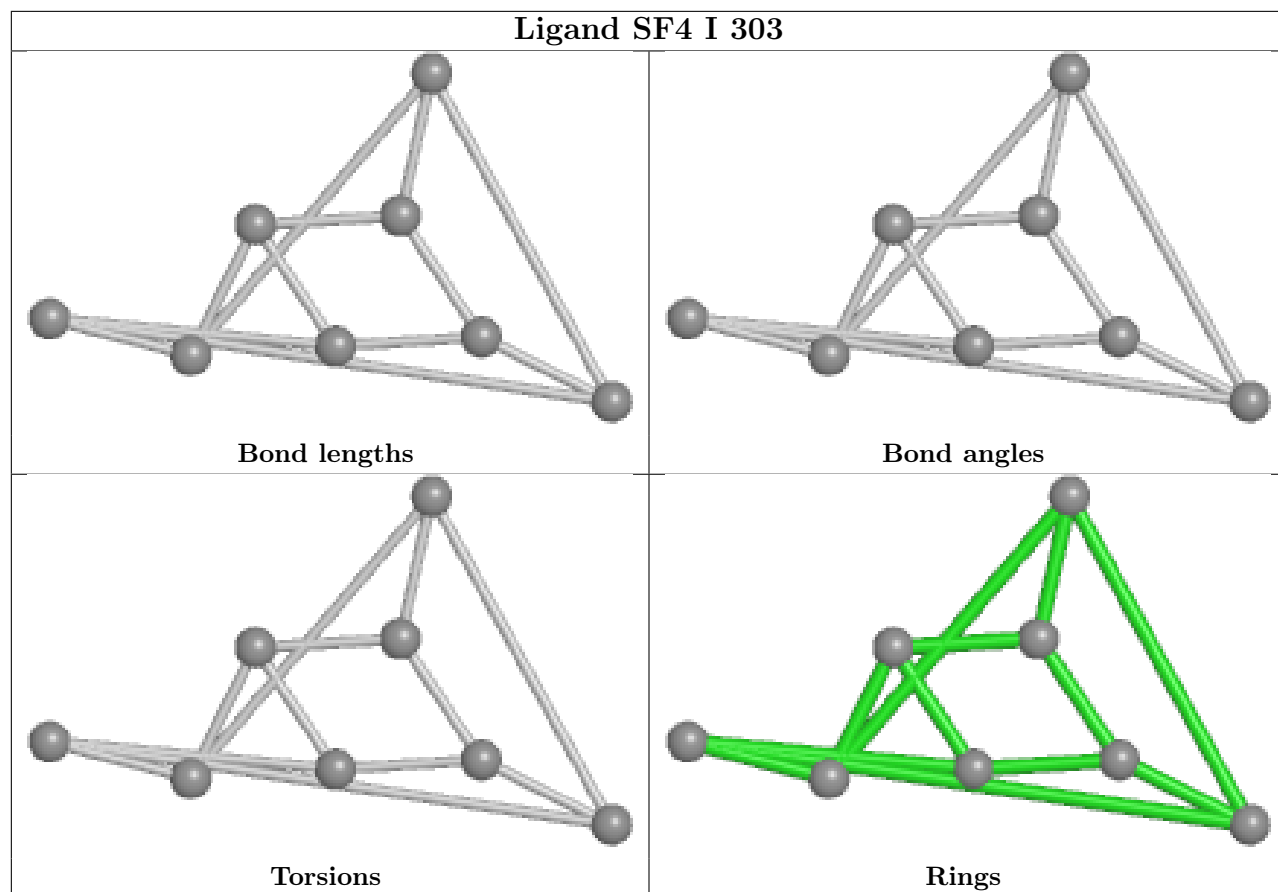
Ligand SF4 F 502

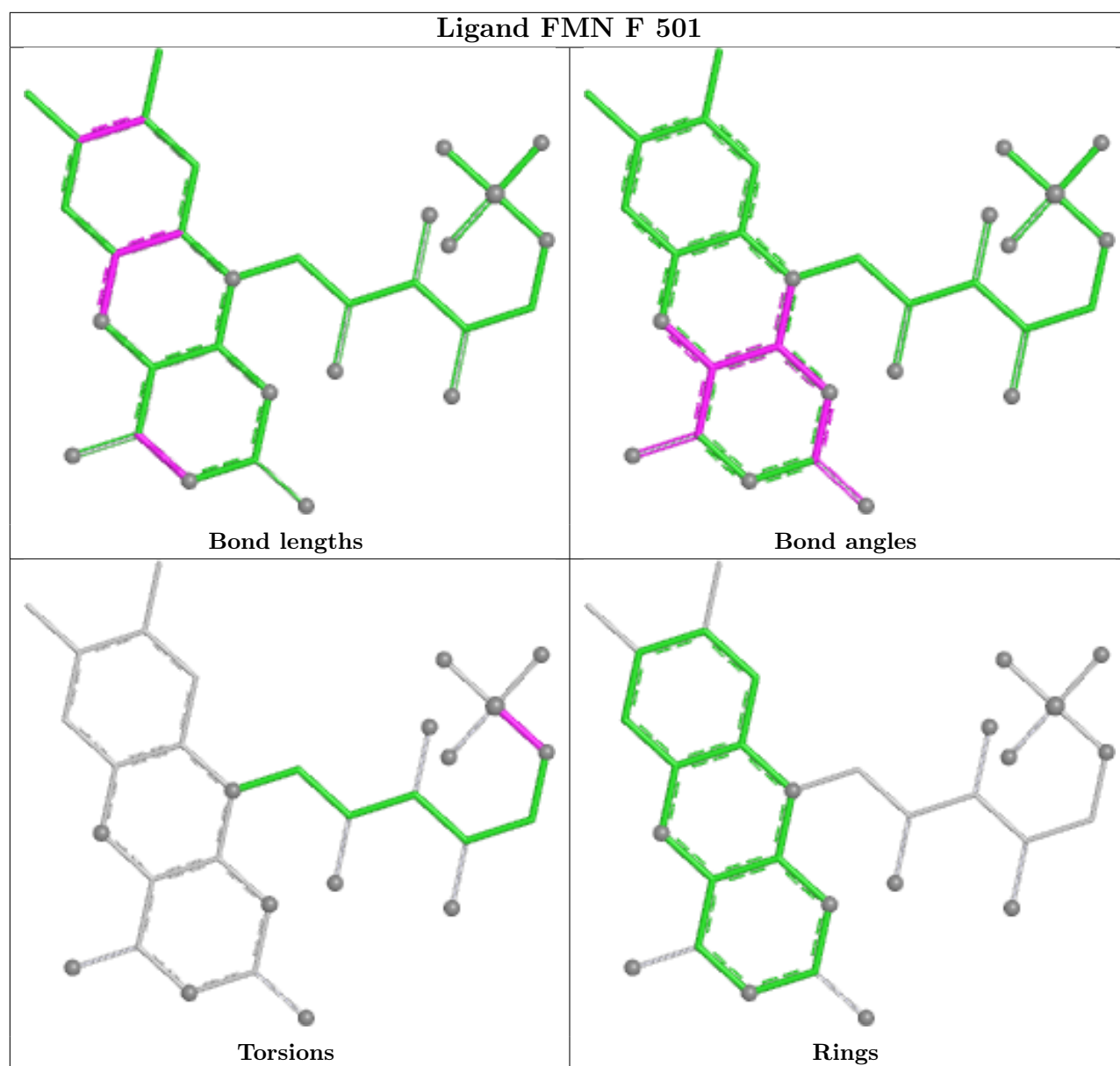












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

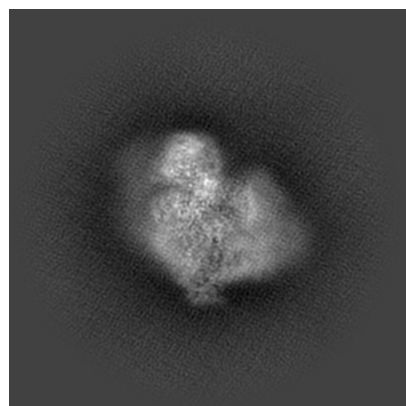
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38515. These allow visual inspection of the internal detail of the map and identification of artifacts.

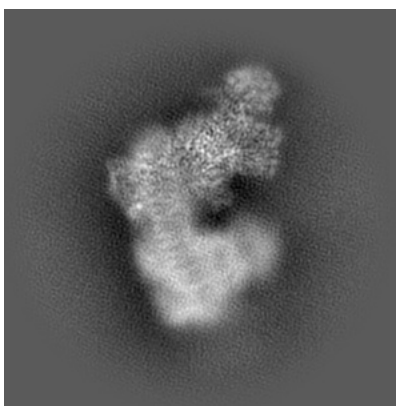
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

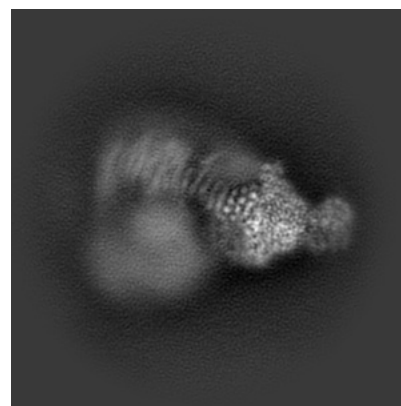
6.1.1 Primary map



X

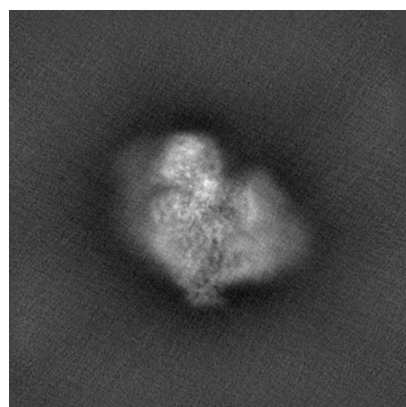


Y

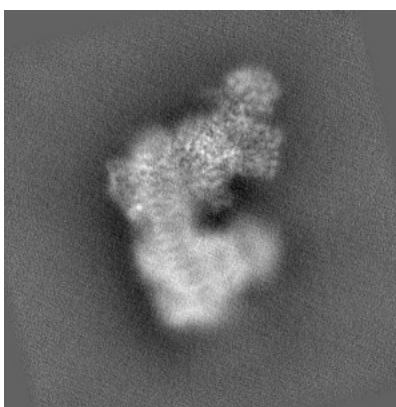


Z

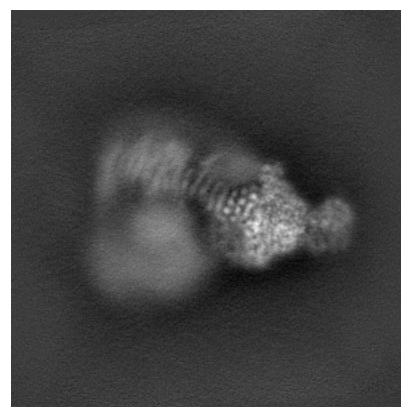
6.1.2 Raw map



X



Y

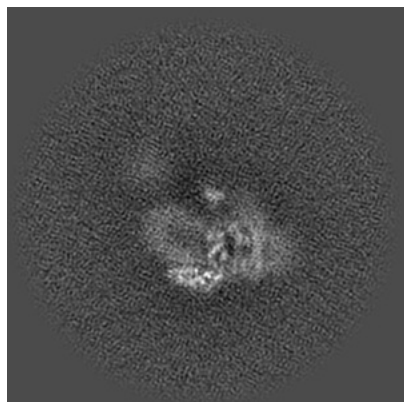


Z

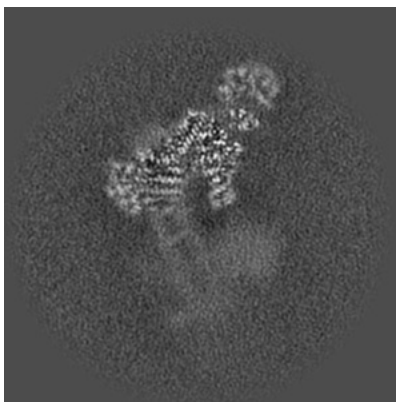
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

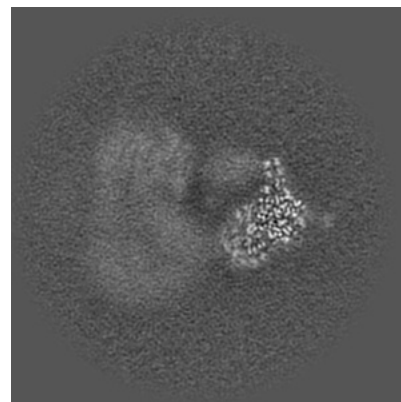
6.2.1 Primary map



X Index: 192

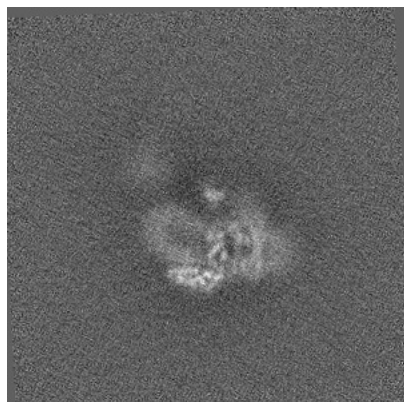


Y Index: 192



Z Index: 192

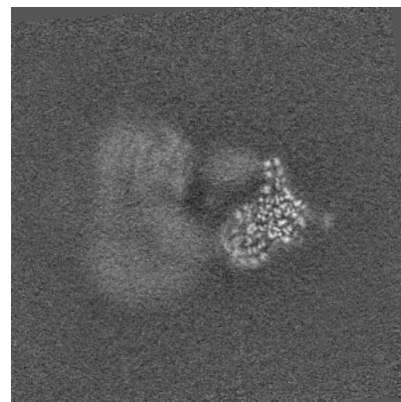
6.2.2 Raw map



X Index: 192



Y Index: 192

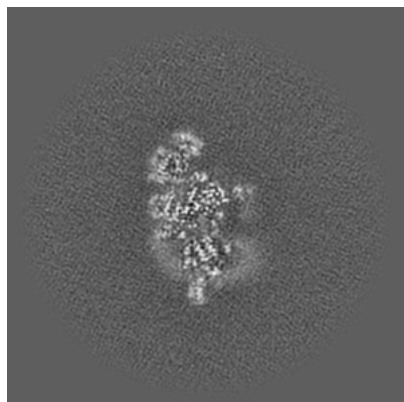


Z Index: 192

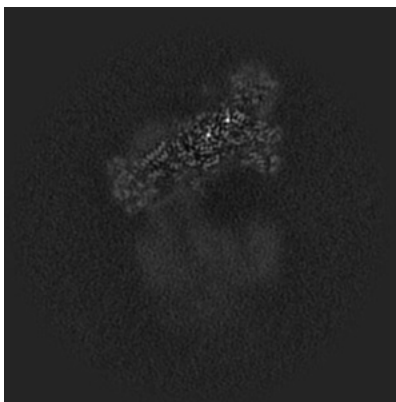
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

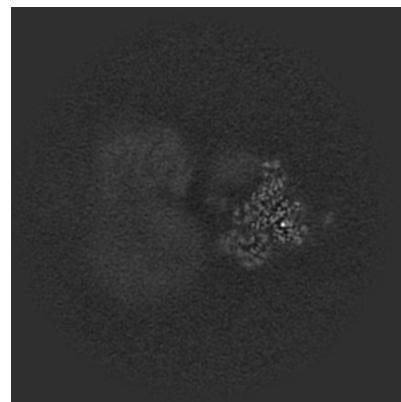
6.3.1 Primary map



X Index: 238

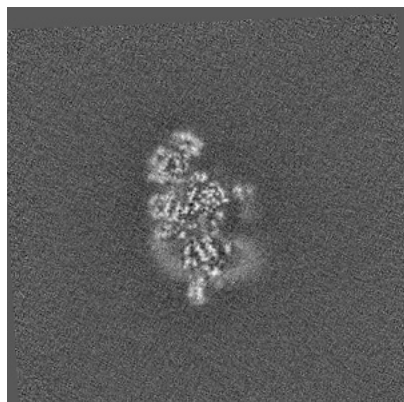


Y Index: 174

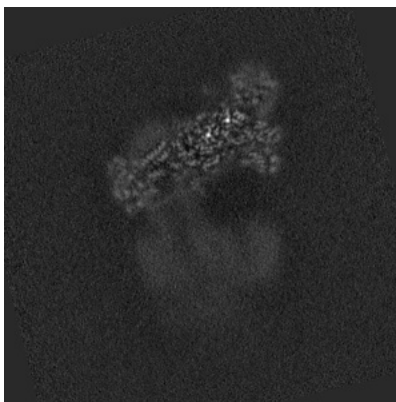


Z Index: 196

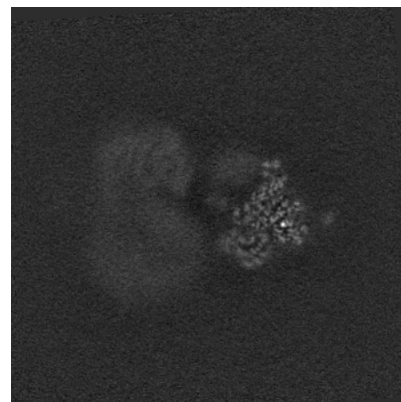
6.3.2 Raw map



X Index: 238



Y Index: 174

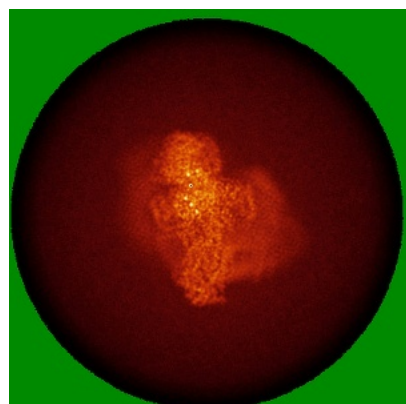


Z Index: 196

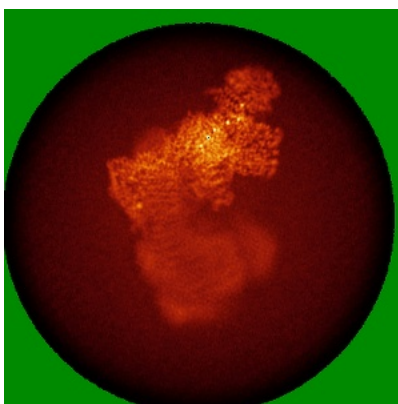
The images above show the largest variance slices of the map in three orthogonal directions.

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

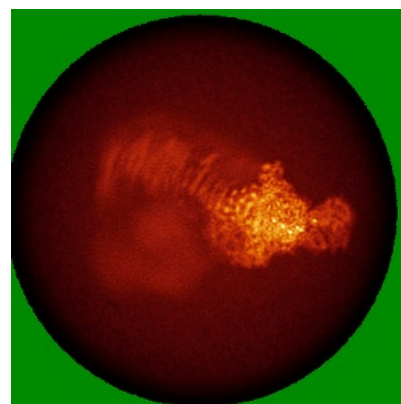
6.4.1 Primary map



X

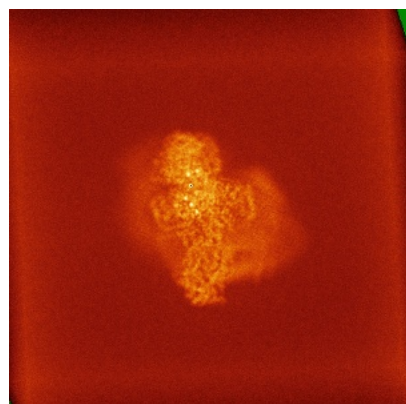


Y

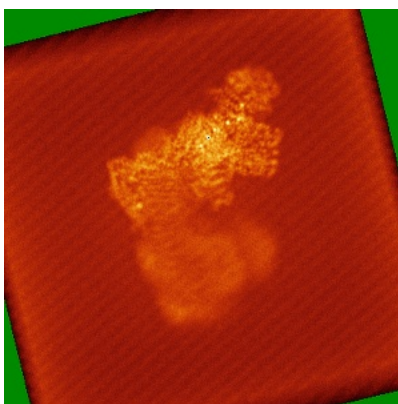


Z

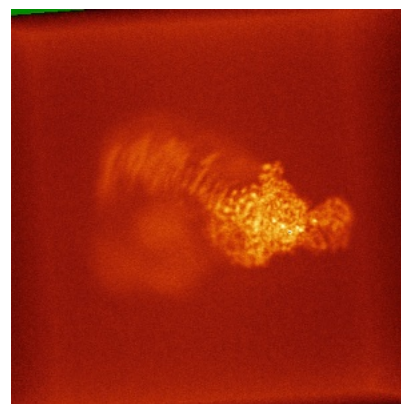
6.4.2 Raw map



X



Y

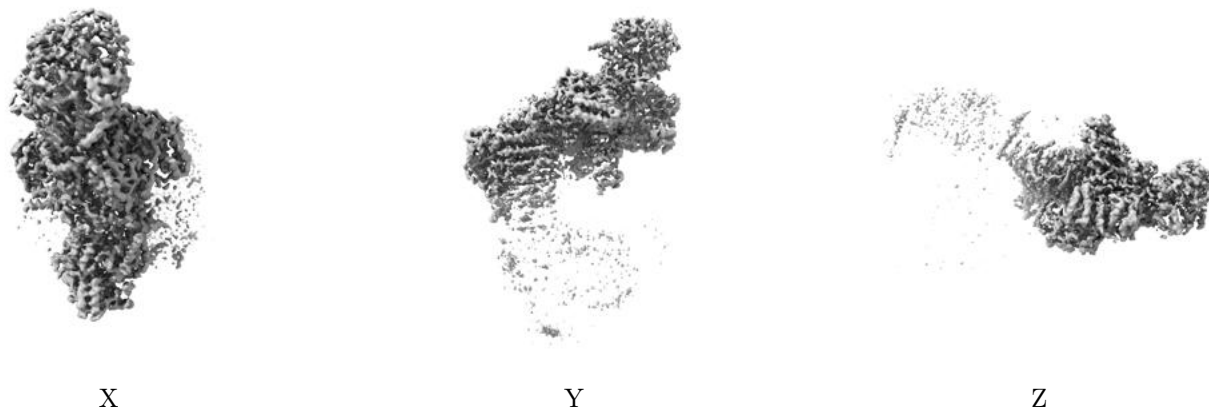


Z

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.

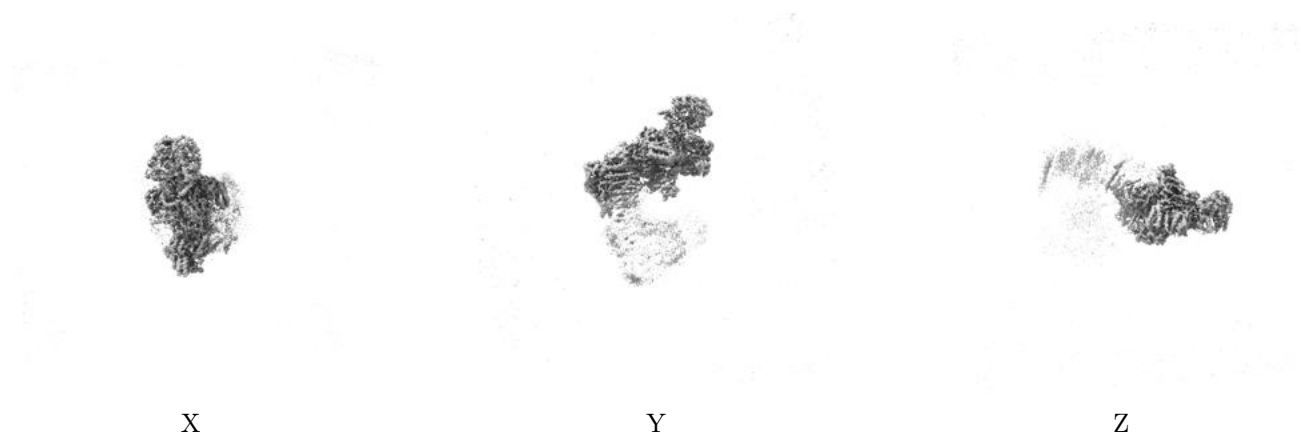
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

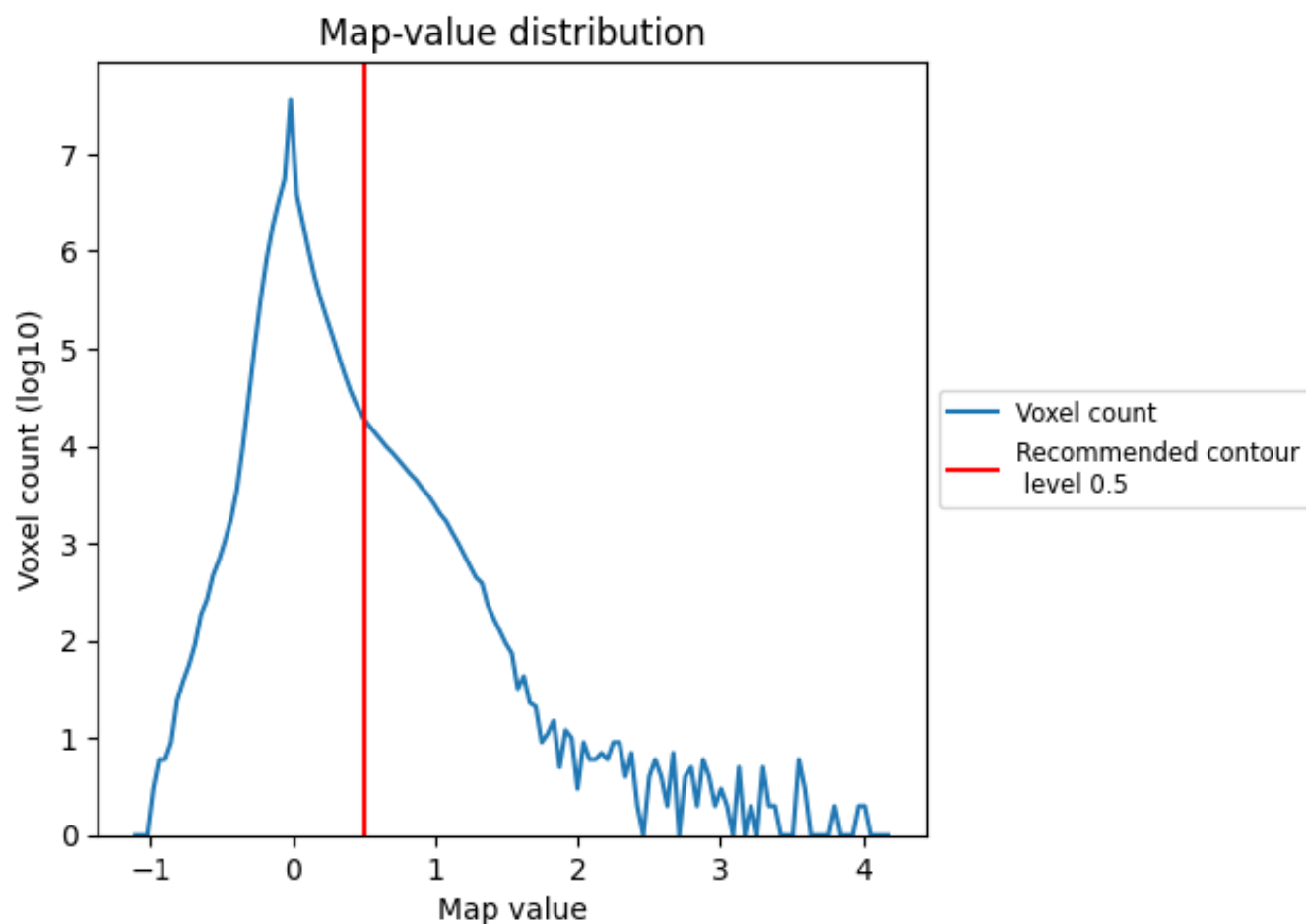
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

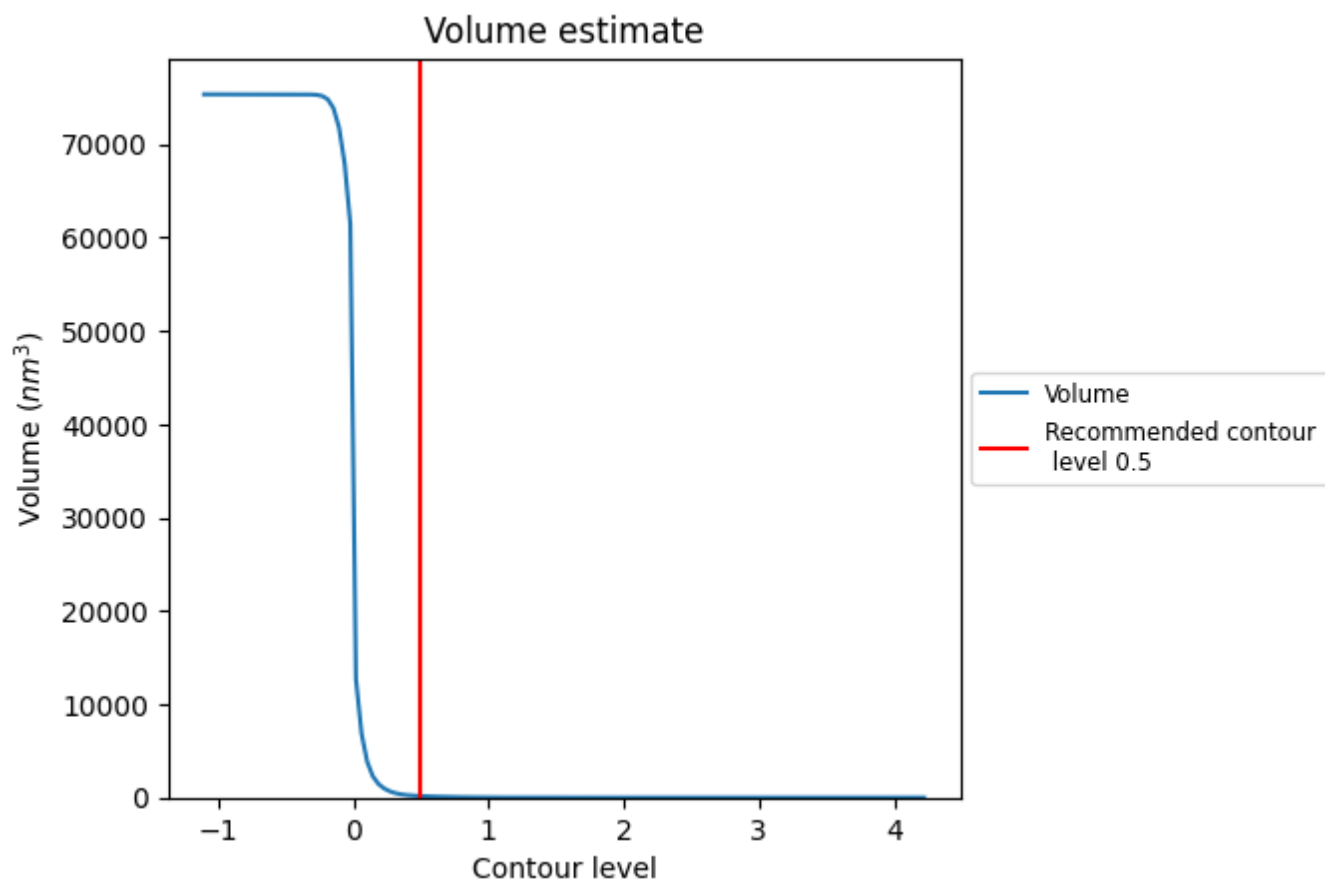
This section contains the results of statistical analysis of the map.

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.

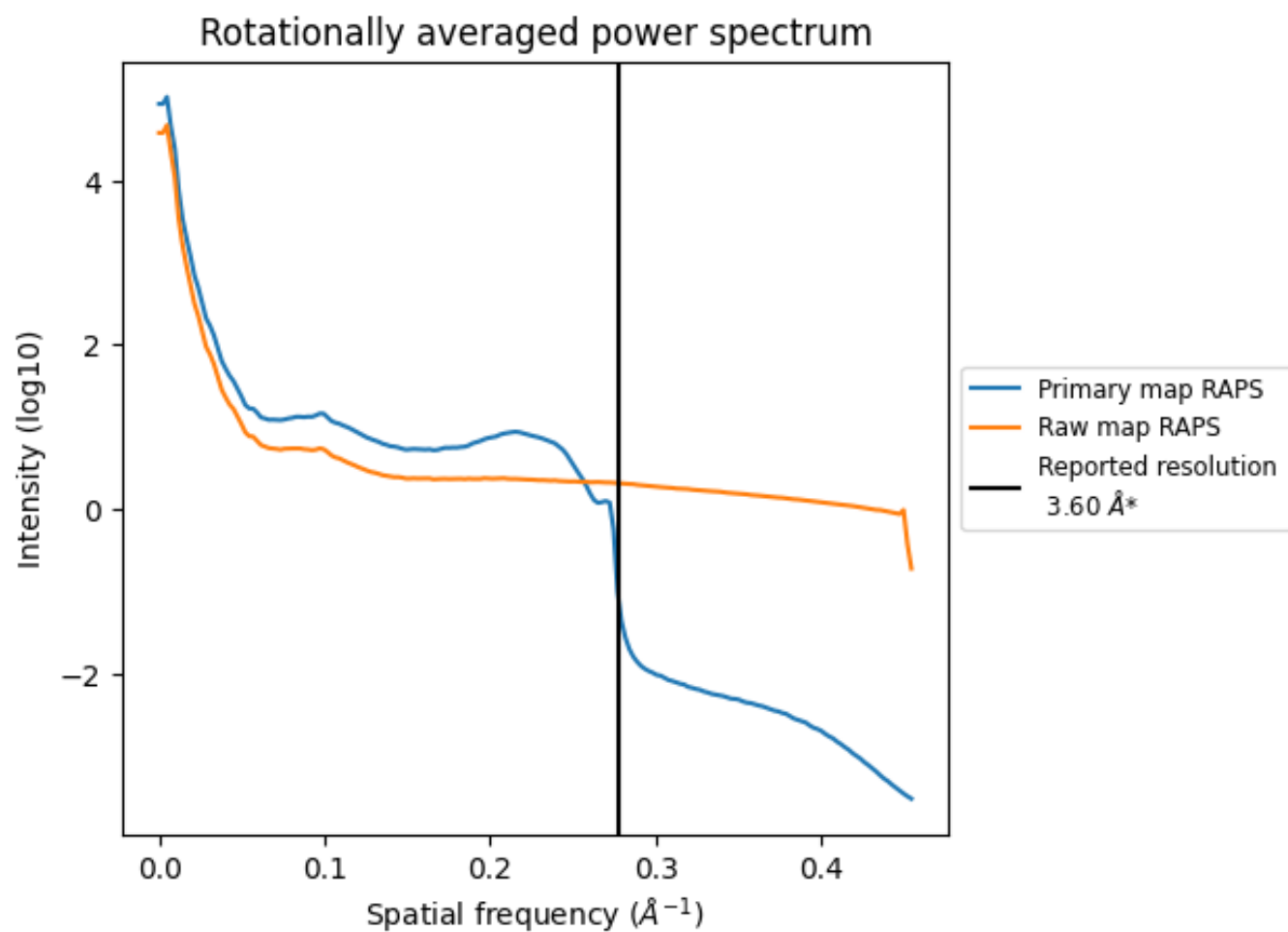
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm^3 ; this corresponds to an approximate mass of 140 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

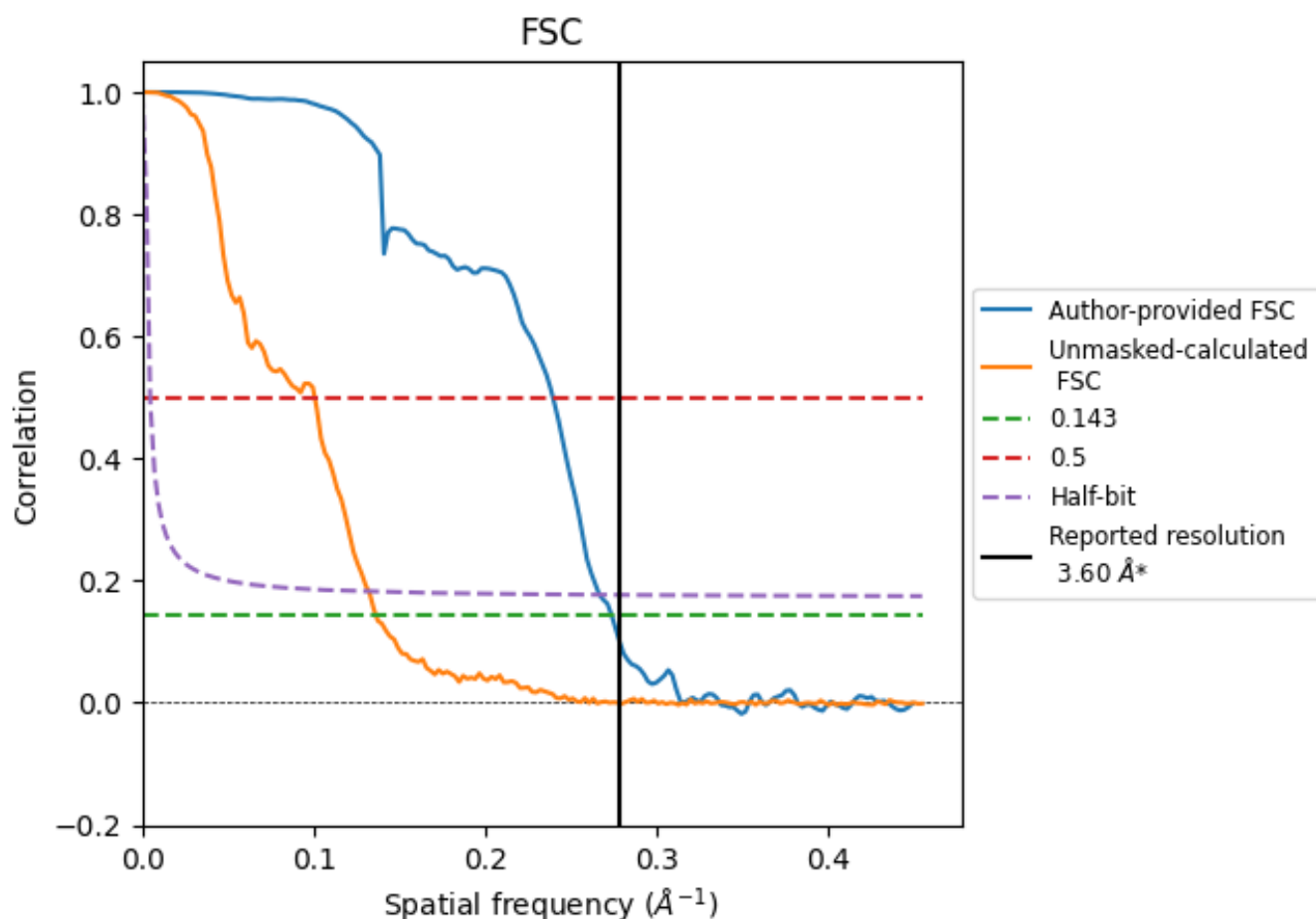


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

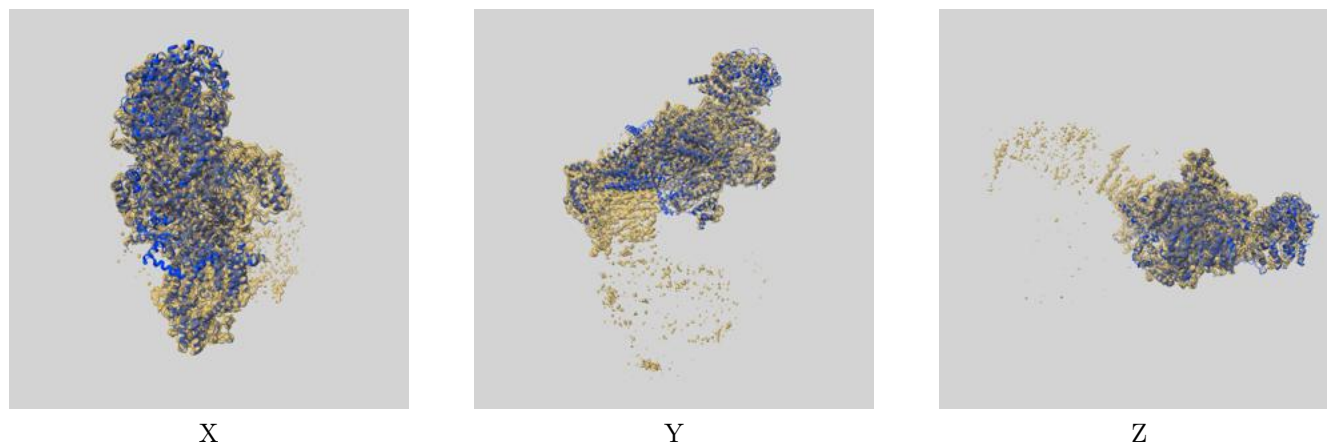
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.65	4.18	3.75
Unmasked-calculated*	7.34	9.95	7.58

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

9 Map-model fit [i](#)

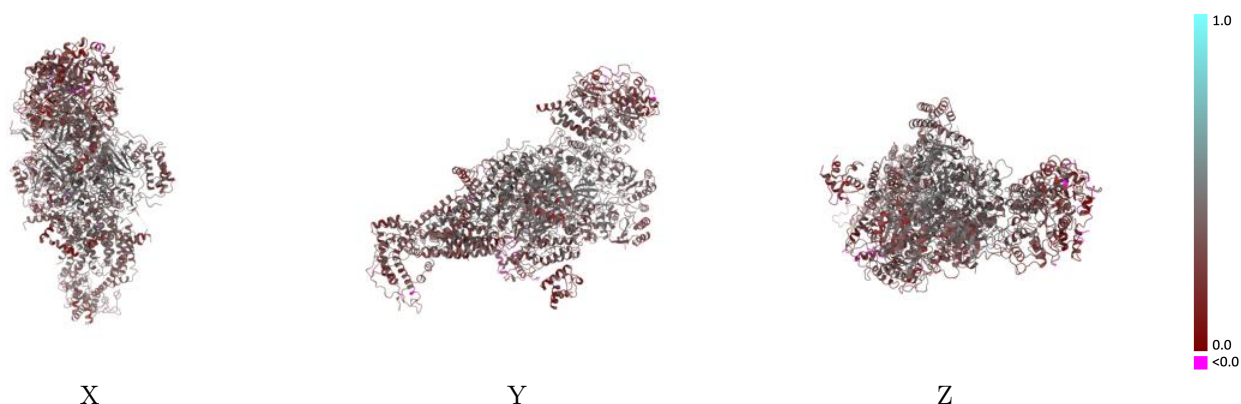
This section contains information regarding the fit between EMDB map EMD-38515 and PDB model 8XNU. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



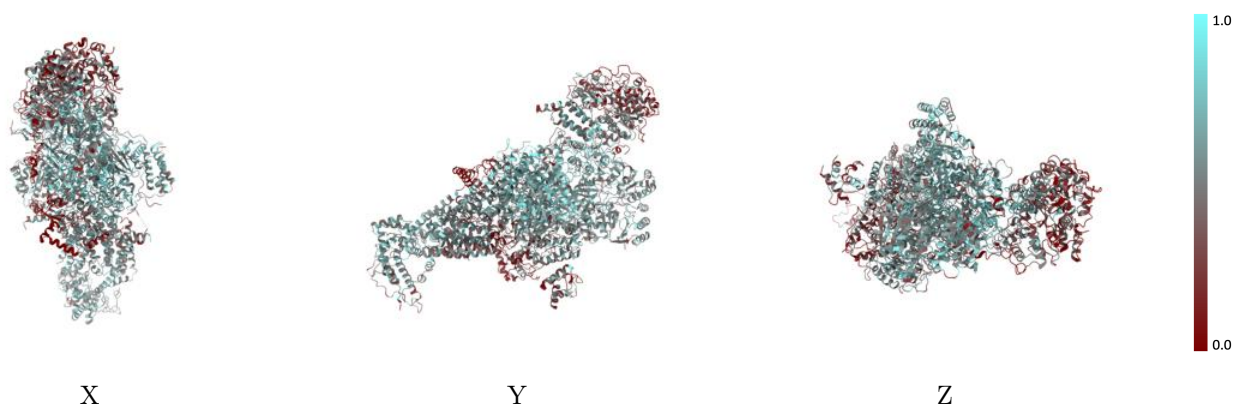
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



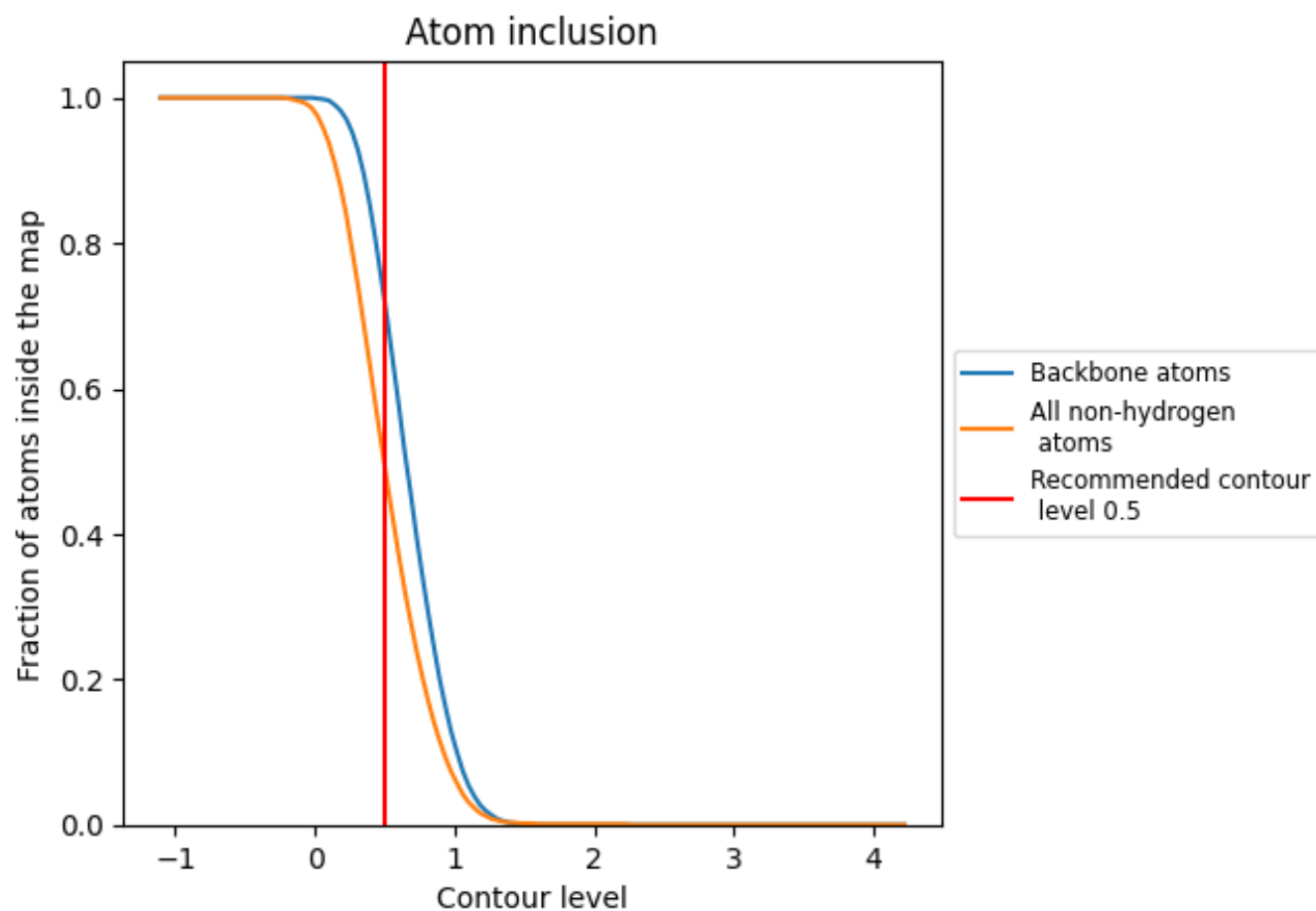
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion ⓘ



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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4930	 0.3500
A	 0.3860	 0.3360
B	 0.6320	 0.4220
C	 0.6340	 0.4310
D	 0.6410	 0.4260
E	 0.3200	 0.2660
F	 0.3990	 0.3050
G	 0.5860	 0.3840
H	 0.5210	 0.3770
I	 0.6520	 0.4150
P	 0.3640	 0.2930
Q	 0.4490	 0.3860
R	 0.2320	 0.2940
S	 0.5420	 0.3160
T	 0.3320	 0.2110
V	 0.5970	 0.3460
W	 0.4920	 0.3420
X	 0.5400	 0.2990
Z	 0.5430	 0.3090
a	 0.6070	 0.3730
b	 0.5090	 0.3180
q	 0.0930	 0.2960
r	 0.2420	 0.2870
s	 0.0360	 0.2390

