



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 05:58 PM JST

PDB ID : 8IAP / pdb_00008iap
EMDB ID : EMD-35314
Title : Respiratory complex Peripheral Arm of CI, focus-refined map of type I, Wild type mouse under thermoneutral temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-09
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

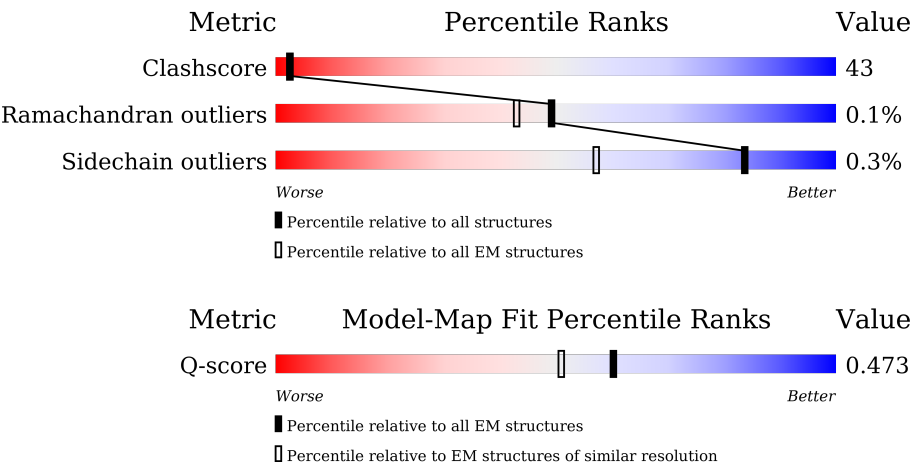
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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

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

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	UQ1	D	501	-	-	X	-
27	FES	E	301	-	-	X	-
27	FES	G	803	-	-	X	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 34534 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	92	Total	C	N	O	S	0	0
			754	523	107	119	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

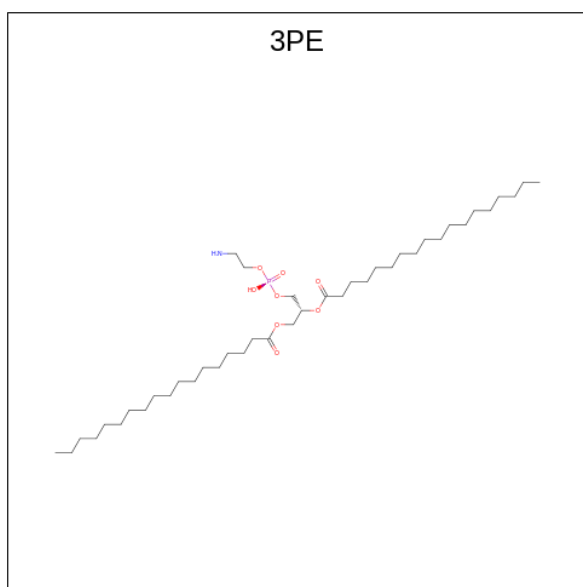
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

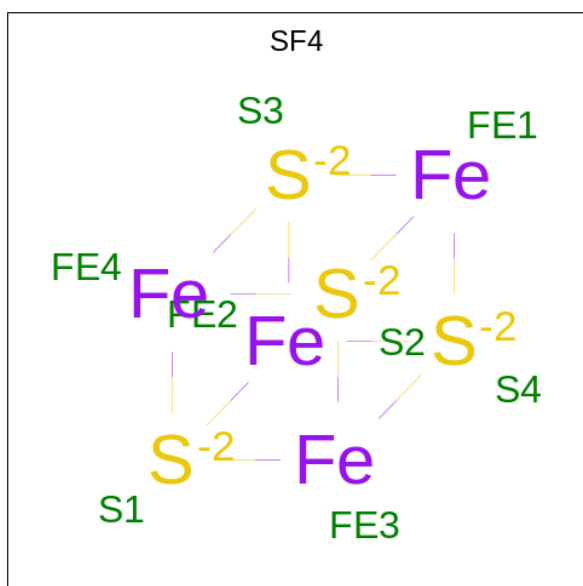
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	22	Total	C	N	O	0	0
			189	124	29	36		

- Molecule 24 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



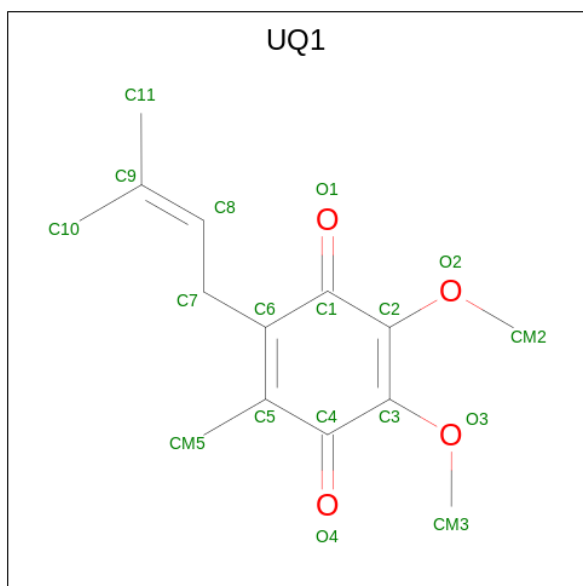
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	b	1	Total	C	N	O	P	0
			46	36	1	8	1	

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



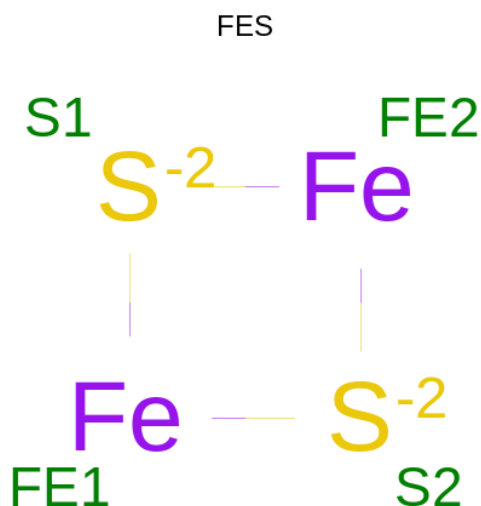
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	Fe	S	0
			8	4	4	
25	F	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	

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



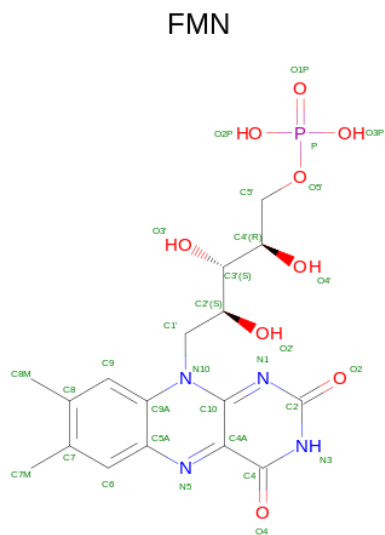
Mol	Chain	Residues	Atoms			AltConf
26	D	1	Total	C	O	0
			18	14	4	

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



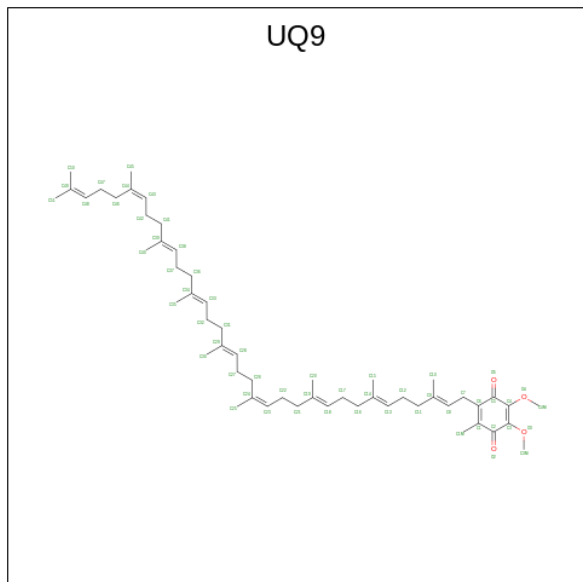
Mol	Chain	Residues	Atoms			AltConf
27	E	1	Total 4	Fe 2	S 2	0
27	G	1	Total 4	Fe 2	S 2	0

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



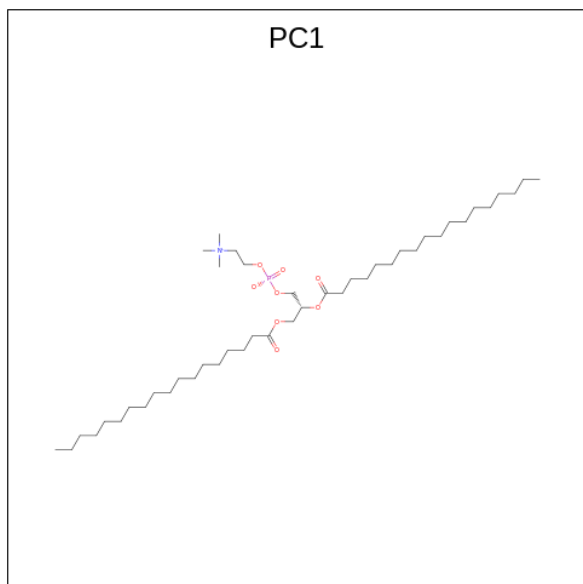
Mol	Chain	Residues	Atoms					AltConf
28	F	1	Total 31	C 17	N 4	O 9	P 1	0

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



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

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



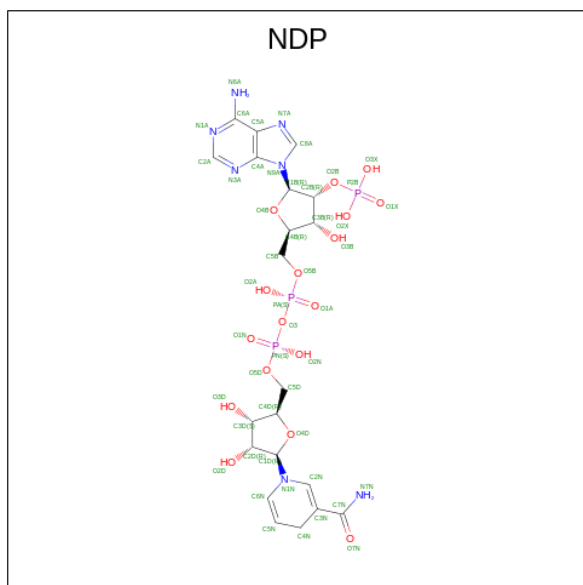
Mol	Chain	Residues	Atoms					AltConf
30	I	1	Total	C	N	O	P	0
			47	37	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
30	q	1	Total	C	N	O	P	0
			35	25	1	8	1	

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

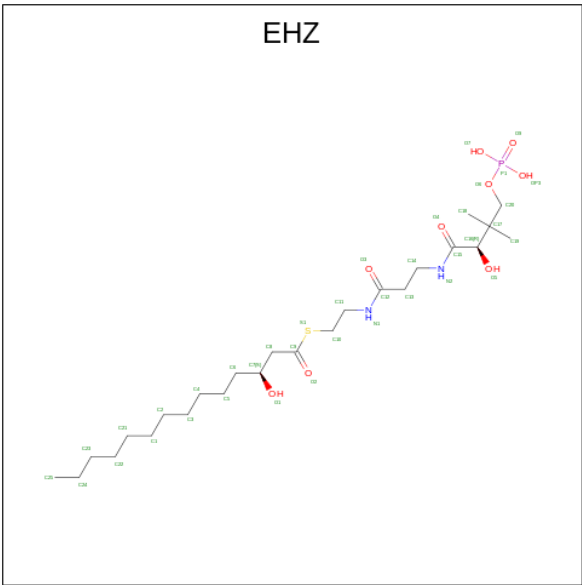


Mol	Chain	Residues	Atoms					AltConf
31	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

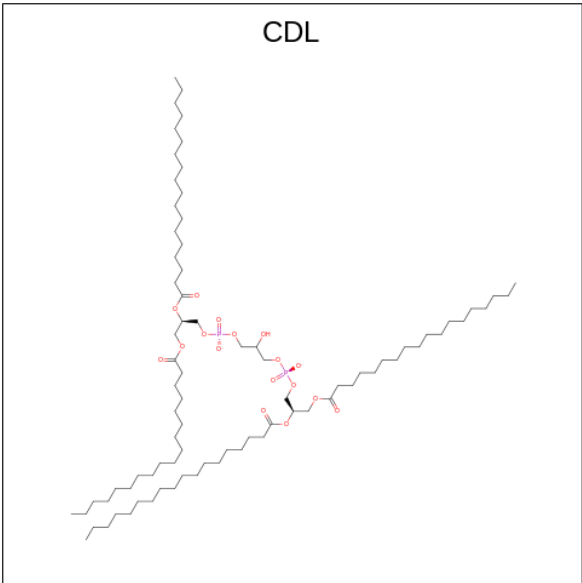
Mol	Chain	Residues	Atoms		AltConf
32	R	1	Total	Zn	0
			1	1	

- Molecule 33 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EH2) (formula: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



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

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

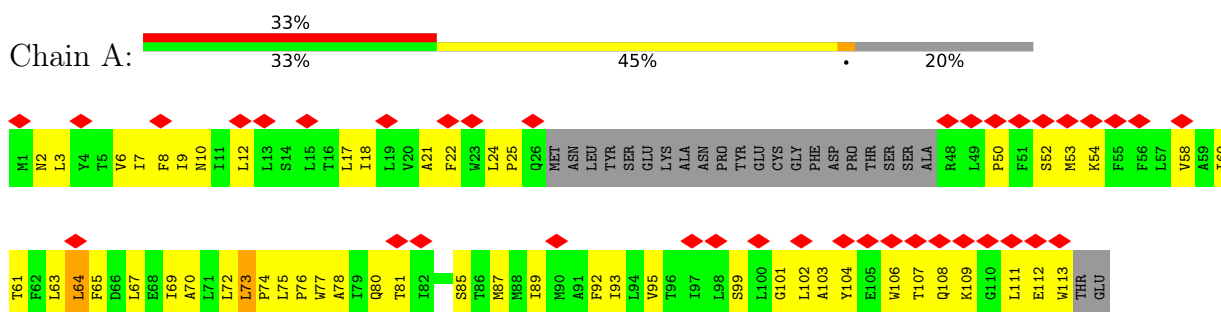


Mol	Chain	Residues	Atoms				AltConf
34	q	1	Total	C	O	P	0
			57	38	17	2	

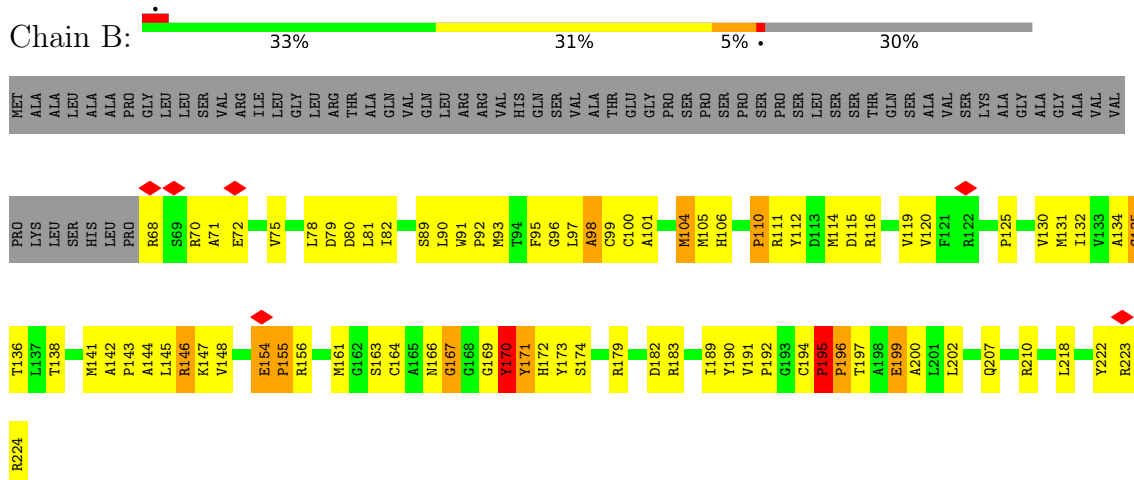
3 Residue-property plots

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.

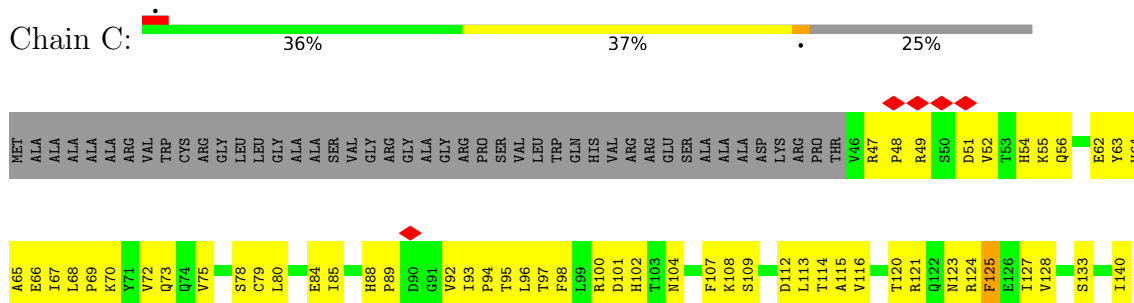
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

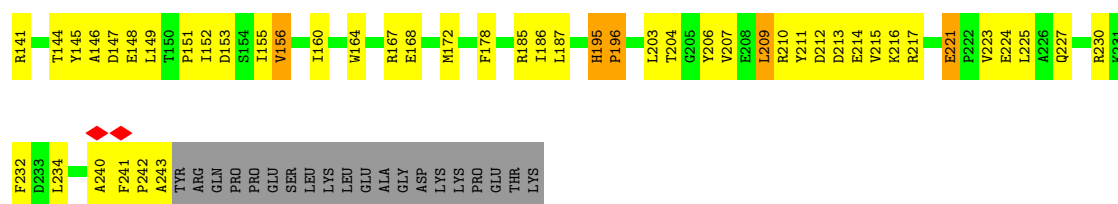


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

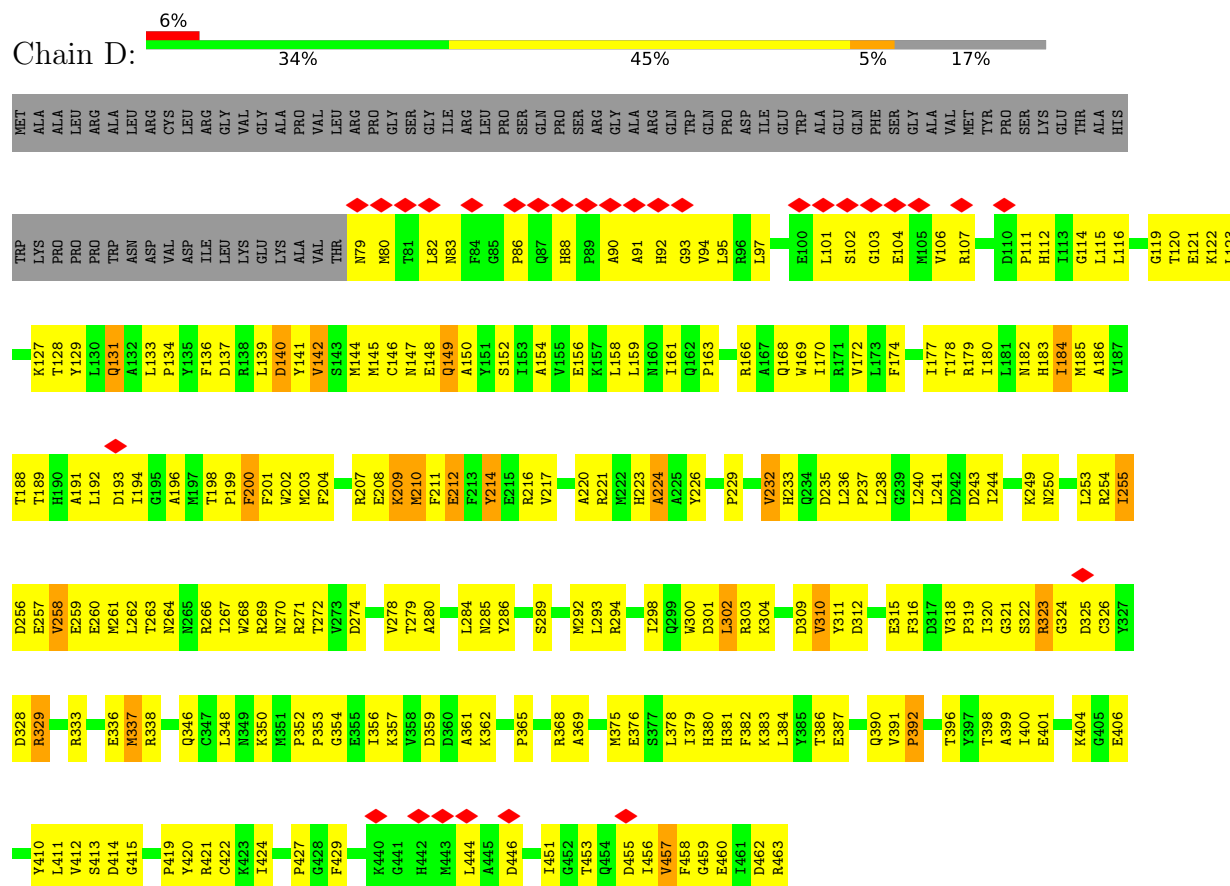


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

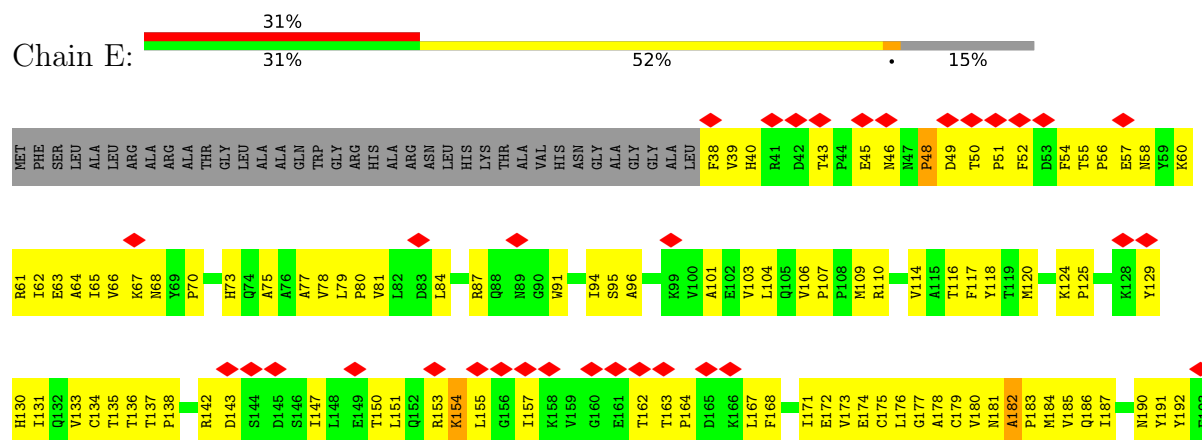




- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

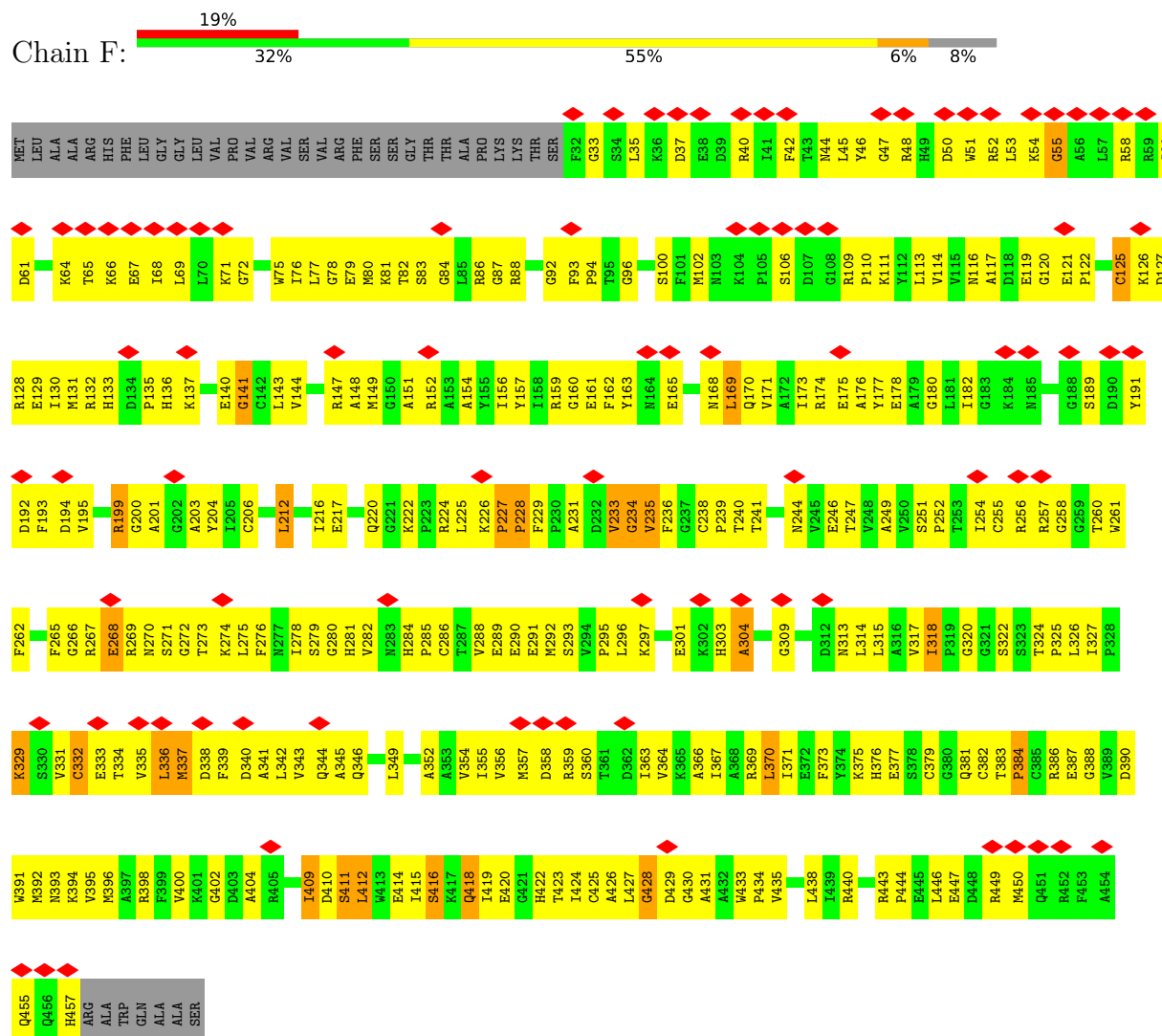


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

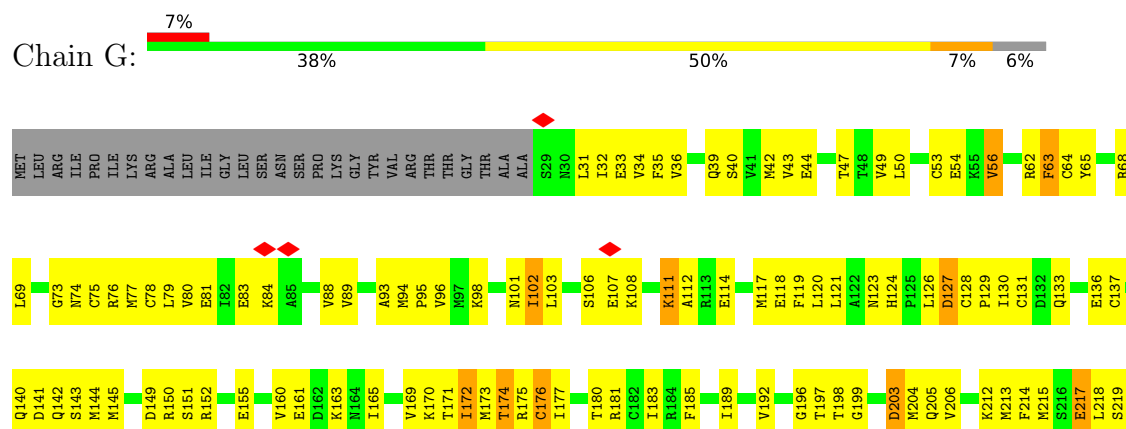




• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

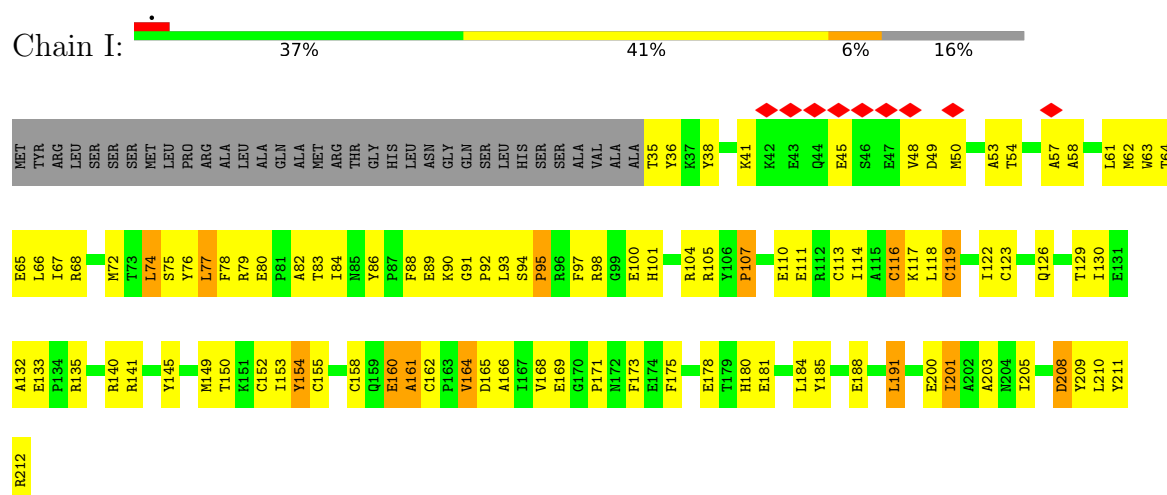


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



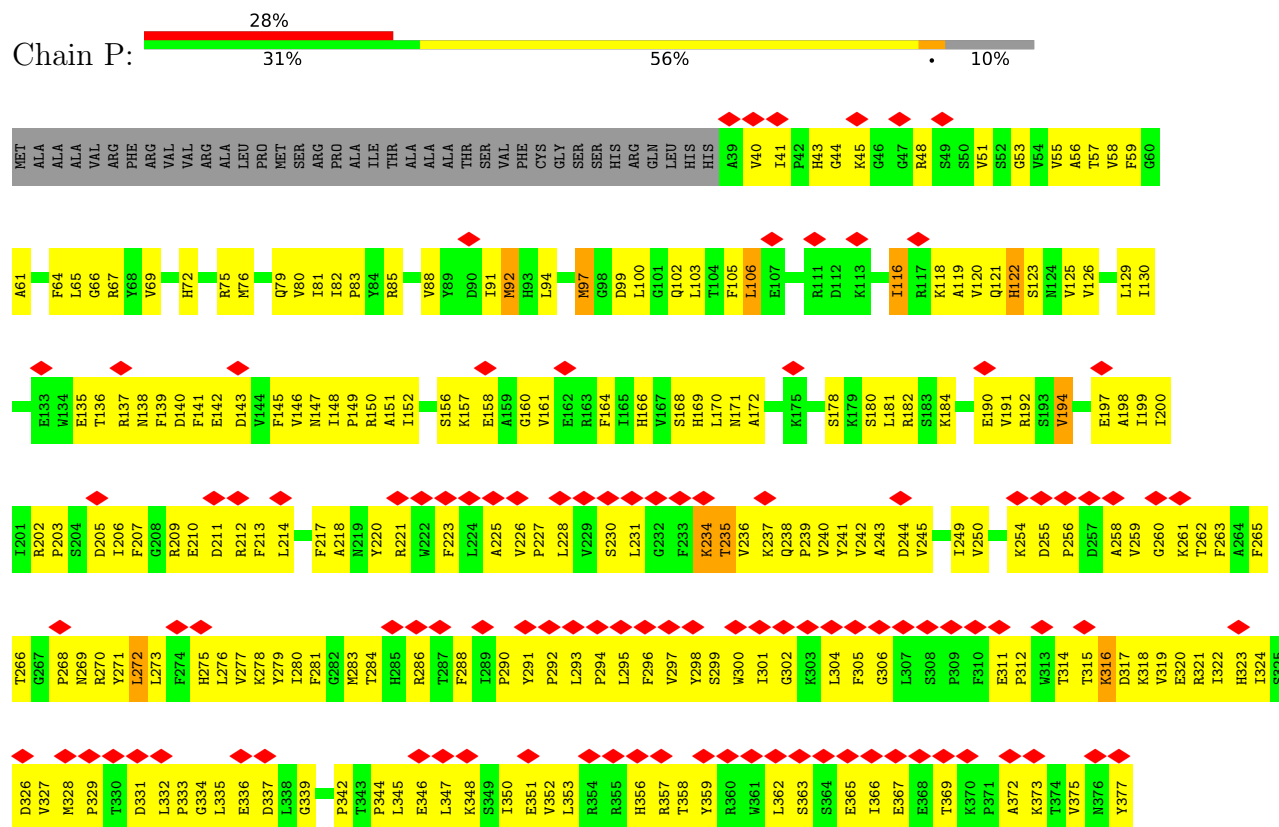
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



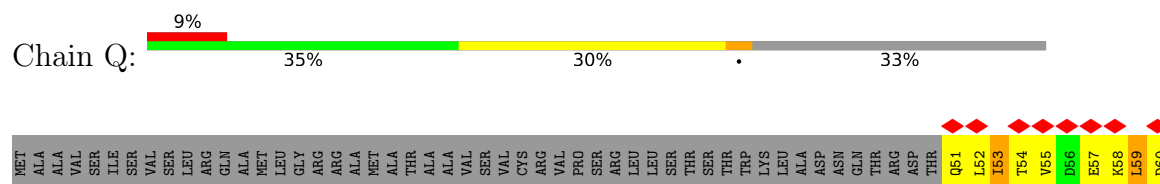
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

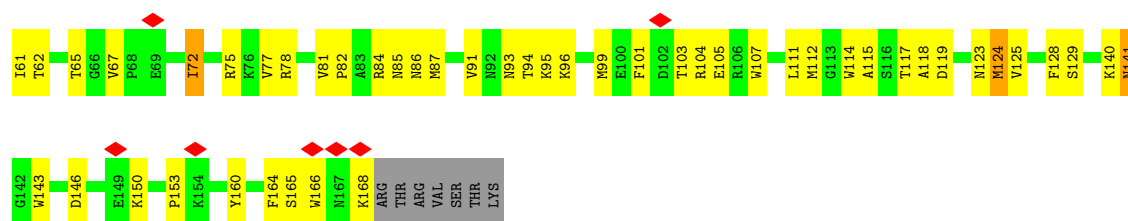
Chain P:



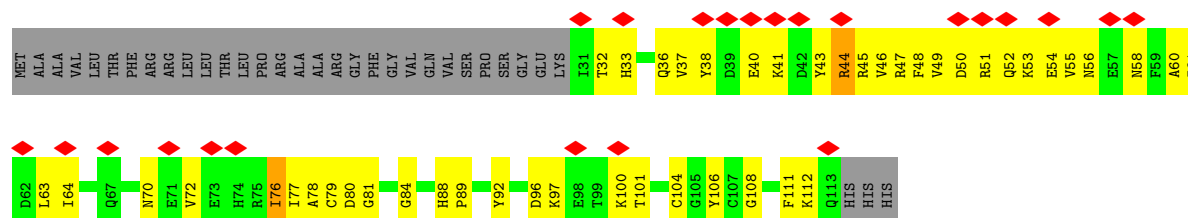
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:

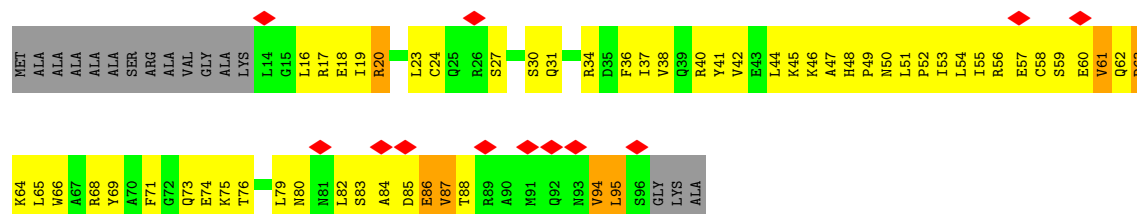




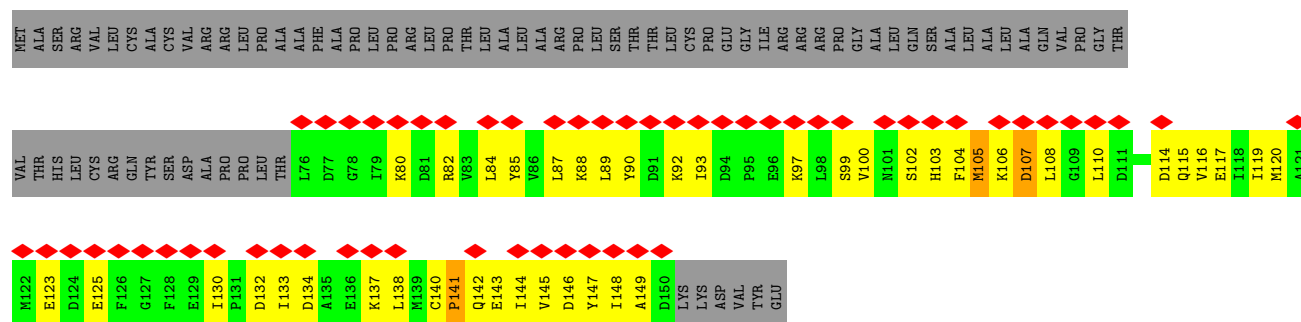
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



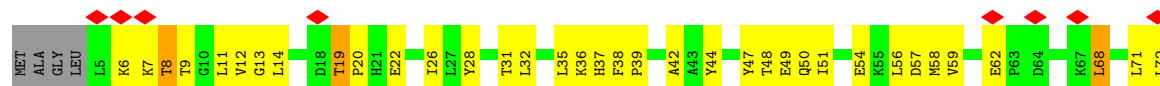
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

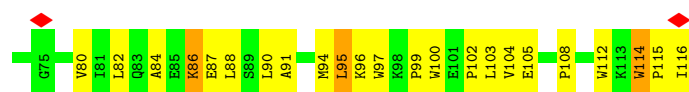


- Molecule 14: Acyl carrier protein, mitochondrial

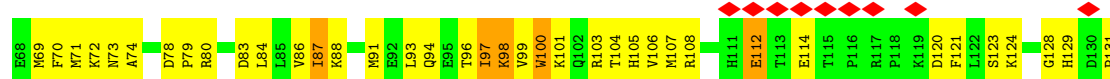
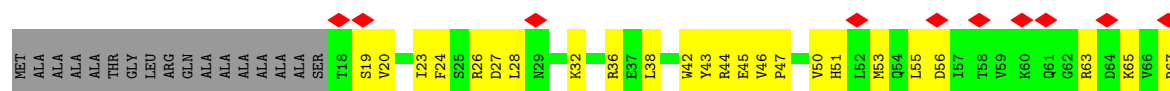


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

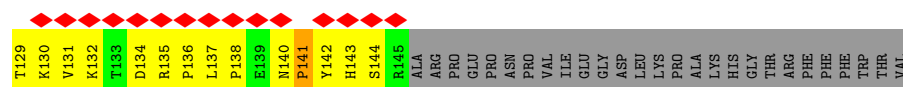
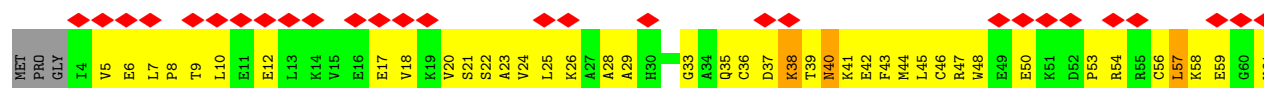




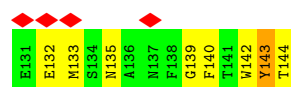
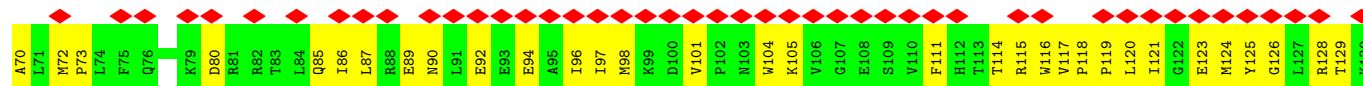
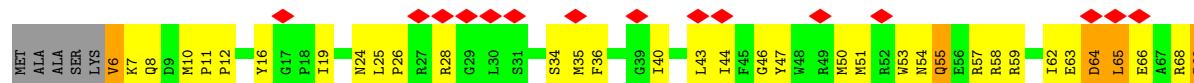
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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

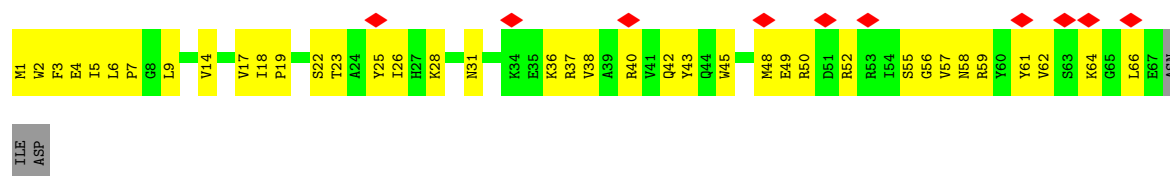


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

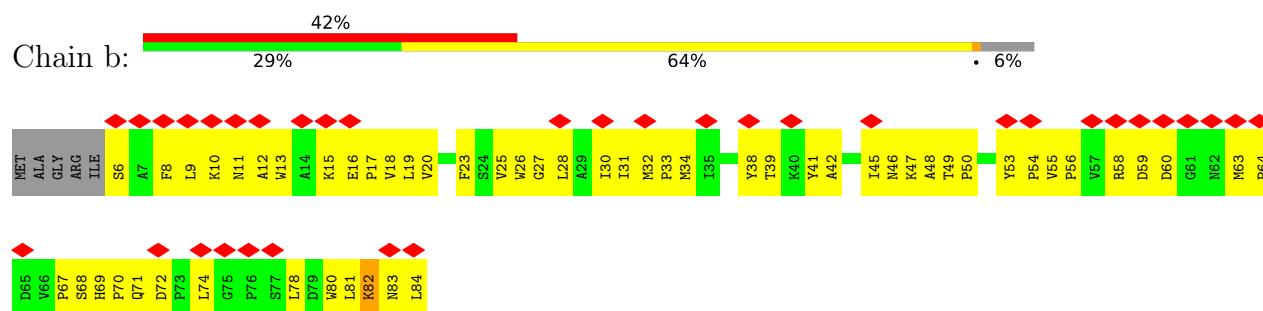


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

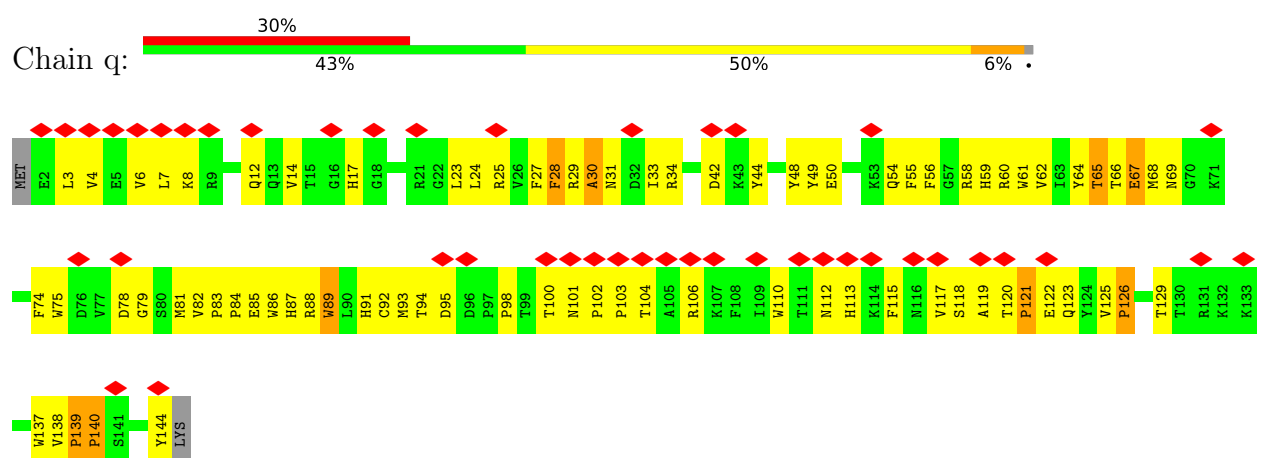




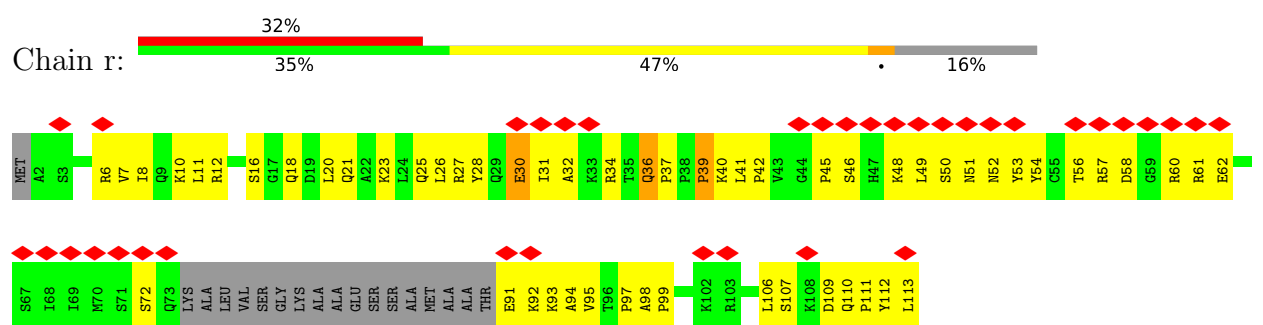
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



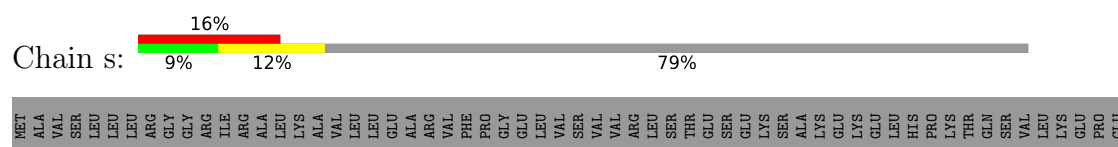
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



PRO	THR	ASP	THR	THR	THR	TYR	LYS	ASN	LEU	GLN	HIS	HIS	D39	Y40	N41	T42	Y43	T44	F45	L46	D47	L48	N49	L50	D51	L52	S53	K54	F55	R56	L57	F58	Q59	P60	SER	SER	GLY	ARG	GLU	SER	PRO	ARG	HIS	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85845	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.298	Depositor
Minimum map value	-2.419	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.8	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, UQ1, SF4, UQ9, NDP, FMN, PC1, CDL, FES, 3PE, EH2

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	0.79	0/774	1.12	7/1056 (0.7%)
2	B	0.93	1/1289 (0.1%)	1.46	20/1744 (1.1%)
3	C	0.87	0/1687	1.26	11/2297 (0.5%)
4	D	0.96	5/3162 (0.2%)	1.50	38/4276 (0.9%)
5	E	0.72	1/1675 (0.1%)	1.11	13/2282 (0.6%)
6	F	0.90	5/3363 (0.1%)	1.43	54/4543 (1.2%)
7	G	0.93	10/5374 (0.2%)	1.56	101/7281 (1.4%)
8	H	1.00	3/2608 (0.1%)	1.42	48/3563 (1.3%)
9	I	0.92	1/1461 (0.1%)	1.51	20/1974 (1.0%)
10	P	0.74	1/2793 (0.0%)	1.12	17/3787 (0.4%)
11	Q	0.89	1/980 (0.1%)	1.24	8/1324 (0.6%)
12	R	0.66	0/671	0.92	2/903 (0.2%)
13	S	0.92	2/678 (0.3%)	1.39	10/915 (1.1%)
14	T	0.68	1/613 (0.2%)	0.95	3/826 (0.4%)
15	V	0.81	0/937	1.38	12/1270 (0.9%)
16	W	0.80	1/993 (0.1%)	1.06	7/1335 (0.5%)
17	X	0.71	0/1191	1.21	13/1605 (0.8%)
18	Z	0.67	1/1183 (0.1%)	1.09	13/1597 (0.8%)
19	a	0.84	0/561	1.11	3/755 (0.4%)
20	b	0.78	1/643 (0.2%)	1.01	3/884 (0.3%)
21	q	0.91	4/1234 (0.3%)	1.27	19/1681 (1.1%)
22	r	0.60	0/782	1.04	6/1058 (0.6%)
23	s	0.43	0/194	0.69	0/264
All	All	0.86	38/34846 (0.1%)	1.33	428/47220 (0.9%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	214	GLU	C-N	15.51	1.56	1.33
21	q	139	PRO	N-CD	-13.37	1.29	1.47
7	G	532	PRO	N-CD	-12.53	1.30	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	q	102	PRO	N-CD	-11.23	1.32	1.47
8	H	42	PRO	N-CD	10.89	1.62	1.47
6	F	234	GLY	CA-C	-10.42	1.40	1.52
6	F	227	PRO	N-CD	10.13	1.61	1.47
6	F	235	VAL	N-CA	-9.65	1.34	1.46
7	G	275	PRO	N-CD	-9.55	1.34	1.47
8	H	75	PRO	N-CD	9.26	1.60	1.47
9	I	107	PRO	N-CD	8.66	1.59	1.47
20	b	64	PRO	N-CD	8.54	1.59	1.47
21	q	121	PRO	N-CD	-8.40	1.35	1.47
4	D	140	ASP	C-O	-8.05	1.14	1.24
13	S	63	PRO	N-CD	-7.94	1.36	1.47
5	E	218	ARG	CA-C	7.93	1.62	1.53
11	Q	53	ILE	C-O	7.84	1.33	1.24
14	T	141	PRO	N-CD	-7.68	1.36	1.47
4	D	365	PRO	N-CD	-7.41	1.37	1.47
21	q	126	PRO	N-CD	-7.10	1.37	1.47
7	G	449	PRO	N-CD	6.71	1.57	1.47
7	G	541	PRO	N-CD	-6.71	1.38	1.47
6	F	233	VAL	CA-C	-6.68	1.44	1.52
7	G	203	ASP	CA-C	6.65	1.62	1.52
4	D	140	ASP	CA-C	-6.45	1.44	1.52
7	G	600	GLU	CA-C	6.43	1.61	1.52
7	G	632	ILE	CA-C	-6.41	1.44	1.52
18	Z	63	GLU	C-N	-6.25	1.24	1.33
7	G	127	ASP	CA-C	6.20	1.62	1.52
6	F	384	PRO	N-CD	-6.13	1.39	1.47
2	B	110	PRO	C-O	-6.09	1.16	1.24
4	D	392	PRO	C-O	-5.96	1.20	1.25
7	G	361	VAL	CA-C	5.85	1.60	1.52
16	W	98	LYS	CA-C	-5.48	1.46	1.52
7	G	683	PRO	N-CD	-5.47	1.40	1.47
13	S	95	LEU	CA-C	5.47	1.59	1.52
10	P	235	THR	CA-C	5.38	1.59	1.53
4	D	310	VAL	C-O	-5.06	1.16	1.23

All (428) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	174	THR	N-CA-C	-17.48	89.04	114.39
6	F	332	CYS	N-CA-C	15.60	130.05	111.02
7	G	632	ILE	N-CA-C	-13.65	88.01	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	q	139	PRO	N-CA-CB	-13.45	95.66	103.19
7	G	251	ILE	N-CA-C	13.29	126.78	108.17
6	F	125	CYS	N-CA-C	-12.93	93.46	113.89
7	G	500	ILE	N-CA-C	-12.51	98.77	110.53
2	B	199	GLU	N-CA-C	-12.20	98.06	111.36
10	P	106	LEU	N-CA-C	12.19	128.70	109.07
16	W	98	LYS	N-CA-C	-12.06	88.99	108.41
6	F	171	VAL	N-CA-C	-11.88	99.36	110.53
2	B	80	ASP	N-CA-C	-11.68	98.58	111.07
6	F	449	ARG	N-CA-C	-11.62	98.69	111.36
7	G	204	MET	N-CA-C	-11.61	91.49	109.25
6	F	334	THR	N-CA-CB	11.50	127.31	109.82
7	G	599	THR	N-CA-C	11.35	126.22	112.38
11	Q	60	ASP	N-CA-C	-11.32	90.34	109.24
8	H	259	PHE	N-CA-C	-11.02	99.35	111.36
7	G	77	MET	N-CA-C	-10.84	97.35	113.61
2	B	105	MET	N-CA-C	-10.72	99.38	111.71
9	I	164	VAL	N-CA-C	-10.67	100.09	113.22
9	I	77	LEU	N-CA-C	-10.47	99.67	111.71
7	G	280	ASP	N-CA-C	10.32	122.53	111.28
7	G	414	PHE	N-CA-C	-10.11	101.44	113.88
9	I	161	ALA	N-CA-C	10.07	122.26	111.28
4	D	114	GLY	N-CA-C	-9.99	100.87	114.95
9	I	166	ALA	N-CA-C	-9.89	100.75	113.12
2	B	195	PRO	N-CA-C	-9.87	98.66	110.70
6	F	178	GLU	N-CA-C	-9.84	99.30	111.11
7	G	325	ARG	N-CA-C	-9.84	100.25	110.97
4	D	311	TYR	N-CA-C	-9.84	98.37	113.02
6	F	141	GLY	N-CA-C	-9.83	101.09	112.50
7	G	654	VAL	N-CA-C	9.81	123.36	111.09
6	F	144	VAL	N-CA-C	-9.71	101.40	110.53
6	F	418	GLN	N-CA-C	-9.64	100.73	111.14
7	G	337	ALA	N-CA-C	-9.55	100.84	114.12
16	W	87	ILE	N-CA-C	-9.55	101.26	110.42
8	H	52	ALA	N-CA-C	-9.54	100.86	111.07
4	D	427	PRO	N-CA-C	-9.53	95.55	110.50
17	X	70	PHE	N-CA-C	-9.49	99.72	111.11
21	q	123	GLN	N-CA-C	9.38	123.83	110.23
21	q	139	PRO	CA-N-CD	9.36	125.11	112.00
7	G	692	LYS	N-CA-C	-9.30	100.51	112.23
7	G	694	PHE	N-CA-C	9.24	121.36	111.28
18	Z	69	ILE	N-CA-C	-9.24	100.66	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	389	THR	N-CA-C	-9.17	96.20	109.96
4	D	212	GLU	N-CA-C	-9.10	100.32	111.33
4	D	323	ARG	N-CA-C	9.08	124.79	112.90
19	a	57	VAL	N-CA-C	-9.02	105.14	113.71
18	Z	143	TYR	N-CA-C	8.98	121.96	108.31
6	F	411	SER	N-CA-C	-8.92	101.53	111.07
2	B	170	TYR	N-CA-C	-8.85	97.76	110.24
7	G	133	GLN	N-CA-CB	8.83	121.58	110.45
7	G	365	ASN	N-CA-C	-8.78	102.12	112.92
7	G	212	LYS	N-CA-C	-8.78	94.59	108.90
9	I	154	TYR	N-CA-CB	-8.67	99.23	111.62
22	r	62	GLU	N-CA-C	-8.61	102.76	113.18
4	D	209	LYS	N-CA-C	-8.58	101.89	111.07
13	S	86	GLU	N-CA-C	-8.55	102.04	111.36
4	D	140	ASP	N-CA-C	-8.45	94.75	108.52
4	D	214	TYR	CB-CA-C	-8.43	97.64	110.88
17	X	99	HIS	N-CA-C	-8.41	102.19	111.36
5	E	154	LYS	N-CA-C	-8.39	101.82	110.97
3	C	108	LYS	N-CA-C	8.39	120.05	111.07
11	Q	54	THR	N-CA-C	8.34	123.31	109.46
7	G	532	PRO	CA-N-CD	8.33	123.66	112.00
7	G	452	LEU	N-CA-C	-8.32	102.21	111.28
7	G	558	GLN	N-CA-C	-8.30	102.19	111.07
5	E	218	ARG	CB-CA-C	-8.23	99.78	112.12
8	H	196	ALA	N-CA-C	8.21	127.94	109.81
8	H	311	THR	N-CA-C	-8.20	102.59	112.59
1	A	64	LEU	N-CA-C	-8.18	102.32	111.07
7	G	691	ILE	N-CA-C	8.18	123.66	111.89
7	G	500	ILE	N-CA-CB	8.15	121.00	110.57
7	G	484	ASP	N-CA-C	8.14	121.08	111.71
3	C	196	PRO	N-CA-C	8.14	124.84	113.53
6	F	411	SER	N-CA-CB	8.12	121.78	110.01
21	q	118	SER	N-CA-C	8.09	120.82	111.11
15	V	86	LYS	N-CA-C	-8.06	102.43	111.14
7	G	534	VAL	N-CA-C	-8.06	104.74	111.91
13	S	76	THR	N-CA-C	8.05	122.02	108.90
5	E	219	SER	N-CA-CB	8.03	124.01	111.56
9	I	201	ILE	N-CA-C	-8.03	102.61	110.72
17	X	43	PHE	N-CA-C	-7.99	102.52	111.07
8	H	271	LEU	N-CA-C	-7.97	102.53	111.14
1	A	9	ILE	N-CA-C	-7.95	102.52	110.62
7	G	651	PRO	CB-CA-C	-7.94	98.45	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	206	ILE	N-CA-C	7.93	120.93	108.87
15	V	6	LYS	N-CA-C	-7.90	100.11	110.53
8	H	311	THR	N-CA-CB	7.86	123.50	110.92
9	I	160	GLU	N-CA-C	7.85	124.25	111.37
7	G	270	VAL	N-CA-CB	-7.84	100.66	110.31
21	q	28	PHE	N-CA-C	7.83	122.60	112.89
10	P	235	THR	CB-CA-C	-7.82	100.03	112.07
7	G	389	THR	N-CA-CB	7.76	121.42	109.85
18	Z	143	TYR	CB-CA-C	-7.76	107.61	116.54
9	I	74	LEU	N-CA-C	-7.75	102.83	111.28
4	D	233	HIS	N-CA-C	7.72	119.48	111.14
6	F	58	ARG	N-CA-C	-7.71	102.95	111.36
8	H	253	GLU	N-CA-C	7.71	121.94	112.54
21	q	89	TRP	N-CA-C	-7.69	102.83	111.14
6	F	334	THR	N-CA-C	-7.67	101.66	111.02
4	D	184	ILE	N-CA-C	-7.67	102.80	110.62
7	G	56	VAL	N-CA-C	-7.66	102.99	110.72
4	D	257	GLU	N-CA-C	7.61	119.57	111.28
7	G	569	GLN	N-CA-C	7.61	122.01	108.24
9	I	119	CYS	N-CA-C	-7.56	103.11	111.36
6	F	171	VAL	N-CA-CB	7.56	120.25	110.57
22	r	30	GLU	N-CA-C	-7.54	104.98	114.56
8	H	214	GLU	N-CA-CB	-7.53	98.86	110.46
9	I	158	CYS	N-CA-C	-7.51	103.09	111.28
8	H	223	PHE	CB-CA-C	-7.51	99.09	110.88
7	G	277	MET	N-CA-C	7.50	120.61	109.59
4	D	180	ILE	N-CA-C	-7.48	103.24	110.42
6	F	430	GLY	N-CA-C	7.45	121.67	112.73
7	G	467	LYS	N-CA-C	-7.44	102.33	111.33
21	q	102	PRO	CA-N-CD	7.43	122.40	112.00
16	W	100	TRP	N-CA-C	-7.42	103.80	114.12
13	S	94	VAL	N-CA-C	7.42	117.54	110.42
2	B	80	ASP	N-CA-CB	7.41	120.76	110.01
7	G	510	TRP	N-CA-CB	7.41	120.89	109.85
8	H	309	ILE	N-CA-C	7.37	117.45	110.30
7	G	303	THR	N-CA-C	7.33	122.92	113.18
7	G	661	GLU	N-CA-C	7.29	118.91	110.97
7	G	384	ASN	N-CA-C	-7.28	103.38	111.82
3	C	195	HIS	CB-CA-C	7.27	117.37	110.17
15	V	68	LEU	N-CA-C	-7.24	103.39	111.28
7	G	374	THR	CB-CA-C	-7.22	99.88	111.28
4	D	210	MET	N-CA-C	7.20	119.12	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	20	ARG	N-CA-C	7.16	120.66	107.99
4	D	177	ILE	N-CA-C	-7.15	103.33	110.62
7	G	461	SER	N-CA-C	7.15	119.98	111.33
8	H	50	ALA	N-CA-C	7.14	118.71	111.07
7	G	465	VAL	N-CA-CB	7.14	118.43	110.51
7	G	497	VAL	N-CA-C	-7.13	103.34	110.62
6	F	455	GLN	N-CA-C	7.12	118.69	111.07
8	H	254	LEU	N-CA-C	-7.10	103.58	111.82
4	D	457	VAL	N-CA-C	-7.09	98.18	108.11
4	D	119	GLY	N-CA-C	-7.08	103.47	115.08
9	I	45	GLU	N-CA-C	7.08	120.87	108.56
15	V	95	LEU	N-CA-C	-7.08	103.57	111.28
7	G	217	GLU	N-CA-C	-7.03	101.76	110.41
8	H	176	LEU	CA-C-N	-7.02	113.57	120.52
8	H	176	LEU	C-N-CA	-7.02	113.57	120.52
21	q	102	PRO	N-CA-CB	-7.00	96.29	103.08
6	F	428	GLY	N-CA-C	-6.99	103.82	112.77
10	P	235	THR	CA-C-O	6.99	128.17	121.67
7	G	294	TYR	N-CA-C	-6.99	104.57	113.23
6	F	246	GLU	N-CA-C	-6.97	103.69	111.28
6	F	418	GLN	N-CA-CB	6.96	120.16	110.07
6	F	169	LEU	N-CA-C	6.96	118.86	111.28
6	F	148	ALA	N-CA-C	-6.95	103.78	111.36
18	Z	34	SER	N-CA-C	-6.94	103.72	111.28
7	G	300	GLN	N-CA-CB	6.93	122.54	112.08
7	G	582	VAL	N-CA-C	6.91	118.42	108.48
8	H	98	LEU	N-CA-CB	-6.90	98.82	110.83
6	F	233	VAL	O-C-N	6.90	131.18	123.10
2	B	78	LEU	N-CA-C	6.90	119.83	111.82
16	W	99	VAL	N-CA-C	6.89	117.16	107.37
8	H	203	GLY	N-CA-C	-6.89	102.72	112.37
7	G	102	ILE	N-CA-C	6.88	119.69	111.09
8	H	292	ASN	N-CA-C	6.88	118.86	111.36
12	R	108	GLY	N-CA-C	-6.88	105.98	114.92
7	G	362	ASP	N-CA-C	6.86	125.40	110.80
7	G	133	GLN	N-CA-C	-6.84	101.18	110.68
8	H	305	ILE	N-CA-C	-6.83	103.36	113.39
6	F	244	ASN	N-CA-C	-6.82	100.88	110.50
6	F	329	LYS	N-CA-C	6.82	119.58	111.33
6	F	233	VAL	CA-C-O	-6.82	113.24	120.53
8	H	300	LEU	N-CA-C	-6.81	104.23	112.54
18	Z	63	GLU	O-C-N	-6.78	114.94	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	196	PRO	N-CA-C	-6.77	100.60	111.03
7	G	268	GLY	N-CA-C	6.77	124.71	115.30
10	P	91	ILE	CB-CA-C	-6.76	102.62	111.88
5	E	154	LYS	N-CA-CB	6.75	119.77	109.91
4	D	329	ARG	CB-CA-C	6.73	121.97	110.79
7	G	434	SER	N-CA-C	-6.73	101.00	110.29
2	B	110	PRO	N-CA-C	6.73	122.73	113.65
9	I	208	ASP	N-CA-C	6.70	121.61	113.17
15	V	114	TRP	N-CA-CB	6.68	120.26	110.30
15	V	8	THR	N-CA-C	6.68	119.01	108.79
6	F	344	GLN	N-CA-C	-6.65	104.03	111.28
10	P	116	ILE	N-CA-C	-6.64	104.01	110.72
15	V	86	LYS	N-CA-CB	6.63	119.68	110.07
17	X	129	THR	N-CA-C	6.62	120.84	110.17
3	C	125	PHE	N-CA-CB	-6.62	100.64	110.17
8	H	267	SER	N-CA-C	-6.61	104.15	111.36
7	G	601	GLY	N-CA-C	6.60	124.81	115.30
6	F	228	PRO	N-CA-C	-6.60	98.88	112.47
11	Q	141	ASN	N-CA-CB	6.59	120.81	110.46
2	B	79	ASP	N-CA-C	-6.57	103.61	111.69
2	B	154	GLU	CA-C-N	-6.56	112.37	119.98
2	B	154	GLU	C-N-CA	-6.56	112.37	119.98
7	G	287	SER	N-CA-C	6.55	119.18	110.53
7	G	435	PRO	N-CA-C	-6.55	100.21	110.50
17	X	97	PHE	N-CA-C	6.55	118.50	111.36
6	F	234	GLY	CA-C-N	-6.55	111.73	120.50
6	F	234	GLY	C-N-CA	-6.55	111.73	120.50
8	H	223	PHE	N-CA-C	-6.54	104.07	111.07
8	H	182	ALA	N-CA-C	-6.53	104.08	111.07
7	G	250	SER	N-CA-C	6.52	116.89	108.34
18	Z	65	LEU	N-CA-C	-6.52	104.25	111.36
4	D	237	PRO	N-CA-C	-6.50	101.65	111.41
10	P	92	MET	N-CA-C	-6.50	104.23	111.71
6	F	336	LEU	N-CA-CB	-6.50	101.10	111.43
7	G	275	PRO	CB-CA-C	-6.49	102.48	110.98
7	G	605	GLN	N-CA-C	6.46	119.05	108.52
4	D	149	GLN	N-CA-C	-6.45	105.57	113.50
8	H	255	TYR	N-CA-CB	6.45	119.36	110.01
9	I	66	LEU	N-CA-C	-6.44	104.34	111.36
8	H	177	PRO	N-CA-C	-6.44	101.54	111.13
17	X	98	ARG	N-CA-C	6.43	120.39	112.54
6	F	178	GLU	N-CA-CB	6.43	119.52	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	205	ILE	N-CA-C	-6.42	104.23	110.72
15	V	49	GLU	N-CA-C	-6.42	104.28	111.28
3	C	125	PHE	N-CA-C	6.42	119.56	110.50
6	F	370	LEU	N-CA-C	-6.41	104.37	111.36
7	G	275	PRO	CA-N-CD	6.41	120.98	112.00
4	D	302	LEU	N-CA-C	-6.41	105.32	113.01
7	G	273	ILE	N-CA-C	-6.37	98.34	107.77
15	V	91	ALA	N-CA-C	-6.36	104.35	111.28
11	Q	59	LEU	N-CA-C	-6.34	100.80	110.30
14	T	107	ASP	N-CA-C	6.33	122.85	110.56
8	H	271	LEU	N-CA-CB	6.33	119.25	110.07
6	F	144	VAL	N-CA-CB	6.33	118.67	110.57
17	X	99	HIS	N-CA-CB	6.29	119.47	110.16
15	V	71	LEU	N-CA-C	6.29	118.13	111.28
2	B	135	GLY	CA-C-O	-6.29	117.92	122.45
7	G	176	CYS	N-CA-C	6.28	119.59	110.42
5	E	50	THR	N-CA-CB	6.28	121.54	110.37
11	Q	141	ASN	N-CA-C	-6.27	105.63	113.28
21	q	65	THR	N-CA-C	6.26	118.11	110.41
19	a	26	ILE	N-CA-C	-6.25	104.57	113.07
6	F	415	ILE	N-CA-C	-6.25	104.41	110.72
16	W	97	ILE	CB-CA-C	-6.25	104.36	111.55
7	G	356	ASP	N-CA-CB	6.25	119.31	110.12
6	F	255	CYS	N-CA-C	-6.25	104.55	111.36
5	E	182	ALA	CA-C-N	-6.24	112.74	119.98
5	E	182	ALA	C-N-CA	-6.24	112.74	119.98
8	H	269	THR	N-CA-C	6.22	118.06	111.28
10	P	118	LYS	N-CA-C	6.22	119.03	111.82
7	G	383	SER	N-CA-C	-6.21	106.92	114.75
8	H	52	ALA	N-CA-CB	6.21	119.02	110.01
18	Z	69	ILE	N-CA-CB	6.21	117.40	110.51
7	G	451	ILE	N-CA-C	-6.20	104.94	113.00
8	H	76	THR	N-CA-C	-6.20	104.53	111.28
1	A	101	GLY	N-CA-C	-6.17	105.34	112.50
6	F	409	ILE	N-CA-C	6.17	116.34	110.42
2	B	98	ALA	N-CA-C	6.16	117.67	108.31
6	F	212	LEU	N-CA-C	-6.16	104.57	111.28
7	G	420	LYS	N-CA-C	6.16	118.78	111.33
7	G	325	ARG	N-CA-CB	6.13	118.86	109.91
13	S	61	VAL	N-CA-C	-6.13	99.65	108.42
4	D	122	LYS	N-CA-C	-6.13	105.96	113.50
7	G	418	ILE	N-CA-C	-6.12	103.47	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	304	ALA	CB-CA-C	-6.10	109.52	116.54
13	S	87	VAL	N-CA-C	-6.09	104.41	110.62
8	H	276	SER	N-CA-C	6.08	118.87	111.82
6	F	268	GLU	CB-CA-C	-6.08	109.55	116.54
4	D	258	VAL	N-CA-C	-6.07	103.31	111.44
8	H	185	TRP	N-CA-C	-6.06	104.03	112.45
7	G	353	ALA	N-CA-C	-6.06	104.60	112.23
18	Z	65	LEU	N-CA-CB	6.05	119.12	110.16
7	G	508	ALA	N-CA-C	6.04	117.87	111.28
8	H	103	LEU	N-CA-C	-6.02	104.80	111.36
14	T	141	PRO	N-CA-CB	-6.01	96.89	103.39
4	D	444	LEU	N-CA-C	-6.01	104.72	111.28
4	D	414	ASP	N-CA-C	-5.99	101.07	110.36
21	q	104	THR	N-CA-C	5.97	118.45	108.96
7	G	532	PRO	N-CA-CB	-5.96	97.12	103.38
7	G	387	LEU	CB-CA-C	-5.95	101.69	111.68
20	b	60	ASP	N-CA-C	-5.95	105.29	112.54
17	X	38	LYS	N-CA-C	-5.94	104.72	111.07
7	G	480	ALA	N-CA-C	-5.92	104.90	111.36
17	X	141	PRO	N-CA-C	-5.91	102.55	111.41
16	W	98	LYS	N-CA-CB	5.91	119.60	110.21
9	I	116	CYS	N-CA-C	-5.87	105.62	112.89
6	F	127	ASP	N-CA-C	5.86	118.45	111.71
22	r	11	LEU	N-CA-C	-5.85	104.82	111.14
8	H	116	ILE	N-CA-C	-5.85	104.81	110.42
3	C	209	LEU	N-CA-CB	-5.82	100.70	110.83
8	H	315	PRO	O-C-N	5.82	123.89	121.15
2	B	98	ALA	CB-CA-C	-5.82	109.85	116.54
10	P	122	HIS	N-CA-C	5.82	120.08	112.92
13	S	86	GLU	N-CA-CB	5.81	118.75	110.16
7	G	672	ALA	N-CA-C	-5.80	104.95	111.28
15	V	19	THR	N-CA-CB	5.79	120.68	110.37
10	P	97	MET	N-CA-C	-5.78	102.35	110.50
21	q	100	THR	N-CA-C	5.78	117.26	111.07
4	D	212	GLU	N-CA-CB	5.77	118.72	110.06
7	G	289	LYS	N-CA-C	5.77	117.57	111.28
22	r	72	SER	N-CA-C	-5.77	106.08	113.23
21	q	121	PRO	N-CA-CB	-5.75	98.06	103.52
17	X	36	CYS	CB-CA-C	-5.74	102.61	111.74
7	G	275	PRO	N-CA-CB	-5.73	98.00	103.33
8	H	126	LYS	N-CA-C	5.73	117.53	111.28
10	P	272	LEU	N-CA-C	-5.73	101.80	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	234	LYS	CB-CA-C	-5.72	103.44	111.80
4	D	337	MET	N-CA-C	-5.72	105.05	111.28
6	F	393	ASN	N-CA-C	-5.71	104.96	111.07
8	H	252	PRO	N-CA-CB	-5.70	98.04	103.51
6	F	176	ALA	N-CA-C	5.68	118.20	111.33
13	S	73	GLN	N-CA-C	-5.68	100.45	109.59
10	P	119	ALA	N-CA-C	-5.67	105.02	111.14
12	R	44	ARG	N-CA-C	-5.66	106.08	112.87
4	D	186	ALA	N-CA-C	5.64	117.10	111.07
6	F	416	SER	N-CA-C	5.63	117.87	111.11
4	D	192	LEU	N-CA-C	-5.62	105.16	111.28
21	q	140	PRO	N-CA-C	-5.62	102.32	110.80
4	D	455	ASP	CB-CA-C	-5.61	103.93	111.89
6	F	457	HIS	N-CA-CB	-5.61	100.97	110.50
7	G	599	THR	CA-C-N	-5.61	114.20	122.83
7	G	599	THR	C-N-CA	-5.61	114.20	122.83
9	I	191	LEU	N-CA-C	-5.58	105.28	111.36
17	X	40	ASN	N-CA-C	-5.58	104.89	110.97
7	G	530	TYR	N-CA-C	-5.58	102.03	110.28
11	Q	124	MET	CA-C-N	-5.57	115.08	122.98
11	Q	124	MET	C-N-CA	-5.57	115.08	122.98
13	S	63	PRO	CA-N-CD	5.56	119.78	112.00
5	E	223	CYS	CB-CA-C	-5.56	110.15	116.54
19	a	25	TYR	N-CA-C	-5.55	107.75	114.75
7	G	127	ASP	CA-C-O	5.55	129.05	121.89
7	G	615	LEU	N-CA-C	-5.51	106.33	113.16
4	D	350	LYS	CB-CA-C	-5.50	103.77	111.85
7	G	313	LEU	N-CA-C	5.46	118.46	109.72
7	G	363	SER	N-CA-C	-5.45	100.29	109.07
7	G	404	GLY	N-CA-C	5.45	121.44	113.48
21	q	126	PRO	N-CA-CB	-5.45	98.46	103.31
17	X	113	ASP	N-CA-C	-5.45	106.57	113.43
2	B	155	PRO	N-CA-C	-5.44	102.13	110.95
7	G	682	ASP	CA-C-N	-5.44	114.16	119.76
7	G	682	ASP	C-N-CA	-5.44	114.16	119.76
18	Z	55	GLN	N-CA-C	-5.44	105.35	111.28
4	D	200	PHE	CA-CB-CG	5.44	119.24	113.80
7	G	420	LYS	N-CA-CB	-5.43	101.92	110.06
2	B	104	MET	N-CA-C	-5.42	107.21	113.88
4	D	255	ILE	N-CA-C	-5.41	105.25	110.72
7	G	510	TRP	N-CA-C	-5.41	101.84	109.96
2	B	146	ARG	N-CA-C	-5.40	105.39	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	q	121	PRO	CA-N-CD	5.39	119.55	112.00
5	E	219	SER	N-CA-C	-5.38	100.56	108.79
2	B	105	MET	N-CA-CB	5.38	118.50	110.22
4	D	131	GLN	CB-CA-C	5.38	120.32	110.11
18	Z	50	MET	N-CA-C	-5.37	105.43	111.28
5	E	48	PRO	N-CA-C	5.35	120.79	113.84
21	q	30	ALA	N-CA-CB	5.35	118.50	110.53
6	F	199	ARG	N-CA-C	5.34	117.45	109.59
5	E	143	ASP	N-CA-C	5.33	118.47	111.28
8	H	98	LEU	N-CA-C	-5.31	100.74	109.40
8	H	252	PRO	CA-N-CD	5.31	119.43	112.00
18	Z	64	ASP	N-CA-C	5.30	119.80	113.23
6	F	84	GLY	N-CA-C	-5.30	107.93	115.30
11	Q	72	ILE	N-CA-C	-5.30	108.34	113.53
21	q	102	PRO	N-CA-C	-5.30	104.24	110.70
8	H	146	MET	N-CA-C	-5.29	105.41	111.07
7	G	449	PRO	N-CA-CB	5.29	109.10	103.39
8	H	284	GLN	N-CA-C	-5.29	105.60	111.36
8	H	214	GLU	N-CA-C	5.28	119.43	113.15
10	P	260	GLY	N-CA-C	-5.28	108.34	115.36
21	q	67	GLU	N-CA-CB	-5.28	102.17	110.77
7	G	356	ASP	N-CA-C	-5.27	105.54	111.28
7	G	111	LYS	N-CA-C	-5.27	105.59	112.23
9	I	160	GLU	N-CA-CB	-5.26	100.77	109.72
6	F	55	GLY	N-CA-C	-5.25	106.42	112.83
5	E	48	PRO	CB-CA-C	-5.25	104.39	111.85
7	G	362	ASP	CA-CB-CG	5.24	117.84	112.60
6	F	412	LEU	N-CA-C	-5.24	105.74	111.82
10	P	339	GLY	N-CA-C	5.24	122.55	115.00
18	Z	118	PRO	CA-C-N	-5.24	113.91	120.51
18	Z	118	PRO	C-N-CA	-5.24	113.91	120.51
4	D	369	ALA	N-CA-C	5.24	116.99	111.28
8	H	46	LEU	N-CA-C	-5.24	106.67	113.16
6	F	318	ILE	CA-C-N	5.22	124.85	119.05
6	F	318	ILE	C-N-CA	5.22	124.85	119.05
7	G	458	GLY	N-CA-C	-5.22	108.12	115.32
15	V	84	ALA	N-CA-C	5.22	116.66	111.07
7	G	277	MET	N-CA-CB	-5.21	101.68	109.71
2	B	167	GLY	N-CA-C	-5.21	106.11	112.68
4	D	312	ASP	N-CA-C	-5.21	107.09	113.50
8	H	310	PHE	N-CA-C	5.21	119.26	113.01
7	G	600	GLU	CB-CA-C	-5.20	103.01	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	194	VAL	N-CA-CB	5.20	118.37	110.58
7	G	713	ALA	N-CA-C	-5.19	105.51	111.07
7	G	435	PRO	CB-CA-C	-5.19	105.91	111.56
7	G	556	THR	N-CA-C	-5.18	101.53	109.41
4	D	103	GLY	N-CA-C	-5.18	100.90	113.18
22	r	18	GLN	N-CA-C	5.17	117.25	109.23
13	S	85	ASP	N-CA-C	5.17	117.82	111.82
22	r	36	GLN	N-CA-C	-5.17	102.51	110.01
3	C	79	CYS	N-CA-C	-5.17	107.04	113.19
6	F	337	MET	CB-CA-C	-5.17	103.00	111.68
17	X	33	GLY	N-CA-C	-5.16	107.92	114.16
7	G	63	PHE	CA-C-O	-5.16	115.08	121.06
7	G	172	ILE	N-CA-C	-5.16	98.61	109.34
6	F	60	GLY	N-CA-C	-5.14	105.94	114.48
20	b	82	LYS	N-CA-C	-5.14	103.74	110.53
3	C	164	TRP	N-CA-C	5.14	116.96	111.36
3	C	156	VAL	N-CA-C	-5.14	104.08	111.17
10	P	198	ALA	N-CA-C	-5.13	100.15	108.52
8	H	101	GLY	N-CA-C	5.13	118.45	112.50
8	H	277	TYR	N-CA-C	5.12	117.94	110.10
8	H	196	ALA	CA-C-N	-5.12	113.53	119.47
8	H	196	ALA	C-N-CA	-5.12	113.53	119.47
1	A	2	ASN	CA-C-N	-5.12	113.02	120.29
1	A	2	ASN	C-N-CA	-5.12	113.02	120.29
20	b	63	MET	N-CA-C	5.11	118.87	109.10
7	G	569	GLN	CB-CA-C	-5.10	104.30	112.05
7	G	387	LEU	N-CA-C	-5.10	98.40	107.98
9	I	95	PRO	N-CA-C	5.09	121.20	113.81
3	C	221	GLU	N-CA-C	-5.08	102.35	108.25
1	A	73	LEU	CA-C-N	-5.08	114.48	120.12
1	A	73	LEU	C-N-CA	-5.08	114.48	120.12
8	H	254	LEU	N-CA-CB	5.07	118.14	110.28
6	F	366	ALA	N-CA-C	-5.06	105.45	110.97
7	G	280	ASP	N-CA-CB	-5.06	102.68	110.12
14	T	105	MET	N-CA-C	-5.06	105.77	111.28
3	C	109	SER	N-CA-C	5.05	118.05	109.76
9	I	61	LEU	N-CA-C	5.05	116.59	111.14
7	G	203	ASP	CA-C-O	5.05	127.17	121.32
8	H	67	SER	N-CA-C	-5.04	103.87	110.53
7	G	393	GLY	N-CA-C	-5.04	107.80	115.66
16	W	112	GLU	N-CA-C	5.03	116.84	111.36
4	D	232	VAL	CA-C-O	-5.02	116.35	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	90	LYS	N-CA-C	5.02	117.58	109.40
5	E	213	PRO	CB-CA-C	-5.01	106.32	112.89
6	F	249	ALA	N-CA-C	5.01	116.74	111.28
4	D	224	ALA	CA-C-O	-5.01	115.54	120.90
21	q	89	TRP	N-CA-CB	5.01	117.33	110.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	754	0	814	65	0
2	B	1258	0	1269	148	0
3	C	1641	0	1596	159	0
4	D	3088	0	3059	303	0
5	E	1635	0	1624	146	0
6	F	3288	0	3243	383	0
7	G	5287	0	5323	561	0
8	H	2532	0	2621	389	0
9	I	1431	0	1385	176	0
10	P	2720	0	2740	241	0
11	Q	957	0	949	75	0
12	R	660	0	639	64	0
13	S	667	0	683	70	0
14	T	604	0	596	65	0
15	V	915	0	954	94	0
16	W	970	0	991	86	0
17	X	1164	0	1154	105	0
18	Z	1152	0	1148	110	0
19	a	548	0	562	43	0
20	b	620	0	617	95	0
21	q	1192	0	1145	92	0
22	r	764	0	789	84	0
23	s	189	0	181	18	0
24	A	46	0	69	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	H	46	0	69	16	0
24	b	46	0	69	13	0
25	B	8	0	0	2	0
25	F	8	0	0	9	0
25	G	16	0	0	3	0
25	I	16	0	0	16	0
26	D	18	0	18	14	0
27	E	4	0	0	3	0
27	G	4	0	0	6	0
28	F	31	0	19	2	0
29	H	35	0	43	10	0
30	I	47	0	71	9	0
30	q	35	0	44	6	0
31	P	48	0	26	2	0
32	R	1	0	0	0	0
33	W	32	0	0	0	0
34	q	57	0	58	8	0
All	All	34534	0	34568	2960	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 43.

All (2960) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.21
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.28	1.20
8:H:251:LEU:HD12	8:H:251:LEU:O	1.42	1.20
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
4:D:189:THR:HB	26:D:501:UQ1:CM2	1.73	1.18
6:F:379:CYS:SG	25:F:502:SF4:FE4	1.38	1.14
4:D:189:THR:HB	26:D:501:UQ1:HM23	1.16	1.12
14:T:104:PHE:HZ	14:T:115:GLN:HG2	1.08	1.11
18:Z:144:THR:CG2	19:a:48:MET:SD	2.38	1.11
18:Z:144:THR:HG21	19:a:48:MET:SD	1.90	1.11
21:q:59:HIS:ND1	21:q:60:ARG:HG3	1.64	1.11
12:R:80:ASP:OD2	12:R:84:GLY:HA2	1.49	1.10
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.32	1.10
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.22	1.09
9:I:123:CYS:SG	25:I:302:SF4:FE1	1.42	1.09
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:THR:HG21	10:P:359:TYR:HD1	1.15	1.09
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.08
3:C:203:LEU:HD11	4:D:123:LEU:HD23	1.30	1.08
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.34	1.08
9:I:152:CYS:SG	25:I:302:SF4:FE2	1.43	1.08
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.08
8:H:65:THR:CG2	10:P:359:TYR:HD1	1.66	1.08
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.08
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.64	1.07
7:G:399:VAL:HG21	7:G:462:PHE:CZ	1.88	1.07
10:P:299:SER:HB3	10:P:316:LYS:HE3	1.37	1.07
2:B:82:ILE:HG23	8:H:57:MET:SD	1.95	1.06
3:C:241:PHE:CD2	22:r:61:ARG:HB2	1.91	1.06
16:W:101:LYS:HG3	16:W:105:HIS:HB2	1.34	1.05
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.05
8:H:89:LEU:HD11	8:H:233:LEU:CD1	1.87	1.05
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.22	1.05
7:G:353:ALA:HA	7:G:636:TYR:OH	1.54	1.05
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.37	1.05
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.04
4:D:238:LEU:HD13	9:I:211:TYR:OH	1.55	1.04
2:B:89:SER:O	8:H:54:LYS:CD	2.06	1.04
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.03
5:E:247:GLY:HA2	6:F:64:LYS:HE2	1.36	1.02
7:G:401:LEU:HD11	7:G:466:LEU:HD21	1.39	1.02
14:T:104:PHE:CZ	14:T:115:GLN:HG2	1.94	1.02
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.75	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.76	1.02
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.42	1.02
10:P:272:LEU:HG	10:P:375:VAL:HG21	1.36	1.01
17:X:48:TRP:CE2	20:b:55:VAL:HG22	1.94	1.01
5:E:247:GLY:CA	6:F:64:LYS:HE2	1.89	1.01
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.01
3:C:241:PHE:HD2	22:r:61:ARG:HB2	1.24	1.00
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.86	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
18:Z:86:ILE:HG23	18:Z:128:ARG:HE	1.24	1.00
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.99
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.99
4:D:259:GLU:HG3	18:Z:25:LEU:HD11	1.43	0.99
7:G:401:LEU:HD11	7:G:462:PHE:CE2	1.98	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.99
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.98
9:I:113:CYS:SG	25:I:303:SF4:FE3	1.55	0.98
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	0.98
16:W:55:LEU:HB3	16:W:107:MET:CE	1.94	0.98
21:q:78:ASP:OD1	21:q:81:MET:HG3	1.61	0.98
9:I:155:CYS:SG	25:I:302:SF4:FE4	1.55	0.97
10:P:363:SER:HB3	16:W:51:HIS:CE1	1.98	0.97
3:C:203:LEU:HD21	4:D:123:LEU:HD21	1.47	0.97
7:G:75:CYS:HG	27:G:803:FES:FE1	0.80	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
4:D:376:GLU:HG3	7:G:121:LEU:HD12	1.47	0.97
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.96
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.79	0.96
7:G:399:VAL:HG21	7:G:462:PHE:HZ	1.30	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.96
4:D:189:THR:CB	26:D:501:UQ1:HM23	1.94	0.96
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.96
21:q:59:HIS:CE1	21:q:60:ARG:HG3	2.00	0.96
6:F:318:ILE:HD11	6:F:355:ILE:HD12	1.47	0.95
8:H:127:TYR:CD1	8:H:207:LEU:HD22	2.00	0.95
14:T:102:SER:O	14:T:141:PRO:HD3	1.66	0.95
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.95
17:X:132:LYS:HB3	20:b:59:ASP:HB2	1.48	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.65	0.95
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.95
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.94
4:D:128:THR:HG22	4:D:131:GLN:HG2	1.45	0.94
2:B:89:SER:O	8:H:54:LYS:HD3	1.67	0.94
4:D:128:THR:CG2	4:D:131:GLN:HG2	1.98	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.94
14:T:104:PHE:HE1	14:T:115:GLN:HB2	1.32	0.94
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
8:H:65:THR:HG21	10:P:359:TYR:CD1	2.04	0.93
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.93
22:r:12:ARG:HB3	22:r:20:LEU:HD21	1.48	0.93
6:F:318:ILE:HG22	6:F:326:LEU:HB3	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:147:ARG:HD3	6:F:191:TYR:CD2	2.03	0.92
3:C:203:LEU:HD11	4:D:123:LEU:CD2	2.00	0.92
4:D:238:LEU:HD11	22:r:39:PRO:HB3	1.49	0.92
6:F:382:CYS:SG	25:F:502:SF4:FE3	1.60	0.92
9:I:152:CYS:HG	25:I:302:SF4:FE2	0.77	0.92
7:G:399:VAL:CG2	7:G:462:PHE:HZ	1.82	0.91
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.01	0.91
4:D:129:TYR:HE1	4:D:411:LEU:HD21	1.36	0.91
4:D:451:ILE:HG23	4:D:456:ILE:HD11	1.52	0.91
4:D:361:ALA:O	4:D:384:LEU:HD11	1.71	0.91
16:W:55:LEU:HB3	16:W:107:MET:HE1	1.52	0.91
21:q:25:ARG:O	21:q:29:ARG:HG2	1.69	0.91
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.36	0.91
10:P:363:SER:HB3	16:W:51:HIS:NE2	1.86	0.91
18:Z:87:LEU:HD21	18:Z:119:PRO:HG3	1.53	0.91
2:B:111:ARG:HB3	4:D:208:GLU:OE1	1.71	0.90
7:G:78:CYS:SG	27:G:803:FES:FE2	1.63	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.06	0.90
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.53	0.90
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.90
7:G:176:CYS:HG	25:G:802:SF4:FE4	0.66	0.90
10:P:333:PRO:HB2	10:P:337:ASP:HB2	1.53	0.90
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.53	0.90
2:B:100:CYS:HB2	2:B:134:ALA:HB1	1.53	0.90
6:F:110:PRO:HB3	6:F:152:ARG:CZ	2.02	0.90
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.89
9:I:67:ILE:HG13	30:I:301:PC1:H251	1.53	0.89
6:F:314:LEU:HD11	6:F:317:VAL:HG23	1.55	0.89
18:Z:111:PHE:CZ	18:Z:117:VAL:HG21	2.06	0.89
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.53	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.08	0.89
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.55	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
6:F:424:ILE:HD11	7:G:73:GLY:O	1.72	0.89
6:F:225:LEU:H	11:Q:160:TYR:HE2	1.21	0.89
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.89
2:B:82:ILE:HG12	8:H:57:MET:CE	2.03	0.88
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.55	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.55	0.88
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.55	0.88
3:C:240:ALA:HB1	22:r:61:ARG:HD2	1.56	0.88
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.38	0.88
8:H:65:THR:CG2	10:P:359:TYR:CD1	2.56	0.88
5:E:134:CYS:HG	27:E:301:FES:FE1	0.68	0.88
6:F:379:CYS:HG	25:F:502:SF4:FE4	0.62	0.88
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.88
8:H:183:MET:HE2	30:I:301:PC1:H2A1	1.56	0.88
6:F:266:GLY:HA3	6:F:271:SER:HA	1.54	0.88
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.74	0.87
6:F:327:ILE:HD11	6:F:331:VAL:HG11	1.56	0.87
1:A:3:LEU:HD23	24:A:401:3PE:H251	1.56	0.87
2:B:89:SER:O	8:H:54:LYS:HE2	1.72	0.87
2:B:202:LEU:HD23	9:I:86:TYR:CG	2.08	0.87
2:B:89:SER:O	8:H:54:LYS:CE	2.22	0.87
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.88	0.87
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.57	0.87
3:C:98:PHE:CA	15:V:90:LEU:HD11	2.04	0.87
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.57	0.87
10:P:296:PHE:CE1	10:P:297:VAL:HG23	2.10	0.87
4:D:146:CYS:SG	4:D:178:THR:OG1	2.32	0.86
26:D:501:UQ1:O1	26:D:501:UQ1:H8	1.74	0.86
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.40	0.86
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	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
16:W:55:LEU:HD22	16:W:107:MET:HE2	1.58	0.86
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.86
7:G:607:LYS:HG3	11:Q:78:ARG:HH12	1.41	0.85
8:H:127:TYR:CD1	8:H:207:LEU:CD2	2.59	0.85
4:D:101:LEU:HD23	4:D:106:VAL:HG22	1.57	0.85
6:F:288:VAL:HG21	6:F:303:HIS:HD2	1.41	0.85
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.40	0.85
3:C:203:LEU:HD21	4:D:123:LEU:CD2	2.06	0.85
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.91	0.85
12:R:72:VAL:HG11	12:R:77:ILE:HD12	1.59	0.85
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.59	0.85
6:F:425:CYS:SG	25:F:502:SF4:FE1	1.68	0.85
2:B:141:MET:HE1	4:D:86:PRO:HB2	1.59	0.84
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.84
14:T:104:PHE:CZ	14:T:115:GLN:CG	2.61	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
4:D:185:MET:HE3	26:D:501:UQ1:HM33	1.58	0.84
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.12	0.84
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.58	0.84
14:T:104:PHE:HD1	14:T:110:LEU:HB3	1.41	0.84
9:I:123:CYS:HG	25:I:302:SF4:FE1	0.58	0.84
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.17	0.84
14:T:93:ILE:HD11	14:T:110:LEU:HD22	1.58	0.84
14:T:104:PHE:HZ	14:T:115:GLN:CG	1.87	0.84
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.84
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.84
14:T:117:GLU:HA	14:T:120:MET:HE3	1.60	0.84
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.60	0.83
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.61	0.83
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.83
9:I:162:CYS:SG	25:I:303:SF4:FE4	1.71	0.83
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.83
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.61	0.83
13:S:48:HIS:CE1	13:S:95:LEU:HD22	2.13	0.83
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.83
7:G:401:LEU:HD11	7:G:462:PHE:HE2	1.41	0.83
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.58	0.83
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
4:D:271:ARG:HD2	8:H:281:ARG:CG	2.09	0.83
4:D:376:GLU:HG3	7:G:121:LEU:CD1	2.09	0.82
8:H:293:PHE:HE1	24:H:402:3PE:H321	1.42	0.82
7:G:651:PRO:HG3	13:S:57:GLU:H	1.44	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
4:D:280:ALA:CB	15:V:11:LEU:HG	2.09	0.82
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.82
7:G:114:GLU:OE2	22:r:53:TYR:HA	1.79	0.82
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.82
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.62	0.81
5:E:84:LEU:HD12	23:s:46:LEU:HD13	1.61	0.81
8:H:94:PRO:HG2	8:H:97:ASN:HB3	1.61	0.81
9:I:162:CYS:HG	25:I:303:SF4:FE4	0.54	0.81
4:D:101:LEU:CD2	4:D:106:VAL:HG22	2.09	0.81
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:614:GLY:HA2	10:P:41:ILE:CD1	2.10	0.81
8:H:89:LEU:HD11	8:H:233:LEU:HD11	1.62	0.81
9:I:135:ARG:HD2	12:R:61:ILE:HG12	1.61	0.81
18:Z:86:ILE:HG23	18:Z:128:ARG:NE	1.95	0.81
7:G:225:ILE:HD11	7:G:285:TRP:CZ3	2.16	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
4:D:102:SER:HB2	4:D:107:ARG:HG3	1.61	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
16:W:55:LEU:CD2	16:W:107:MET:HE2	2.09	0.81
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.81
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.69	0.81
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.81
4:D:304:LYS:HE2	9:I:35:THR:N	1.96	0.81
6:F:296:LEU:HB2	6:F:337:MET:HE3	1.61	0.81
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.61	0.81
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.60	0.80
14:T:104:PHE:CD1	14:T:110:LEU:HB3	2.16	0.80
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.44	0.80
7:G:607:LYS:HG3	11:Q:78:ARG:NH1	1.94	0.80
12:R:80:ASP:OD2	12:R:84:GLY:CA	2.27	0.80
20:b:20:VAL:HG13	24:b:201:3PE:H2A1	1.64	0.80
5:E:247:GLY:HA2	6:F:64:LYS:CE	2.12	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.80
8:H:251:LEU:O	8:H:251:LEU:CD1	2.28	0.80
4:D:88:HIS:CE1	8:H:205:SER:O	2.34	0.80
8:H:311:THR:HB	18:Z:51:MET:SD	2.21	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
7:G:226:CYS:HG	25:G:802:SF4:FE1	0.99	0.80
7:G:614:GLY:HA2	10:P:41:ILE:HD13	1.63	0.80
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
14:T:108:LEU:O	14:T:108:LEU:HD23	1.82	0.79
16:W:96:THR:HG22	16:W:101:LYS:HD2	1.64	0.79
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.13	0.79
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.17	0.79
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
30:I:301:PC1:H2D1	30:I:301:PC1:H291	1.64	0.79
16:W:101:LYS:HG3	16:W:105:HIS:CB	2.12	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.79
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.79
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.79
8:H:127:TYR:CE1	8:H:207:LEU:HD23	2.17	0.79
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
9:I:211:TYR:CE2	22:r:39:PRO:HG3	2.17	0.79
10:P:44:GLY:HA2	11:Q:107:TRP:CZ3	2.18	0.79
6:F:174:ARG:HA	23:s:52:LEU:HD21	1.65	0.78
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.13	0.78
4:D:170:ILE:HD13	4:D:236:LEU:CD1	2.13	0.78
15:V:48:THR:OG1	15:V:87:GLU:OE2	2.01	0.78
6:F:66:LYS:HZ3	6:F:189:SER:HA	1.48	0.78
7:G:401:LEU:CD1	7:G:466:LEU:HD21	2.13	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.66	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.78
21:q:85:GLU:OE2	21:q:103:PRO:HD3	1.83	0.78
8:H:17:MET:HE1	8:H:225:MET:HE3	1.66	0.78
8:H:39:ILE:HD11	30:q:202:PC1:H131	1.65	0.78
14:T:90:TYR:HD2	14:T:93:ILE:HG12	1.48	0.78
2:B:82:ILE:HA	8:H:57:MET:HE1	1.65	0.78
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.78
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.78
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.48	0.78
4:D:271:ARG:NH2	8:H:206:GLU:OE2	2.17	0.78
5:E:136:THR:HB	27:E:301:FES:S2	2.24	0.78
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.78
17:X:48:TRP:CD1	20:b:55:VAL:HG13	2.19	0.78
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
18:Z:111:PHE:CZ	18:Z:117:VAL:CG2	2.66	0.77
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.65	0.77
4:D:128:THR:HG22	4:D:131:GLN:CG	2.13	0.77
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77
13:S:19:ILE:HB	13:S:53:ILE:CD1	2.15	0.77
6:F:297:LYS:HB2	6:F:333:GLU:CB	2.15	0.77
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.65	0.77
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.77
4:D:271:ARG:HD2	8:H:281:ARG:HG3	1.66	0.77
10:P:231:LEU:HD13	10:P:292:PRO:HD3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:THR:CG2	8:H:32:GLN:HE21	1.98	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.77
20:b:20:VAL:HA	24:b:201:3PE:H282	1.67	0.77
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.20	0.76
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.76
21:q:24:LEU:HD22	21:q:28:PHE:HE2	1.50	0.76
6:F:234:GLY:HA3	6:F:238:CYS:O	1.85	0.76
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.76
7:G:225:ILE:HD11	7:G:285:TRP:HZ3	1.48	0.76
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.67	0.76
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.99	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
3:C:88:HIS:CE1	15:V:105:GLU:HB3	2.20	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
8:H:200:LEU:HD22	8:H:282:TYR:HA	1.64	0.76
10:P:143:ASP:HA	10:P:147:ASN:HB2	1.67	0.76
7:G:126:LEU:CD1	12:R:89:PRO:HB3	2.16	0.76
14:T:104:PHE:CE1	14:T:115:GLN:HB2	2.21	0.76
3:C:241:PHE:HD2	22:r:61:ARG:CB	1.97	0.76
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.20	0.76
5:E:75:ALA:O	5:E:78:VAL:HG23	1.85	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
4:D:321:GLY:HA3	4:D:328:ASP:OD1	1.86	0.76
5:E:120:MET:HE1	6:F:160:GLY:HA3	1.66	0.76
6:F:192:ASP:HB3	23:s:57:LEU:HD11	1.67	0.76
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.21	0.76
9:I:113:CYS:HG	25:I:303:SF4:FE3	0.45	0.76
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.76
4:D:129:TYR:CE1	4:D:411:LEU:HD21	2.20	0.75
7:G:173:MET:HE2	7:G:231:LEU:HD23	1.68	0.75
9:I:68:ARG:NH2	18:Z:26:PRO:O	2.19	0.75
16:W:97:ILE:HG13	16:W:98:LYS:N	2.02	0.75
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.67	0.75
2:B:173:TYR:O	3:C:203:LEU:HD22	1.86	0.75
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.21	0.75
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.75
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.21	0.75
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.75
4:D:259:GLU:CG	18:Z:25:LEU:HD11	2.16	0.75
8:H:292:ASN:HD21	24:H:402:3PE:H122	1.50	0.75
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:362:LYS:HE2	22:r:54:TYR:CE2	2.22	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
16:W:55:LEU:HB3	16:W:107:MET:HE2	1.66	0.75
6:F:297:LYS:HD3	6:F:333:GLU:CB	2.17	0.74
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.74
13:S:19:ILE:HB	13:S:53:ILE:HD12	1.68	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.74
14:T:110:LEU:HG	14:T:114:ASP:CB	2.17	0.74
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.74
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.69	0.74
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.67	0.74
8:H:97:ASN:ND2	19:a:38:VAL:HG13	2.02	0.74
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.74
10:P:336:GLU:HG3	10:P:342:PRO:HD3	1.67	0.74
20:b:31:ILE:HA	20:b:34:MET:HE2	1.69	0.74
3:C:203:LEU:CD1	4:D:123:LEU:HD23	2.15	0.74
7:G:75:CYS:SG	27:G:803:FES:FE1	1.79	0.74
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.22	0.74
8:H:295:PRO:HB3	24:b:201:3PE:H3A1	1.69	0.74
14:T:103:HIS:ND1	14:T:140:CYS:HB3	2.01	0.74
3:C:100:ARG:HH12	15:V:86:LYS:HZ1	1.32	0.74
6:F:288:VAL:HG21	6:F:303:HIS:CD2	2.22	0.74
14:T:103:HIS:HB2	14:T:106:LYS:HG2	1.67	0.74
7:G:88:VAL:HG13	7:G:108:LYS:HE2	1.67	0.74
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.22	0.74
10:P:351:GLU:HB3	16:W:56:ASP:OD2	1.87	0.74
1:A:24:LEU:N	1:A:25:PRO:HD2	2.03	0.74
4:D:238:LEU:CD1	22:r:39:PRO:HB3	2.17	0.74
6:F:318:ILE:CG2	6:F:326:LEU:HB3	2.17	0.74
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.15	0.74
2:B:163:SER:HB2	9:I:150:THR:O	1.88	0.73
4:D:375:MET:HE1	7:G:126:LEU:HA	1.70	0.73
9:I:211:TYR:CZ	22:r:39:PRO:HG3	2.23	0.73
10:P:293:LEU:HD12	10:P:294:PRO:HD2	1.69	0.73
5:E:68:ASN:HD21	23:s:49:ASN:HD21	1.35	0.73
6:F:66:LYS:NZ	6:F:189:SER:HA	2.03	0.73
7:G:382:ARG:HD2	13:S:56:ARG:CD	2.18	0.73
1:A:106:TRP:CE3	24:b:201:3PE:H342	2.24	0.73
4:D:279:THR:HA	15:V:12:VAL:HG13	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:94:LEU:HA	10:P:97:MET:HE2	1.68	0.73
19:a:7:PRO:HG3	34:q:201:CDL:H181	1.68	0.73
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.73
10:P:44:GLY:HA2	11:Q:107:TRP:CE3	2.23	0.73
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.73
4:D:326:CYS:HB3	4:D:453:THR:HG21	1.69	0.73
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73
6:F:392:MET:CE	6:F:419:ILE:HD12	2.19	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.73
17:X:48:TRP:CZ2	20:b:55:VAL:HG22	2.23	0.73
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.87	0.73
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.70	0.73
2:B:166:ASN:O	9:I:150:THR:HB	1.89	0.73
4:D:323:ARG:O	15:V:12:VAL:HG21	1.88	0.73
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.73
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.73
10:P:169:HIS:H	10:P:184:LYS:HE3	1.54	0.72
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.72
8:H:181:MET:CE	8:H:304:HIS:CE1	2.72	0.72
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.71	0.72
6:F:273:THR:HG22	6:F:291:GLU:HA	1.70	0.72
14:T:120:MET:HG2	16:W:44:ARG:HH11	1.53	0.72
14:T:140:CYS:SG	14:T:143:GLU:HB2	2.29	0.72
18:Z:65:LEU:O	18:Z:69:ILE:HG12	1.89	0.72
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.72	0.72
9:I:57:ALA:HB2	20:b:13:TRP:O	1.88	0.72
18:Z:6:VAL:CG1	22:r:40:LYS:HB3	2.19	0.72
4:D:392:PRO:HG3	22:r:60:ARG:O	1.89	0.72
6:F:327:ILE:HG23	6:F:332:CYS:SG	2.29	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.19	0.72
20:b:23:PHE:HD2	24:b:201:3PE:H281	1.54	0.72
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.72
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.20	0.72
24:H:402:3PE:H322	9:I:63:TRP:HE1	1.55	0.72
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	2.05	0.72
4:D:136:PHE:HZ	4:D:422:CYS:SG	2.13	0.72
8:H:17:MET:SD	8:H:225:MET:HB3	2.30	0.72
1:A:73:LEU:O	1:A:76:PRO:HD2	1.90	0.72
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:35:LEU:HD22	6:F:273:THR:HG21	1.72	0.72
6:F:318:ILE:O	6:F:318:ILE:HG13	1.90	0.72
16:W:42:TRP:CH2	16:W:93:LEU:HA	2.24	0.72
5:E:155:LEU:HB3	5:E:157:ILE:HG22	1.72	0.71
7:G:544:MET:HE3	7:G:565:PHE:HE2	1.54	0.71
8:H:17:MET:HE1	8:H:225:MET:HB3	1.72	0.71
8:H:96:ILE:HG23	18:Z:143:TYR:OH	1.90	0.71
9:I:64:THR:HG22	30:I:301:PC1:H222	1.72	0.71
9:I:107:PRO:HG3	21:q:106:ARG:NH1	2.05	0.71
18:Z:6:VAL:HG13	18:Z:7:LYS:H	1.53	0.71
6:F:110:PRO:HD2	6:F:238:CYS:SG	2.30	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
8:H:310:PHE:HA	20:b:39:THR:HA	1.72	0.71
3:C:217:ARG:NH1	16:W:112:GLU:HB2	2.04	0.71
9:I:135:ARG:HH11	12:R:61:ILE:HG23	1.55	0.71
2:B:210:ARG:NH1	21:q:78:ASP:HB3	2.05	0.71
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.71
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.71
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.20	0.71
3:C:67:ILE:HD11	15:V:47:TYR:HD2	1.55	0.71
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.72	0.71
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.54	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
8:H:21:THR:HG21	29:H:401:UQ9:H16A	1.72	0.71
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.71
6:F:318:ILE:HG22	6:F:326:LEU:CB	2.20	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.26	0.71
6:F:44:ASN:ND2	6:F:133:HIS:O	2.24	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.79	0.71
8:H:306:SER:OG	20:b:33:PRO:HG3	1.90	0.71
10:P:170:LEU:O	10:P:171:ASN:OD1	2.09	0.71
18:Z:144:THR:HG22	19:a:48:MET:SD	2.30	0.71
4:D:238:LEU:CD1	9:I:211:TYR:OH	2.35	0.70
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.70
9:I:188:GLU:OE1	12:R:56:ASN:N	2.24	0.70
22:r:46:SER:C	22:r:52:ASN:HD21	1.99	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:ARG:HG2	8:H:36:GLY:O	1.91	0.70
4:D:198:THR:HG22	8:H:32:GLN:NE2	2.07	0.70
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.56	0.70
3:C:67:ILE:HD11	15:V:47:TYR:CD2	2.25	0.70
4:D:82:LEU:HD12	8:H:126:LYS:HD2	1.73	0.70
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.55	0.70
6:F:110:PRO:O	6:F:238:CYS:HB3	1.91	0.70
2:B:166:ASN:HB2	2:B:190:TYR:HD2	1.55	0.70
7:G:81:GLU:OE2	7:G:108:LYS:HD3	1.92	0.70
8:H:127:TYR:HD1	8:H:207:LEU:HD22	1.50	0.70
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.73	0.70
9:I:155:CYS:HG	25:I:302:SF4:FE4	1.08	0.70
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.70
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.44	0.70
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.21	0.70
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.70
13:S:16:LEU:HD21	13:S:19:ILE:HD11	1.74	0.70
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.69
2:B:120:VAL:HG21	29:H:401:UQ9:C1M	2.22	0.69
3:C:100:ARG:HH12	15:V:86:LYS:NZ	1.88	0.69
4:D:255:ILE:HG12	4:D:337:MET:HE2	1.72	0.69
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.57	0.69
7:G:614:GLY:CA	10:P:41:ILE:HD13	2.22	0.69
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.69
22:r:98:ALA:HB1	22:r:99:PRO:HD2	1.74	0.69
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.07	0.69
4:D:120:THR:HG21	4:D:139:LEU:HD21	1.74	0.69
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.69
8:H:97:ASN:HD21	19:a:38:VAL:HG13	1.58	0.69
10:P:365:GLU:HB2	10:P:367:GLU:OE2	1.92	0.69
18:Z:6:VAL:HG13	22:r:40:LYS:HB3	1.75	0.69
4:D:88:HIS:HE1	8:H:205:SER:O	1.74	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
10:P:171:ASN:OD1	10:P:171:ASN:O	2.11	0.69
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.08	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.74	0.69
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.75	0.69
5:E:61:ARG:NE	23:s:47:ASP:OD1	2.22	0.69
6:F:278:ILE:HG12	6:F:304:ALA:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:17:MET:CE	8:H:225:MET:HB3	2.23	0.69
8:H:293:PHE:CE1	24:H:402:3PE:H321	2.25	0.69
13:S:51:LEU:HD13	13:S:95:LEU:HD12	1.75	0.69
17:X:122:LEU:HD21	20:b:81:LEU:HD23	1.73	0.69
7:G:117:MET:HE3	7:G:143:SER:HA	1.74	0.69
7:G:171:THR:HB	7:G:173:MET:HG3	1.74	0.69
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.69
6:F:236:PHE:O	11:Q:166:TRP:HE3	1.76	0.69
4:D:88:HIS:CD2	8:H:208:VAL:HG13	2.27	0.68
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.75	0.68
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.68
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.68
7:G:401:LEU:HD11	7:G:462:PHE:CZ	2.28	0.68
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.23	0.68
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.74	0.68
3:C:217:ARG:HH12	16:W:112:GLU:HB2	1.58	0.68
4:D:156:GLU:HG2	4:D:161:ILE:HD11	1.74	0.68
14:T:90:TYR:HE2	14:T:110:LEU:HD11	1.58	0.68
2:B:111:ARG:CB	4:D:208:GLU:OE1	2.40	0.68
5:E:233:LEU:H	6:F:37:ASP:CG	2.02	0.68
6:F:382:CYS:HG	25:F:502:SF4:FE3	1.10	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
10:P:191:VAL:HA	10:P:194:VAL:HG22	1.72	0.68
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.68
4:D:95:LEU:HG	4:D:97:LEU:HG	1.76	0.68
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.68
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.68
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.08	0.68
22:r:112:TYR:O	22:r:113:LEU:HB2	1.93	0.68
13:S:42:VAL:HB	13:S:46:LYS:HE3	1.75	0.68
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.29	0.68
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.68
9:I:93:LEU:O	21:q:93:MET:HG2	1.94	0.68
4:D:156:GLU:HG3	4:D:229:PRO:O	1.93	0.68
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.76	0.68
10:P:263:PHE:HD2	10:P:333:PRO:O	1.77	0.68
7:G:78:CYS:HG	27:G:803:FES:FE2	0.46	0.68
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.59	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
14:T:104:PHE:HB2	14:T:110:LEU:HB2	1.74	0.68
18:Z:65:LEU:HB3	20:b:50:PRO:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:PRO:HG2	8:H:58:LYS:HA	1.75	0.68
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.68
6:F:147:ARG:HD3	6:F:191:TYR:CE2	2.29	0.68
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.68
9:I:110:GLU:OE1	12:R:64:ILE:HB	1.94	0.68
4:D:142:VAL:HG11	4:D:185:MET:HG2	1.76	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.28	0.67
16:W:45:GLU:CD	16:W:97:ILE:HG22	2.19	0.67
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.60	0.67
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
10:P:197:GLU:HB3	10:P:259:VAL:CG2	2.24	0.67
13:S:20:ARG:HB2	13:S:66:TRP:HB2	1.75	0.67
2:B:202:LEU:CD2	9:I:86:TYR:CB	2.73	0.67
7:G:651:PRO:CD	13:S:56:ARG:HB3	2.23	0.67
10:P:296:PHE:CZ	10:P:297:VAL:HG23	2.29	0.67
22:r:12:ARG:HH21	22:r:20:LEU:CD1	2.07	0.67
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.24	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.77	0.67
7:G:73:GLY:HA2	27:G:803:FES:S1	2.35	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.67
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.77	0.67
10:P:302:GLY:HA2	10:P:314:THR:HG23	1.77	0.67
18:Z:62:ILE:HD12	20:b:81:LEU:HD22	1.76	0.67
21:q:138:VAL:CG2	21:q:139:PRO:HD2	2.25	0.67
4:D:451:ILE:CG2	4:D:456:ILE:HD11	2.25	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.24	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
8:H:207:LEU:O	8:H:208:VAL:C	2.38	0.67
6:F:233:VAL:HG11	11:Q:164:PHE:HB2	1.76	0.67
17:X:7:LEU:HD13	18:Z:87:LEU:HB3	1.77	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
8:H:185:TRP:CD1	8:H:238:THR:HG1	2.13	0.67
14:T:97:LYS:HZ3	14:T:108:LEU:N	1.93	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.66
9:I:62:MET:HE1	18:Z:36:PHE:HA	1.77	0.66
9:I:200:GLU:OE2	21:q:93:MET:SD	2.53	0.66
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	1.77	0.66
2:B:81:LEU:CG	8:H:53:MET:HE1	2.25	0.66
2:B:95:PHE:HB3	2:B:97:LEU:CD1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:PHE:HE1	15:V:44:TYR:CE1	2.13	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
10:P:122:HIS:HB2	12:R:46:VAL:HG12	1.77	0.66
17:X:130:LYS:HG2	20:b:68:SER:HA	1.77	0.66
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.26	0.66
2:B:170:TYR:HB2	9:I:153:ILE:CG2	2.24	0.66
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.66
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.66
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.76	0.66
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.60	0.66
10:P:262:THR:H	10:P:332:LEU:HD12	1.61	0.66
3:C:47:ARG:HG3	3:C:48:PRO:HD2	1.77	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
4:D:279:THR:HA	15:V:12:VAL:CG1	2.25	0.66
6:F:275:LEU:HA	6:F:289:GLU:HA	1.77	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
8:H:300:LEU:HD23	20:b:25:VAL:HG11	1.76	0.66
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.28	0.66
16:W:121:PHE:HA	16:W:124:LYS:HE2	1.76	0.66
17:X:48:TRP:CE2	20:b:55:VAL:CG2	2.75	0.66
17:X:57:LEU:HG	17:X:61:LYS:NZ	2.10	0.66
4:D:83:ASN:OD1	4:D:83:ASN:O	2.14	0.66
8:H:187:ILE:HD12	24:H:402:3PE:H242	1.77	0.66
10:P:320:GLU:O	10:P:324:ILE:HG12	1.96	0.66
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.66
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.66
4:D:359:ASP:HB3	7:G:150:ARG:NH2	2.11	0.66
6:F:48:ARG:HH11	6:F:48:ARG:HA	1.61	0.66
6:F:297:LYS:HD3	6:F:333:GLU:HB3	1.77	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
10:P:169:HIS:H	10:P:184:LYS:CE	2.09	0.66
2:B:81:LEU:HG	8:H:53:MET:HE1	1.77	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.74	0.66
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.66
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.26	0.66
8:H:283:ASP:OD1	8:H:284:GLN:N	2.29	0.66
4:D:102:SER:CB	4:D:107:ARG:HG3	2.26	0.65
7:G:360:LYS:HB2	7:G:632:ILE:CD1	2.22	0.65
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.65
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:114:THR:O	18:Z:114:THR:HG22	1.94	0.65
4:D:178:THR:HG22	4:D:214:TYR:OH	1.96	0.65
4:D:384:LEU:CD2	7:G:144:MET:HE1	2.26	0.65
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.94	0.65
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.30	0.65
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.32	0.65
10:P:59:PHE:HB2	10:P:130:ILE:HD11	1.79	0.65
6:F:293:SER:HA	6:F:338:ASP:HB3	1.78	0.65
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.65
8:H:17:MET:HE1	8:H:225:MET:CE	2.25	0.65
13:S:58:CYS:HB2	13:S:61:VAL:HG12	1.78	0.65
18:Z:143:TYR:CD1	18:Z:144:THR:N	2.65	0.65
4:D:198:THR:HG22	8:H:32:GLN:CG	2.26	0.65
4:D:211:PHE:O	4:D:214:TYR:HB2	1.96	0.65
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65
10:P:199:ILE:HD11	10:P:258:ALA:O	1.96	0.65
13:S:16:LEU:HD11	13:S:19:ILE:HD11	1.78	0.65
1:A:106:TRP:CZ2	8:H:291:LYS:HA	2.32	0.65
2:B:95:PHE:CZ	2:B:145:LEU:HA	2.31	0.65
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.65
4:D:376:GLU:OE1	7:G:151:SER:HB2	1.97	0.65
8:H:310:PHE:O	20:b:38:TYR:HB2	1.96	0.65
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.31	0.65
4:D:315:GLU:HB3	4:D:346:GLN:HE22	1.61	0.65
8:H:292:ASN:HD21	24:H:402:3PE:C12	2.10	0.65
10:P:236:VAL:CG1	10:P:270:ARG:HH21	2.10	0.65
12:R:40:GLU:HA	12:R:45:ARG:NH1	2.12	0.65
17:X:53:PRO:HB3	18:Z:80:ASP:OD2	1.97	0.65
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.65
17:X:141:PRO:O	17:X:142:TYR:HB2	1.96	0.65
2:B:154:GLU:HB3	2:B:155:PRO:HD3	1.77	0.65
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.61	0.65
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.96	0.65
8:H:287:HIS:HE1	24:H:402:3PE:N	1.94	0.65
7:G:89:VAL:HB	7:G:94:MET:HG3	1.78	0.64
9:I:181:GLU:HB2	21:q:126:PRO:HG3	1.79	0.64
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.79	0.64
7:G:614:GLY:C	10:P:41:ILE:HG21	2.22	0.64
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.64
24:H:402:3PE:H322	9:I:63:TRP:NE1	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:THR:HG22	8:H:32:GLN:HG3	1.79	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
8:H:249:ILE:HD13	17:X:99:HIS:CG	2.32	0.64
10:P:226:VAL:HG21	10:P:281:PHE:CZ	2.32	0.64
13:S:48:HIS:CE1	13:S:95:LEU:CD2	2.80	0.64
21:q:3:LEU:O	21:q:6:VAL:HG22	1.97	0.64
3:C:68:LEU:HD13	3:C:95:THR:HG23	1.80	0.64
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.33	0.64
17:X:65:GLY:HA2	17:X:68:LEU:HD12	1.78	0.64
1:A:7:ILE:HG21	24:A:401:3PE:H292	1.80	0.64
3:C:241:PHE:CD2	22:r:61:ARG:CB	2.75	0.64
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.80	0.64
6:F:388:GLY:HA3	6:F:419:ILE:HD11	1.80	0.64
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.64
14:T:80:LYS:HD3	14:T:100:VAL:HG11	1.79	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.64
4:D:104:GLU:HG3	8:H:130:PHE:HZ	1.63	0.64
5:E:58:ASN:HB3	5:E:84:LEU:HD21	1.80	0.64
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.61	0.64
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.64
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.64
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.60	0.64
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.78	0.64
2:B:202:LEU:HD21	9:I:86:TYR:CB	2.28	0.64
4:D:451:ILE:HG23	4:D:456:ILE:CD1	2.28	0.64
6:F:379:CYS:SG	25:F:502:SF4:S1	2.96	0.64
7:G:557:ARG:HD3	21:q:144:TYR:CE1	2.32	0.64
4:D:102:SER:HB2	4:D:107:ARG:CG	2.26	0.64
4:D:217:VAL:HG22	4:D:226:TYR:CZ	2.33	0.64
7:G:152:ARG:HD2	22:r:49:LEU:HA	1.80	0.64
8:H:249:ILE:HG21	17:X:99:HIS:CE1	2.33	0.64
10:P:296:PHE:CZ	10:P:297:VAL:CG2	2.81	0.64
17:X:50:GLU:HG2	17:X:138:PRO:HG3	1.79	0.64
4:D:156:GLU:HG2	4:D:161:ILE:CD1	2.28	0.64
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.80	0.64
6:F:227:PRO:HG3	7:G:94:MET:SD	2.38	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.64
21:q:29:ARG:O	30:q:202:PC1:C14	2.46	0.64
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.80	0.64

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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	0.64
10:P:150:ARG:HE	10:P:190:GLU:HG2	1.62	0.64
10:P:299:SER:CB	10:P:316:LYS:HE3	2.22	0.64
13:S:20:ARG:HG2	13:S:54:LEU:HD12	1.79	0.64
17:X:37:ASP:OD1	17:X:38:LYS:N	2.31	0.64
5:E:48:PRO:HA	5:E:95:SER:HB2	1.80	0.63
5:E:129:TYR:CE2	5:E:167:LEU:HG	2.33	0.63
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.61	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
7:G:449:PRO:HG3	7:G:483:ARG:HH22	1.62	0.63
10:P:180:SER:O	10:P:184:LYS:HG3	1.98	0.63
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.78	0.63
2:B:202:LEU:CD2	9:I:86:TYR:HB2	2.29	0.63
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.63	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
8:H:90:PRO:HB2	8:H:166:ILE:HD11	1.80	0.63
8:H:181:MET:CE	8:H:304:HIS:ND1	2.62	0.63
8:H:310:PHE:HB3	20:b:33:PRO:HA	1.80	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
8:H:85:LEU:HD21	8:H:108:THR:HB	1.80	0.63
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.80	0.63
2:B:116:ARG:HA	8:H:37:PRO:HA	1.80	0.63
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.63
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.63
14:T:104:PHE:CE1	14:T:115:GLN:CB	2.80	0.63
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.63
2:B:194:CYS:O	25:B:301:SF4:S4	2.56	0.63
10:P:284:THR:HG23	10:P:356:HIS:HB2	1.79	0.63
10:P:365:GLU:CB	10:P:367:GLU:OE2	2.46	0.63
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.79	0.63
10:P:66:GLY:O	10:P:67:ARG:C	2.42	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.98	0.63
7:G:126:LEU:HD11	12:R:89:PRO:HB3	1.80	0.63
12:R:44:ARG:HG2	12:R:47:ARG:NH1	2.14	0.63
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.79	0.63
14:T:104:PHE:HE1	14:T:115:GLN:CB	2.07	0.63
18:Z:65:LEU:O	18:Z:68:ARG:HG2	1.98	0.63
21:q:29:ARG:O	30:q:202:PC1:H141	1.97	0.63
2:B:91:TRP:CE3	29:H:401:UQ9:H1MA	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:275:LEU:HG	6:F:289:GLU:HB3	1.80	0.63
6:F:425:CYS:SG	25:F:502:SF4:S4	2.96	0.63
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.63
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.79	0.63
1:A:52:SER:HB2	1:A:54:LYS:HG2	1.79	0.63
2:B:98:ALA:O	4:D:141:TYR:CZ	2.52	0.63
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.63
4:D:198:THR:HA	8:H:32:GLN:HG2	1.80	0.63
1:A:7:ILE:HG13	24:A:401:3PE:H271	1.81	0.62
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.32	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.29	0.62
16:W:55:LEU:CB	16:W:107:MET:CE	2.75	0.62
18:Z:6:VAL:HG11	22:r:40:LYS:HD3	1.80	0.62
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.59	0.62
4:D:384:LEU:HD21	7:G:144:MET:HE1	1.79	0.62
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.62
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.35	0.62
7:G:360:LYS:CE	7:G:632:ILE:HB	2.27	0.62
5:E:238:LYS:HE2	5:E:242:PHE:CE2	2.34	0.62
6:F:87:GLY:H	6:F:92:GLY:HA2	1.64	0.62
7:G:382:ARG:HD2	13:S:56:ARG:HD3	1.82	0.62
4:D:102:SER:HB2	4:D:107:ARG:CD	2.29	0.62
4:D:139:LEU:O	4:D:460:GLU:N	2.32	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.81	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
9:I:92:PRO:HG2	21:q:56:PHE:CE2	2.35	0.62
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.62
16:W:55:LEU:CB	16:W:107:MET:HE2	2.30	0.62
18:Z:69:ILE:HG23	20:b:54:PRO:HD3	1.81	0.62
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.62
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.40	0.62
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.80	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
2:B:142:ALA:HB3	2:B:143:PRO:HD3	1.82	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.82	0.62
2:B:161:MET:HG2	2:B:196:PRO:HG2	1.80	0.62
6:F:87:GLY:O	6:F:88:ARG:HB2	1.99	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.15	0.62
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.62
3:C:212:ASP:OD2	10:P:75:ARG:NH2	2.32	0.62
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.34	0.62
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.29	0.62
10:P:240:VAL:HB	10:P:266:THR:O	2.00	0.62
17:X:7:LEU:CD1	18:Z:87:LEU:HB3	2.30	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
8:H:17:MET:HE3	8:H:225:MET:HG2	1.82	0.62
8:H:186:PHE:CD1	8:H:270:PHE:HE1	2.14	0.62
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.64	0.62
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.24	0.62
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.62
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.62
18:Z:143:TYR:HD1	18:Z:144:THR:H	1.46	0.62
4:D:368:ARG:NH1	9:I:160:GLU:O	2.33	0.61
5:E:180:VAL:HG13	5:E:181:ASN:N	2.15	0.61
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.61
7:G:636:TYR:CD1	7:G:642:VAL:HG22	2.34	0.61
9:I:92:PRO:HA	21:q:91:HIS:O	2.00	0.61
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.81	0.61
34:q:201:CDL:H331	34:q:201:CDL:H722	1.82	0.61
2:B:97:LEU:HD11	2:B:141:MET:HE2	1.82	0.61
4:D:145:MET:HA	4:D:148:GLU:HG2	1.82	0.61
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.80	0.61
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.30	0.61
13:S:48:HIS:HE1	13:S:95:LEU:HD22	1.63	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.81	0.61
12:R:72:VAL:HG21	12:R:77:ILE:HD13	1.82	0.61
17:X:18:VAL:HG11	17:X:25:LEU:HD21	1.80	0.61
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.61
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.28	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.61
20:b:11:ASN:O	20:b:15:LYS:N	2.31	0.61
21:q:84:PRO:HD2	21:q:113:HIS:CD2	2.36	0.61
5:E:65:ILE:HD11	23:s:46:LEU:HD22	1.83	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:271:ARG:HD2	8:H:281:ARG:HG2	1.82	0.61
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.81	0.61
10:P:363:SER:CB	16:W:51:HIS:NE2	2.60	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	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	1.81	0.61
17:X:46:CYS:SG	17:X:59:GLU:HG3	2.41	0.61
2:B:120:VAL:HG11	29:H:401:UQ9:H1MB	1.83	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.61
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.30	0.61
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.61
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.66	0.61
8:H:89:LEU:HD11	8:H:233:LEU:HD13	1.80	0.61
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.30	0.61
10:P:169:HIS:HD2	10:P:181:LEU:HD11	1.65	0.61
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.61
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.66	0.61
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.61
8:H:39:ILE:HG13	21:q:31:ASN:ND2	2.15	0.61
4:D:128:THR:HG23	4:D:131:GLN:HG2	1.81	0.60
4:D:256:ASP:O	4:D:259:GLU:HB3	2.02	0.60
4:D:323:ARG:O	15:V:12:VAL:CG2	2.49	0.60
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.60
6:F:69:LEU:HD11	6:F:143:LEU:CD2	2.31	0.60
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.14	0.60
4:D:170:ILE:CD1	4:D:236:LEU:CD1	2.79	0.60
4:D:261:MET:HE1	8:H:276:SER:HA	1.83	0.60
5:E:91:TRP:CE3	5:E:125:PRO:HB3	2.36	0.60
5:E:154:LYS:HE3	5:E:201:GLU:HB2	1.83	0.60
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.84	0.60
22:r:12:ARG:HH21	22:r:20:LEU:HD11	1.65	0.60
5:E:134:CYS:SG	5:E:175:CYS:HA	2.41	0.60
6:F:318:ILE:HD11	6:F:355:ILE:CD1	2.28	0.60
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.60
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.60
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.81	0.60
18:Z:144:THR:O	19:a:36:LYS:HD2	2.02	0.60
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.84	0.60
5:E:150:THR:O	5:E:154:LYS:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.83	0.60
10:P:136:THR:CG2	10:P:139:PHE:HB2	2.31	0.60
12:R:72:VAL:CG1	12:R:77:ILE:HD12	2.30	0.60
12:R:97:LYS:HD2	12:R:100:LYS:HB2	1.84	0.60
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.60
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.60
8:H:42:PRO:HG3	21:q:28:PHE:CE1	2.36	0.60
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.60
2:B:95:PHE:HZ	2:B:148:VAL:HB	1.67	0.60
6:F:414:GLU:OE1	22:r:50:SER:HA	2.02	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.60
2:B:101:ALA:HB1	26:D:501:UQ1:H112	1.83	0.60
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.32	0.60
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.36	0.60
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.83	0.60
5:E:63:GLU:O	5:E:67:LYS:HG3	2.02	0.60
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.36	0.60
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.60
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.60
2:B:169:GLY:O	2:B:170:TYR:C	2.44	0.59
5:E:70:PRO:HB3	23:s:60:PRO:HG3	1.82	0.59
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.59
16:W:42:TRP:CZ2	16:W:93:LEU:HA	2.37	0.59
17:X:37:ASP:HA	17:X:40:ASN:HB2	1.84	0.59
3:C:84:GLU:OE2	3:C:141:ARG:NH1	2.35	0.59
3:C:141:ARG:NH1	4:D:410:TYR:HE1	2.00	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
7:G:114:GLU:OE2	22:r:54:TYR:N	2.31	0.59
7:G:117:MET:HE3	7:G:143:SER:CA	2.32	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
7:G:614:GLY:HA2	10:P:41:ILE:HD12	1.84	0.59
7:G:617:ARG:NH1	16:W:128:GLY:C	2.59	0.59
5:E:226:PRO:HG2	5:E:231:THR:H	1.67	0.59
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.38	0.59
8:H:306:SER:HG	8:H:310:PHE:HE2	1.32	0.59
9:I:72:MET:HE1	22:r:16:SER:HB2	1.84	0.59
9:I:80:GLU:HG3	19:a:1:MET:SD	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
2:B:95:PHE:CE1	2:B:145:LEU:HD12	2.36	0.59
2:B:202:LEU:CD2	9:I:86:TYR:CG	2.83	0.59
6:F:418:GLN:HE22	7:G:111:LYS:HG3	1.65	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
12:R:45:ARG:HA	12:R:48:PHE:HD2	1.67	0.59
13:S:16:LEU:HD11	13:S:19:ILE:CD1	2.32	0.59
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.84	0.59
4:D:207:ARG:O	4:D:211:PHE:HD1	1.84	0.59
6:F:270:ASN:HD21	6:F:340:ASP:H	1.50	0.59
6:F:318:ILE:CG1	6:F:355:ILE:HB	2.32	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
8:H:127:TYR:CE1	8:H:207:LEU:CD2	2.84	0.59
9:I:188:GLU:OE1	12:R:56:ASN:HB2	2.01	0.59
20:b:8:PHE:HA	20:b:11:ASN:ND2	2.18	0.59
20:b:20:VAL:HG22	24:b:201:3PE:H261	1.84	0.59
6:F:314:LEU:O	6:F:329:LYS:HB2	2.03	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
2:B:95:PHE:CZ	2:B:148:VAL:HB	2.38	0.59
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.36	0.59
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.67	0.59
6:F:87:GLY:HA3	6:F:92:GLY:HA2	1.84	0.59
6:F:410:ASP:OD1	6:F:411:SER:N	2.36	0.59
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
10:P:318:LYS:HG2	10:P:322:ILE:HD11	1.84	0.59
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.84	0.59
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.67	0.59
4:D:170:ILE:HD13	4:D:236:LEU:HD11	1.84	0.59
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.67	0.59
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.83	0.59
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.59
12:R:32:THR:OG1	12:R:36:GLN:HB3	2.03	0.59
20:b:6:SER:O	20:b:9:LEU:HB3	2.03	0.59
23:s:57:LEU:HG	23:s:58:PRO:HD2	1.84	0.59
3:C:100:ARG:NH1	15:V:86:LYS:NZ	2.51	0.59
3:C:242:PRO:O	3:C:243:ALA:C	2.45	0.59
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.59
4:D:411:LEU:HD11	4:D:419:PRO:HB3	1.85	0.59
6:F:318:ILE:HG12	6:F:355:ILE:HB	1.85	0.59
10:P:178:SER:O	10:P:182:ARG:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.59
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.59
22:r:20:LEU:C	22:r:20:LEU:HD12	2.27	0.59
4:D:326:CYS:CB	4:D:453:THR:HG21	2.32	0.58
6:F:267:ARG:HH12	6:F:340:ASP:HB3	1.68	0.58
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.85	0.58
21:q:66:THR:HG22	21:q:67:GLU:OE2	2.03	0.58
2:B:99:CYS:HB3	4:D:141:TYR:CB	2.33	0.58
6:F:225:LEU:N	11:Q:160:TYR:HE2	1.95	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.58
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.87	0.58
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.32	0.58
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.85	0.58
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.58
10:P:57:THR:HG23	10:P:123:SER:CB	2.33	0.58
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.58
17:X:123:GLY:HA2	18:Z:66:GLU:OE2	2.03	0.58
21:q:59:HIS:CE1	21:q:60:ARG:CG	2.83	0.58
4:D:97:LEU:CD2	4:D:111:PRO:HB3	2.33	0.58
6:F:270:ASN:ND2	6:F:340:ASP:H	2.00	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.16	0.58
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.68	0.58
10:P:57:THR:HG23	10:P:123:SER:HB2	1.86	0.58
16:W:104:THR:O	16:W:108:ARG:HG3	2.02	0.58
6:F:51:TRP:CB	6:F:133:HIS:O	2.52	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
6:F:119:GLU:OE1	6:F:125:CYS:HA	2.03	0.58
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.38	0.58
6:F:303:HIS:O	6:F:304:ALA:C	2.45	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.86	0.58
4:D:112:HIS:HE1	16:W:100:TRP:CD1	2.22	0.58
4:D:203:MET:HE2	4:D:258:VAL:HG13	1.86	0.58
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.81	0.58
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.34	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.66	0.58
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:125:VAL:HG23	21:q:125:VAL:O	2.03	0.58
4:D:94:VAL:HB	4:D:115:LEU:HB2	1.86	0.58
4:D:159:LEU:CG	4:D:391:VAL:HG12	2.34	0.58
4:D:217:VAL:HG22	4:D:226:TYR:CE1	2.39	0.58
5:E:227:ALA:HB3	6:F:284:HIS:ND1	2.19	0.58
4:D:121:GLU:HG2	4:D:424:ILE:HD12	1.86	0.58
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.86	0.58
8:H:17:MET:CE	8:H:225:MET:HG2	2.34	0.58
14:T:90:TYR:CE2	14:T:110:LEU:HD11	2.39	0.58
4:D:145:MET:HA	4:D:148:GLU:CG	2.34	0.58
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.58
6:F:297:LYS:O	6:F:301:GLU:HG2	2.03	0.57
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.12	0.57
10:P:245:VAL:O	10:P:249:ILE:HG13	2.04	0.57
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.57
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.57
1:A:80:GLN:NE2	8:H:315:PRO:O	2.37	0.57
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.04	0.57
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.57
8:H:200:LEU:HD21	8:H:285:LEU:HD13	1.86	0.57
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.57
10:P:220:TYR:HA	10:P:223:PHE:HD2	1.68	0.57
10:P:363:SER:O	16:W:51:HIS:CD2	2.58	0.57
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.57
12:R:37:VAL:O	12:R:37:VAL:HG13	2.03	0.57
4:D:159:LEU:HG	4:D:391:VAL:HG12	1.86	0.57
4:D:163:PRO:HG2	4:D:168:GLN:HE21	1.68	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.57
7:G:372:PHE:H	7:G:532:PRO:HB2	1.69	0.57
8:H:17:MET:SD	8:H:225:MET:O	2.62	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
3:C:186:ILE:HG13	3:C:187:LEU:N	2.18	0.57
5:E:107:PRO:HB2	5:E:110:ARG:HG2	1.87	0.57
6:F:291:GLU:HG2	6:F:292:MET:O	2.05	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.57
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.66	0.57
7:G:632:ILE:HG13	7:G:632:ILE:O	2.04	0.57
12:R:52:GLN:NE2	12:R:54:GLU:HA	2.19	0.57
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.34	0.57
3:C:67:ILE:HD12	15:V:44:TYR:HA	1.85	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:180:PRO:HD3	18:Z:43:LEU:HD21	1.87	0.57
2:B:106:HIS:HE1	4:D:207:ARG:HB3	1.69	0.57
4:D:92:HIS:CD2	26:D:501:UQ1:C2	2.87	0.57
4:D:170:ILE:CD1	4:D:236:LEU:HD13	2.34	0.57
4:D:320:ILE:O	4:D:320:ILE:HG13	2.03	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.05	0.57
18:Z:59:ARG:NH2	20:b:84:LEU:HB3	2.18	0.57
2:B:202:LEU:HD23	9:I:86:TYR:CB	2.34	0.57
4:D:280:ALA:CB	15:V:11:LEU:CG	2.83	0.57
4:D:320:ILE:HG12	9:I:36:TYR:HD2	1.69	0.57
6:F:87:GLY:N	6:F:92:GLY:HA2	2.19	0.57
6:F:270:ASN:HD22	6:F:338:ASP:CG	2.13	0.57
6:F:296:LEU:O	6:F:297:LYS:C	2.47	0.57
8:H:14:LEU:HG	29:H:401:UQ9:H23	1.86	0.57
8:H:65:THR:HG22	10:P:359:TYR:HD1	1.64	0.57
8:H:175:LEU:HD21	30:I:301:PC1:H2C1	1.86	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
20:b:23:PHE:HE1	24:b:201:3PE:H3A2	1.69	0.57
21:q:86:TRP:CG	21:q:98:PRO:HG2	2.39	0.57
21:q:129:THR:O	21:q:129:THR:HG22	2.03	0.57
2:B:112:TYR:CZ	2:B:199:GLU:HG2	2.40	0.57
4:D:154:ALA:HB2	4:D:398:THR:HG21	1.87	0.57
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.35	0.57
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.57
6:F:296:LEU:HD23	6:F:332:CYS:HB3	1.86	0.57
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.57
1:A:60:ILE:O	1:A:61:THR:C	2.46	0.57
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.64	0.57
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.87	0.57
6:F:382:CYS:HA	7:G:74:ASN:O	2.05	0.57
7:G:399:VAL:HG22	7:G:462:PHE:HZ	1.68	0.57
8:H:17:MET:SD	8:H:225:MET:CA	2.93	0.57
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.85	0.57
3:C:209:LEU:HD21	16:W:108:ARG:NH1	2.20	0.56
5:E:73:HIS:HB3	6:F:236:PHE:CE1	2.40	0.56
6:F:69:LEU:HD11	6:F:143:LEU:HD21	1.87	0.56
8:H:69:SER:C	8:H:71:PHE:H	2.13	0.56
17:X:5:VAL:HG13	17:X:7:LEU:HG	1.87	0.56
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.85	0.56
2:B:110:PRO:HB3	8:H:33:LEU:O	2.05	0.56
2:B:154:GLU:O	2:B:155:PRO:C	2.48	0.56
2:B:164:CYS:SG	25:B:301:SF4:S3	3.03	0.56
6:F:278:ILE:CD1	6:F:304:ALA:HB1	2.35	0.56
7:G:362:ASP:HB2	13:S:71:PHE:CD1	2.39	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
7:G:625:ALA:O	7:G:629:ILE:HG12	2.04	0.56
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.69	0.56
9:I:88:PHE:CZ	21:q:30:ALA:HA	2.40	0.56
12:R:44:ARG:HG2	12:R:47:ARG:HH12	1.70	0.56
17:X:53:PRO:HD3	18:Z:116:TRP:CD1	2.40	0.56
18:Z:8:GLN:HG3	22:r:41:LEU:HD12	1.86	0.56
3:C:123:ASN:HD22	15:V:108:PRO:HG2	1.69	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.56
7:G:62:ARG:H	7:G:142:GLN:HE22	1.53	0.56
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.84	0.56
8:H:4:ILE:O	8:H:8:THR:HG23	2.05	0.56
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.40	0.56
17:X:103:GLN:HA	17:X:106:LYS:HD3	1.88	0.56
17:X:122:LEU:HD23	20:b:82:LYS:HG2	1.88	0.56
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.06	0.56
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.35	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
10:P:64:PHE:HE1	10:P:209:ARG:O	1.88	0.56
10:P:315:THR:HG22	10:P:317:ASP:H	1.69	0.56
10:P:323:HIS:ND1	10:P:323:HIS:O	2.39	0.56
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.36	0.56
5:E:226:PRO:HD3	6:F:46:TYR:CE2	2.40	0.56
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.56
34:q:201:CDL:H141	34:q:201:CDL:H321	1.87	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
8:H:127:TYR:CD1	8:H:207:LEU:HD23	2.36	0.56
20:b:67:PRO:HB3	20:b:74:LEU:HB2	1.87	0.56
5:E:176:LEU:HB2	5:E:184:MET:HE1	1.87	0.56
6:F:154:ALA:HB2	6:F:193:PHE:HZ	1.71	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.56
7:G:399:VAL:CG2	7:G:462:PHE:CE1	2.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:615:LEU:HG	10:P:41:ILE:HG23	1.86	0.56
7:G:651:PRO:HG3	13:S:57:GLU:N	2.19	0.56
9:I:82:ALA:HA	22:r:26:LEU:HD21	1.88	0.56
22:r:106:LEU:HD21	22:r:111:PRO:CB	2.36	0.56
3:C:240:ALA:HB1	22:r:61:ARG:CD	2.34	0.56
4:D:271:ARG:NH1	8:H:279:ARG:O	2.38	0.56
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.36	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56
18:Z:85:GLN:O	18:Z:89:GLU:HG3	2.06	0.56
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.87	0.56
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.87	0.56
8:H:65:THR:O	8:H:124:ASN:HB2	2.05	0.56
10:P:375:VAL:HG12	10:P:377:TYR:HB3	1.87	0.56
12:R:58:ASN:HB3	12:R:63:LEU:HD11	1.88	0.55
14:T:93:ILE:HA	14:T:108:LEU:HD21	1.88	0.55
17:X:124:GLN:C	17:X:125:LEU:HD12	2.31	0.55
22:r:106:LEU:HD21	22:r:111:PRO:HB2	1.86	0.55
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.35	0.55
5:E:231:THR:HG21	6:F:303:HIS:HA	1.88	0.55
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.55
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.45	0.55
10:P:140:ASP:OD1	10:P:142:GLU:HB2	2.06	0.55
17:X:47:ARG:NH2	17:X:53:PRO:HG3	2.21	0.55
1:A:113:TRP:HH2	8:H:287:HIS:CD2	2.25	0.55
3:C:62:GLU:O	3:C:66:GLU:HG3	2.06	0.55
3:C:151:PRO:HG2	16:W:23:ILE:HG13	1.86	0.55
4:D:128:THR:HG22	4:D:131:GLN:CD	2.31	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.55
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.36	0.55
10:P:145:PHE:O	10:P:149:PRO:HG2	2.05	0.55
17:X:142:TYR:HA	18:Z:115:ARG:HD3	1.86	0.55
20:b:69:HIS:HB3	20:b:72:ASP:OD1	2.05	0.55
4:D:380:HIS:O	4:D:384:LEU:HG	2.07	0.55
14:T:146:ASP:O	14:T:149:ALA:HB3	2.06	0.55
17:X:39:THR:HG23	17:X:40:ASN:N	2.20	0.55
4:D:375:MET:HE1	7:G:126:LEU:CA	2.35	0.55
13:S:27:SER:N	13:S:34:ARG:HH22	2.05	0.55
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.70	0.55
4:D:189:THR:HG21	26:D:501:UQ1:HM32	1.89	0.55
4:D:217:VAL:CG2	4:D:226:TYR:CZ	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:264:ASN:O	9:I:65:GLU:OE1	2.25	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
8:H:123:SER:HB3	8:H:214:GLU:HG3	1.88	0.55
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.89	0.55
8:H:212:ASN:HA	8:H:215:TYR:HB2	1.89	0.55
9:I:68:ARG:HH21	18:Z:26:PRO:HD2	1.72	0.55
21:q:3:LEU:O	21:q:7:LEU:HG	2.07	0.55
2:B:91:TRP:CZ3	29:H:401:UQ9:H1MA	2.42	0.55
2:B:194:CYS:HB2	9:I:153:ILE:O	2.07	0.55
6:F:51:TRP:CZ3	6:F:168:ASN:HB3	2.41	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.71	0.55
19:a:1:MET:HB2	19:a:3:PHE:CZ	2.42	0.55
3:C:240:ALA:HB1	22:r:61:ARG:HH11	1.71	0.55
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.42	0.55
5:E:247:GLY:C	6:F:64:LYS:HE2	2.30	0.55
6:F:147:ARG:CD	6:F:191:TYR:CE2	2.90	0.55
14:T:141:PRO:O	14:T:145:VAL:HG23	2.06	0.55
16:W:53:MET:HB2	16:W:55:LEU:HG	1.89	0.55
20:b:8:PHE:CG	20:b:9:LEU:N	2.74	0.55
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.42	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
8:H:69:SER:C	8:H:71:PHE:N	2.61	0.55
8:H:183:MET:HE2	30:I:301:PC1:H271	1.88	0.55
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.55
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.71	0.55
14:T:85:TYR:O	14:T:89:LEU:HD13	2.07	0.55
21:q:56:PHE:HD2	22:r:27:ARG:HH11	1.53	0.55
6:F:424:ILE:CG1	7:G:76:ARG:HD3	2.37	0.55
6:F:425:CYS:HG	25:F:502:SF4:FE1	0.48	0.55
8:H:9:LEU:O	8:H:13:ILE:HG12	2.06	0.55
10:P:237:LYS:HE3	10:P:322:ILE:O	2.07	0.55
12:R:43:TYR:O	12:R:46:VAL:HG22	2.07	0.55
19:a:31:ASN:HD21	19:a:36:LYS:HB2	1.71	0.55
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.71	0.54
12:R:45:ARG:HA	12:R:48:PHE:CD2	2.41	0.54
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.54
18:Z:92:GLU:O	18:Z:96:ILE:HG13	2.07	0.54
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.54
2:B:161:MET:CG	2:B:196:PRO:HG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:PHE:HB2	15:V:94:MET:CE	2.37	0.54
4:D:293:LEU:HD22	4:D:300:TRP:HB3	1.89	0.54
7:G:617:ARG:HH12	16:W:128:GLY:C	2.15	0.54
8:H:307:LEU:HD11	18:Z:47:TYR:CG	2.42	0.54
10:P:44:GLY:H	11:Q:105:GLU:CD	2.15	0.54
10:P:236:VAL:HG13	10:P:270:ARG:HH21	1.71	0.54
18:Z:40:ILE:O	18:Z:44:ILE:HG12	2.07	0.54
2:B:166:ASN:O	2:B:166:ASN:OD1	2.25	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.36	0.54
6:F:388:GLY:CA	6:F:419:ILE:HD11	2.37	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
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.54
9:I:49:ASP:O	9:I:50:MET:C	2.50	0.54
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
11:Q:165:SER:HB2	11:Q:168:LYS:HG2	1.89	0.54
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.22	0.54
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.88	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
7:G:655:ARG:NH1	13:S:59:SER:CB	2.70	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
8:H:43:TYR:CE2	21:q:27:PHE:HZ	2.25	0.54
19:a:58:ASN:HB2	19:a:61:TYR:CD2	2.43	0.54
21:q:50:GLU:HA	21:q:59:HIS:O	2.07	0.54
4:D:150:ALA:HB2	4:D:400:ILE:HG12	1.89	0.54
4:D:189:THR:HB	26:D:501:UQ1:HM21	1.82	0.54
4:D:310:VAL:HG23	4:D:310:VAL:O	2.06	0.54
6:F:286:CYS:SG	6:F:304:ALA:HA	2.47	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:655:ARG:NH1	13:S:59:SER:HB3	2.21	0.54
10:P:207:PHE:CE1	10:P:214:LEU:HD22	2.43	0.54
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.90	0.54
13:S:47:ALA:O	13:S:49:PRO:HD3	2.08	0.54
14:T:84:LEU:O	14:T:88:LYS:HG3	2.07	0.54
17:X:124:GLN:O	20:b:70:PRO:HB2	2.08	0.54
3:C:104:ASN:ND2	22:r:94:ALA:HB1	2.22	0.54
4:D:158:LEU:HD12	4:D:411:LEU:HD23	1.90	0.54
4:D:240:LEU:HG	4:D:244:ILE:CD1	2.38	0.54
6:F:297:LYS:HD3	6:F:333:GLU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
7:G:62:ARG:H	7:G:142:GLN:NE2	2.05	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
10:P:58:VAL:O	10:P:83:PRO:HD2	2.08	0.54
10:P:172:ALA:H	10:P:202:ARG:NH2	2.06	0.54
12:R:48:PHE:CD1	12:R:53:LYS:HB2	2.43	0.54
14:T:115:GLN:O	14:T:119:ILE:HG12	2.08	0.54
17:X:64:ASN:O	17:X:68:LEU:HG	2.07	0.54
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.54
18:Z:143:TYR:O	18:Z:144:THR:HB	2.08	0.54
2:B:100:CYS:CB	2:B:134:ALA:HB1	2.34	0.54
4:D:159:LEU:HD21	4:D:391:VAL:HG12	1.89	0.54
5:E:199:ASP:O	5:E:203:ILE:HG13	2.08	0.54
6:F:278:ILE:HG12	6:F:304:ALA:CB	2.38	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
10:P:306:GLY:HA2	10:P:312:PRO:HB3	1.90	0.54
18:Z:120:LEU:HB2	18:Z:123:GLU:HG3	1.89	0.54
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.43	0.54
4:D:202:TRP:HH2	4:D:261:MET:HG3	1.73	0.54
5:E:84:LEU:HD12	23:s:46:LEU:CD1	2.34	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.08	0.54
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.54
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.54
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.08	0.54
20:b:8:PHE:O	20:b:9:LEU:C	2.50	0.54
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.54
1:A:69:ILE:O	1:A:73:LEU:HG	2.08	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
22:r:54:TYR:CZ	22:r:58:ASP:HB3	2.42	0.54
5:E:116:THR:O	7:G:199:GLY:HA2	2.07	0.54
5:E:133:VAL:HA	5:E:185:VAL:HG12	1.90	0.54
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.90	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
24:H:402:3PE:H2E2	30:I:301:PC1:H2A2	1.90	0.54
4:D:446:ASP:OD2	8:H:281:ARG:NH2	2.41	0.53
5:E:62:ILE:HD11	5:E:84:LEU:HD22	1.90	0.53
6:F:87:GLY:CA	6:F:92:GLY:HA2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:102:MET:SD	6:F:149:MET:HB2	2.48	0.53
6:F:119:GLU:OE1	6:F:125:CYS:CA	2.56	0.53
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.53
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.39	0.53
10:P:231:LEU:HD13	10:P:292:PRO:CD	2.37	0.53
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.53
16:W:23:ILE:HG23	16:W:24:PHE:N	2.22	0.53
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.53
22:r:36:GLN:HB3	22:r:37:PRO:HD2	1.90	0.53
5:E:52:PHE:CD2	5:E:96:ALA:HA	2.43	0.53
5:E:91:TRP:CZ2	5:E:125:PRO:HD3	2.43	0.53
6:F:293:SER:HA	6:F:336:LEU:HD13	1.89	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.52	0.53
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.90	0.53
14:T:93:ILE:HG23	14:T:108:LEU:CD1	2.38	0.53
21:q:49:TYR:HB2	21:q:61:TRP:CE2	2.42	0.53
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.53
5:E:226:PRO:HD3	6:F:46:TYR:CZ	2.44	0.53
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
10:P:142:GLU:HA	10:P:146:VAL:HG12	1.90	0.53
21:q:31:ASN:HD21	30:q:202:PC1:H151	1.73	0.53
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.38	0.53
4:D:140:ASP:CB	4:D:147:ASN:HD21	2.07	0.53
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.53
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.73	0.53
10:P:363:SER:CB	16:W:51:HIS:CE1	2.84	0.53
18:Z:105:LYS:HD2	18:Z:105:LYS:N	2.24	0.53
2:B:182:ASP:OD1	2:B:183:ARG:N	2.41	0.53
4:D:92:HIS:HB2	4:D:458:PHE:HE2	1.73	0.53
4:D:172:VAL:HG21	4:D:310:VAL:HG23	1.90	0.53
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.53
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.09	0.53
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.53
8:H:17:MET:SD	8:H:225:MET:CB	2.96	0.53
8:H:180:PRO:CD	18:Z:43:LEU:HD21	2.39	0.53
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.53
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:17:GLU:HG3	17:X:64:ASN:HD22	1.73	0.53
3:C:101:ASP:OD1	15:V:86:LYS:HE3	2.08	0.53
5:E:118:TYR:HE1	6:F:206:CYS:SG	2.31	0.53
7:G:617:ARG:HH12	16:W:129:HIS:N	2.06	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.39	0.53
9:I:54:THR:HG22	20:b:13:TRP:HE1	1.74	0.53
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.44	0.53
10:P:353:LEU:HA	10:P:356:HIS:HD2	1.74	0.53
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.53
16:W:42:TRP:CZ2	16:W:93:LEU:CA	2.91	0.53
17:X:70:PHE:O	17:X:74:ILE:HG13	2.09	0.53
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.44	0.53
2:B:116:ARG:O	8:H:39:ILE:HG22	2.08	0.53
3:C:234:LEU:O	4:D:387:GLU:HG3	2.08	0.53
4:D:136:PHE:HZ	4:D:422:CYS:HG	1.56	0.53
4:D:390:GLN:HG3	4:D:415:GLY:O	2.09	0.53
5:E:177:GLY:O	5:E:178:ALA:HB3	2.08	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53
16:W:42:TRP:CD2	16:W:93:LEU:HD13	2.44	0.53
18:Z:140:PHE:HD1	19:a:45:TRP:HB2	1.72	0.53
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.90	0.53
6:F:86:ARG:NH1	6:F:339:PHE:HB2	2.24	0.53
7:G:364:ASP:C	7:G:364:ASP:OD1	2.52	0.53
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.53
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.42	0.53
1:A:112:GLU:C	1:A:113:TRP:CG	2.86	0.53
2:B:199:GLU:HB2	9:I:173:PHE:HE2	1.74	0.53
4:D:289:SER:HA	4:D:293:LEU:HD13	1.91	0.53
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.53
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.53
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.53
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.39	0.53
18:Z:59:ARG:HH21	20:b:84:LEU:HB3	1.72	0.53
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.91	0.53
3:C:51:ASP:OD1	3:C:54:HIS:HB3	2.08	0.53
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.27	0.53
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.53
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.53
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.90	0.53
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.53
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.91	0.53
10:P:336:GLU:CG	10:P:342:PRO:HD3	2.38	0.53
19:a:42:GLN:O	19:a:43:TYR:C	2.50	0.53
21:q:44:TYR:OH	21:q:112:ASN:CG	2.52	0.53
22:r:6:ARG:O	22:r:10:LYS:HG3	2.09	0.53
3:C:63:TYR:HE1	15:V:47:TYR:CG	2.26	0.52
7:G:275:PRO:HB2	11:Q:86:ASN:ND2	2.24	0.52
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.52
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.91	0.52
12:R:43:TYR:O	12:R:46:VAL:HG13	2.09	0.52
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.09	0.52
1:A:103:ALA:O	1:A:107:THR:HG23	2.09	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
8:H:153:VAL:HG11	8:H:241:ILE:HG23	1.90	0.52
8:H:311:THR:O	18:Z:51:MET:HG3	2.08	0.52
11:Q:53:ILE:O	16:W:20:VAL:HG22	2.09	0.52
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.52
16:W:23:ILE:HG23	16:W:24:PHE:H	1.74	0.52
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
7:G:161:GLU:O	7:G:163:LYS:HE3	2.10	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
8:H:287:HIS:HE1	24:H:402:3PE:HN1	1.55	0.52
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.52
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.52
2:B:163:SER:HA	2:B:166:ASN:OD1	2.10	0.52
2:B:170:TYR:CB	9:I:153:ILE:HG21	2.36	0.52
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.07	0.52
4:D:348:LEU:O	18:Z:11:PRO:HB3	2.09	0.52
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.42	0.52
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.74	0.52
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.52
10:P:265:PHE:HD1	10:P:334:GLY:HA3	1.74	0.52
12:R:40:GLU:HA	12:R:45:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:129:THR:HB	18:Z:132:GLU:HG3	1.91	0.52
2:B:115:ASP:OD1	8:H:25:ARG:NH2	2.42	0.52
3:C:63:TYR:HB2	22:r:95:VAL:CG2	2.40	0.52
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.10	0.52
4:D:139:LEU:O	4:D:459:GLY:C	2.53	0.52
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52
8:H:65:THR:HG22	10:P:359:TYR:CD1	2.41	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.52
17:X:57:LEU:HG	17:X:61:LYS:HZ1	1.74	0.52
19:a:4:GLU:O	19:a:7:PRO:HD2	2.09	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52
3:C:64:VAL:HG11	3:C:85:ILE:CD1	2.32	0.52
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.28	0.52
6:F:109:ARG:HB3	6:F:238:CYS:SG	2.50	0.52
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.52
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.52
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.73	0.52
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.52
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.52
2:B:199:GLU:HB2	9:I:173:PHE:CE2	2.44	0.52
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.61	0.52
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.91	0.52
6:F:414:GLU:OE2	22:r:51:ASN:N	2.29	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
10:P:236:VAL:HG11	10:P:270:ARG:HH21	1.75	0.52
14:T:90:TYR:CD2	14:T:93:ILE:HG12	2.38	0.52
14:T:130:ILE:HG23	14:T:147:TYR:HE2	1.75	0.52
18:Z:126:GLY:HA2	18:Z:133:MET:HE2	1.91	0.52
2:B:95:PHE:O	4:D:93:GLY:HA2	2.09	0.52
2:B:161:MET:HE2	2:B:196:PRO:HD2	1.92	0.52
4:D:193:ASP:O	8:H:205:SER:OG	2.27	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
20:b:23:PHE:CD2	24:b:201:3PE:H281	2.40	0.52
21:q:138:VAL:HG23	21:q:139:PRO:HD2	1.92	0.52
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.90	0.52
2:B:101:ALA:O	2:B:104:MET:HG2	2.10	0.52
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.52
5:E:179:CYS:HA	27:E:301:FES:S1	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:192:ASP:HB3	23:s:57:LEU:CD1	2.38	0.52
6:F:288:VAL:HG11	6:F:303:HIS:CB	2.40	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.52
7:G:81:GLU:O	7:G:103:LEU:HB2	2.09	0.52
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.52
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.91	0.52
10:P:305:PHE:HB2	10:P:314:THR:HG22	1.92	0.52
12:R:50:ASP:O	12:R:51:ARG:HG3	2.10	0.52
17:X:137:LEU:HA	20:b:58:ARG:HH22	1.75	0.52
20:b:48:ALA:O	20:b:49:THR:C	2.53	0.52
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.52
2:B:202:LEU:HD23	9:I:86:TYR:CD1	2.45	0.51
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.25	0.51
4:D:303:ARG:HH11	4:D:401:GLU:HG2	1.75	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.46	0.51
6:F:391:TRP:HH2	7:G:118:GLU:OE2	1.92	0.51
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.51
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.92	0.51
21:q:101:ASN:OD1	21:q:101:ASN:O	2.28	0.51
2:B:95:PHE:HE1	2:B:131:MET:HE2	1.75	0.51
4:D:97:LEU:HD23	4:D:111:PRO:HB3	1.91	0.51
5:E:129:TYR:HE2	5:E:167:LEU:HG	1.74	0.51
5:E:196:THR:O	5:E:197:PRO:C	2.54	0.51
8:H:99:ASN:OD1	19:a:40:ARG:HG3	2.11	0.51
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.51
10:P:45:LYS:HB2	11:Q:118:ALA:CB	2.41	0.51
14:T:104:PHE:CE1	14:T:115:GLN:CG	2.94	0.51
16:W:42:TRP:CE3	16:W:93:LEU:HD13	2.45	0.51
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.51
4:D:235:ASP:HA	4:D:356:ILE:HG21	1.92	0.51
6:F:288:VAL:HG11	6:F:303:HIS:HB3	1.91	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
8:H:200:LEU:O	8:H:201:THR:C	2.52	0.51
10:P:157:LYS:O	10:P:158:GLU:C	2.53	0.51
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.51
18:Z:69:ILE:CG2	20:b:54:PRO:HD3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:ILE:HD12	2:B:207:GLN:HB3	1.93	0.51
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.92	0.51
4:D:172:VAL:HG21	4:D:310:VAL:CG2	2.40	0.51
4:D:179:ARG:HG2	4:D:183:HIS:CD2	2.46	0.51
7:G:614:GLY:HA2	10:P:41:ILE:HG21	1.91	0.51
9:I:88:PHE:O	21:q:62:VAL:HG12	2.10	0.51
9:I:152:CYS:SG	25:I:302:SF4:S3	3.09	0.51
10:P:315:THR:HB	10:P:318:LYS:HB2	1.92	0.51
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.41	0.51
18:Z:86:ILE:HA	18:Z:128:ARG:HH21	1.74	0.51
4:D:202:TRP:CH2	4:D:261:MET:HG3	2.46	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
6:F:267:ARG:HD3	6:F:338:ASP:OD2	2.10	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.93	0.51
9:I:210:LEU:HD22	22:r:39:PRO:HD2	1.92	0.51
10:P:272:LEU:HG	10:P:375:VAL:CG2	2.26	0.51
14:T:141:PRO:HD2	14:T:142:GLN:H	1.75	0.51
21:q:8:LYS:O	21:q:12:GLN:HG2	2.10	0.51
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.24	0.51
7:G:33:GLU:HB3	7:G:98:LYS:HE2	1.92	0.51
8:H:145:THR:HG22	8:H:289:LEU:HD11	1.91	0.51
8:H:222:LEU:O	8:H:223:PHE:C	2.51	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.51
16:W:65:LYS:HE3	16:W:69:MET:HE2	1.92	0.51
18:Z:143:TYR:HD1	18:Z:144:THR:N	2.04	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
1:A:81:THR:O	20:b:46:ASN:ND2	2.44	0.51
4:D:320:ILE:CD1	9:I:36:TYR:CD2	2.93	0.51
5:E:68:ASN:ND2	23:s:49:ASN:HD21	2.07	0.51
5:E:183:PRO:HG2	5:E:194:ASP:HA	1.92	0.51
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.51
7:G:140:GLN:HG3	7:G:141:ASP:OD1	2.10	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.10	0.51
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.41	0.51
8:H:17:MET:CE	8:H:225:MET:CB	2.88	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.92	0.51
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:MET:HE3	2:B:119:VAL:CG1	2.40	0.51
5:E:180:VAL:HG11	5:E:224:CYS:HB3	1.92	0.51
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.51
6:F:238:CYS:O	6:F:239:PRO:C	2.51	0.51
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.76	0.51
7:G:239:THR:HA	9:I:132:ALA:O	2.11	0.51
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.51
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.51
4:D:159:LEU:CD2	4:D:391:VAL:HG12	2.41	0.51
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.40	0.51
6:F:42:PHE:CE2	6:F:275:LEU:HD11	2.46	0.51
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:90:PRO:HG2	8:H:240:ILE:HG21	1.92	0.51
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.51
10:P:234:LYS:HG2	10:P:234:LYS:O	2.10	0.51
12:R:43:TYR:C	12:R:45:ARG:N	2.69	0.51
18:Z:111:PHE:CE1	18:Z:117:VAL:HG21	2.45	0.51
21:q:65:THR:OG1	21:q:66:THR:N	2.44	0.51
4:D:174:PHE:CZ	4:D:240:LEU:HD21	2.45	0.51
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.92	0.51
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.46	0.51
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.51
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.46	0.51
17:X:56:CYS:HA	17:X:135:ARG:HH12	1.76	0.51
18:Z:72:MET:SD	20:b:53:TYR:HB2	2.51	0.51
20:b:11:ASN:OD1	20:b:12:ALA:N	2.44	0.51
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.93	0.50
4:D:274:ASP:H	4:D:325:ASP:CB	2.24	0.50
6:F:109:ARG:HH21	6:F:239:PRO:HG3	1.75	0.50
6:F:225:LEU:HB3	6:F:227:PRO:CD	2.37	0.50
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.42	0.50
6:F:279:SER:O	6:F:355:ILE:HA	2.11	0.50
6:F:280:GLY:O	6:F:356:VAL:HB	2.11	0.50
6:F:315:LEU:HA	6:F:359:ARG:CZ	2.42	0.50
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.11	0.50
16:W:103:ARG:O	16:W:104:THR:C	2.54	0.50
18:Z:28:ARG:HG3	18:Z:28:ARG:O	2.11	0.50
4:D:179:ARG:NH2	4:D:303:ARG:HD3	2.25	0.50
7:G:35:PHE:O	7:G:101:ASN:HA	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.50
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.50
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.50
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.50
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.50
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.50
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.50
10:P:65:LEU:HD23	10:P:129:LEU:HD22	1.93	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
2:B:95:PHE:HB3	2:B:97:LEU:HD13	1.92	0.50
6:F:78:GLY:O	6:F:82:THR:HG23	2.12	0.50
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.50
7:G:643:ARG:O	7:G:644:ASN:C	2.55	0.50
10:P:300:TRP:O	10:P:304:LEU:HG	2.11	0.50
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.50
17:X:38:LYS:O	17:X:42:GLU:HG3	2.11	0.50
4:D:263:THR:HG22	4:D:263:THR:O	2.11	0.50
5:E:120:MET:HE2	6:F:201:ALA:HA	1.94	0.50
5:E:235:GLU:HB2	5:E:236:PRO:HD2	1.93	0.50
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
8:H:8:THR:O	8:H:12:PRO:HG2	2.11	0.50
8:H:85:LEU:CD2	8:H:108:THR:HB	2.41	0.50
9:I:58:ALA:HB2	18:Z:36:PHE:CZ	2.45	0.50
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.91	0.50
10:P:150:ARG:O	10:P:151:ALA:C	2.54	0.50
12:R:38:TYR:CE1	12:R:44:ARG:HD2	2.47	0.50
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.50
15:V:44:TYR:O	15:V:48:THR:HG22	2.11	0.50
1:A:113:TRP:CH2	8:H:287:HIS:HD2	2.29	0.50
4:D:189:THR:CB	26:D:501:UQ1:CM2	2.64	0.50
4:D:462:ASP:O	4:D:463:ARG:C	2.54	0.50
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.50
7:G:277:MET:HE1	11:Q:153:PRO:HD3	1.94	0.50
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.50
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.50
7:G:621:LYS:HZ3	16:W:131:PRO:HD3	1.76	0.50
10:P:209:ARG:N	10:P:352:VAL:HG22	2.26	0.50
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.93	0.50
22:r:48:LYS:HB2	22:r:52:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TRP:HD1	1:A:111:LEU:HD12	1.76	0.50
4:D:255:ILE:HG22	4:D:338:ARG:NH2	2.26	0.50
5:E:180:VAL:HG13	5:E:181:ASN:H	1.77	0.50
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.47	0.50
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.50
18:Z:66:GLU:HA	18:Z:69:ILE:HG12	1.93	0.50
19:a:14:VAL:O	19:a:18:ILE:HG13	2.10	0.50
22:r:48:LYS:O	22:r:49:LEU:HB2	2.12	0.50
2:B:104:MET:HE1	2:B:132:ILE:HD12	1.92	0.50
6:F:270:ASN:HD22	6:F:338:ASP:HB2	1.76	0.50
6:F:297:LYS:CD	6:F:333:GLU:HB2	2.42	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
10:P:205:ASP:OD1	10:P:205:ASP:O	2.30	0.50
10:P:207:PHE:HE1	10:P:214:LEU:HD22	1.76	0.50
14:T:82:ARG:HD2	14:T:125:GLU:OE2	2.10	0.50
17:X:57:LEU:HD12	17:X:57:LEU:O	2.12	0.50
3:C:104:ASN:O	22:r:97:PRO:HD3	2.12	0.50
3:C:210:ARG:CD	10:P:48:ARG:HD3	2.42	0.50
4:D:333:ARG:HH12	4:D:453:THR:HA	1.77	0.50
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
7:G:617:ARG:NH1	16:W:129:HIS:N	2.60	0.50
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50
14:T:97:LYS:NZ	14:T:107:ASP:C	2.69	0.50
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.50
6:F:42:PHE:HE2	6:F:275:LEU:HD11	1.75	0.50
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.50
8:H:173:TRP:CZ2	8:H:262:GLU:OE2	2.65	0.50
9:I:36:TYR:HE2	9:I:38:TYR:CZ	2.29	0.50
17:X:70:PHE:CE2	17:X:74:ILE:HD11	2.46	0.50
17:X:78:CYS:C	17:X:81:PRO:HD2	2.36	0.50
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.50
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.50
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.49
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.49
4:D:133:LEU:HB3	4:D:134:PRO:HD3	1.94	0.49
4:D:163:PRO:HG2	4:D:168:GLN:NE2	2.27	0.49
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.49
4:D:399:ALA:HB1	4:D:406:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:247:GLY:O	6:F:64:LYS:HE2	2.12	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.47	0.49
6:F:297:LYS:HB2	6:F:333:GLU:HA	1.94	0.49
6:F:297:LYS:HB2	6:F:333:GLU:HB3	1.90	0.49
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.36	0.49
9:I:181:GLU:HB2	21:q:126:PRO:CG	2.41	0.49
10:P:135:GLU:CG	10:P:140:ASP:HA	2.41	0.49
10:P:172:ALA:H	10:P:202:ARG:HH21	1.59	0.49
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.49
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.94	0.49
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.49
2:B:166:ASN:CB	2:B:190:TYR:HD2	2.24	0.49
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.47	0.49
6:F:204:TYR:CE1	28:F:501:FMN:H6	2.47	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.49
8:H:17:MET:HE1	8:H:225:MET:CB	2.42	0.49
10:P:238:GLN:HB2	10:P:270:ARG:HG2	1.94	0.49
10:P:375:VAL:C	10:P:377:TYR:H	2.19	0.49
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.49
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.49
18:Z:90:ASN:O	18:Z:94:GLU:HB2	2.12	0.49
21:q:55:PHE:CD2	22:r:26:LEU:HD22	2.47	0.49
21:q:85:GLU:HG2	21:q:98:PRO:HB3	1.94	0.49
2:B:95:PHE:CD2	2:B:141:MET:HE3	2.47	0.49
5:E:39:VAL:CG2	7:G:205:GLN:HE22	2.23	0.49
8:H:127:TYR:HE1	8:H:207:LEU:HD23	1.75	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
10:P:275:HIS:CE1	10:P:373:LYS:HG2	2.47	0.49
20:b:23:PHE:CE2	24:b:201:3PE:H252	2.47	0.49
2:B:222:TYR:O	10:P:137:ARG:NH1	2.45	0.49
3:C:97:THR:O	15:V:90:LEU:HD12	2.12	0.49
3:C:124:ARG:HD2	11:Q:140:LYS:HZ1	1.78	0.49
4:D:209:LYS:HG2	22:r:27:ARG:NH2	2.27	0.49
4:D:324:GLY:O	4:D:329:ARG:NH1	2.45	0.49
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.93	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
7:G:611:THR:CG2	11:Q:105:GLU:HA	2.22	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
9:I:54:THR:CG2	20:b:13:TRP:HE1	2.26	0.49
10:P:235:THR:O	10:P:236:VAL:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.49
1:A:54:LYS:O	1:A:58:VAL:HG23	2.12	0.49
3:C:73:GLN:NE2	15:V:112:TRP:HE1	2.09	0.49
3:C:75:VAL:HG22	3:C:85:ILE:HG23	1.94	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
7:G:632:ILE:O	7:G:632:ILE:CG1	2.60	0.49
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.49
10:P:197:GLU:HB3	10:P:259:VAL:HG23	1.93	0.49
2:B:170:TYR:O	2:B:171:TYR:CB	2.60	0.49
6:F:278:ILE:HG22	6:F:354:VAL:HB	1.94	0.49
6:F:297:LYS:HE2	6:F:333:GLU:HB2	1.94	0.49
7:G:643:ARG:O	7:G:646:LEU:N	2.46	0.49
10:P:318:LYS:O	10:P:322:ILE:HG13	2.13	0.49
18:Z:58:ARG:CB	20:b:45:ILE:HD11	2.42	0.49
22:r:45:PRO:O	22:r:46:SER:HB2	2.13	0.49
5:E:131:ILE:HA	5:E:187:ILE:HA	1.93	0.49
6:F:117:ALA:HB1	6:F:131:MET:SD	2.53	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:240:ALA:HA	9:I:117:LYS:HZ3	1.77	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.93	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
2:B:115:ASP:O	2:B:116:ARG:C	2.55	0.49
3:C:121:ARG:NH2	15:V:114:TRP:HA	2.28	0.49
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.95	0.49
4:D:378:LEU:HD21	7:G:129:PRO:HD2	1.95	0.49
6:F:170:GLN:HB3	23:s:48:LEU:HD22	1.95	0.49
9:I:79:ARG:CZ	22:r:20:LEU:HD22	2.43	0.49
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.94	0.49
10:P:64:PHE:CZ	10:P:211:ASP:HB3	2.47	0.49
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.94	0.49
17:X:44:MET:O	17:X:48:TRP:CD1	2.66	0.49
21:q:74:PHE:HD2	21:q:75:TRP:CD2	2.31	0.49
4:D:260:GLU:OE2	9:I:68:ARG:HG2	2.13	0.49
5:E:77:ALA:C	5:E:80:PRO:HD2	2.38	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.94	0.49
6:F:37:ASP:HA	6:F:40:ARG:HD2	1.94	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.49
7:G:240:ALA:HA	9:I:117:LYS:NZ	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
8:H:9:LEU:HD11	8:H:86:TRP:HB3	1.93	0.49
10:P:315:THR:HB	10:P:318:LYS:H	1.78	0.49
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.49
12:R:81:GLY:HA2	12:R:88:HIS:CD2	2.47	0.49
2:B:144:ALA:O	2:B:145:LEU:C	2.55	0.49
4:D:199:PRO:HG3	4:D:262:LEU:HD11	1.95	0.49
6:F:233:VAL:CG1	11:Q:164:PHE:HB2	2.43	0.49
6:F:295:PRO:HA	6:F:336:LEU:CB	2.43	0.49
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.49
8:H:26:LYS:HB3	19:a:5:ILE:HG22	1.94	0.49
8:H:200:LEU:CD2	8:H:285:LEU:HD13	2.43	0.49
10:P:59:PHE:CB	10:P:130:ILE:HD11	2.42	0.49
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.94	0.49
17:X:47:ARG:CZ	17:X:53:PRO:HG3	2.42	0.49
21:q:48:TYR:OH	21:q:83:PRO:HD2	2.13	0.49
2:B:68:ARG:NH1	2:B:70:ARG:HB3	2.28	0.48
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.48
3:C:210:ARG:HD2	10:P:48:ARG:HD3	1.94	0.48
4:D:203:MET:HE2	4:D:258:VAL:CG1	2.43	0.48
4:D:274:ASP:H	4:D:325:ASP:HB2	1.78	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.48
7:G:612:PRO:HG2	16:W:129:HIS:CD2	2.48	0.48
8:H:196:ALA:HA	8:H:199:ASP:HB2	1.95	0.48
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.48
10:P:278:LYS:HB3	10:P:288:PHE:CE2	2.48	0.48
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.48
10:P:318:LYS:HA	10:P:321:ARG:HH12	1.78	0.48
17:X:53:PRO:CD	18:Z:116:TRP:CD1	2.96	0.48
22:r:7:VAL:HG13	22:r:8:ILE:N	2.28	0.48
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.74	0.48
7:G:614:GLY:CA	10:P:41:ILE:HG21	2.43	0.48
7:G:617:ARG:NH1	16:W:129:HIS:HA	2.25	0.48
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.47	0.48
9:I:116:CYS:O	9:I:117:LYS:HB2	2.12	0.48
9:I:210:LEU:HD23	22:r:39:PRO:O	2.13	0.48
11:Q:111:LEU:HA	12:R:47:ARG:NH1	2.29	0.48
14:T:93:ILE:HG23	14:T:108:LEU:HD11	1.95	0.48
16:W:46:VAL:N	16:W:47:PRO:HD2	2.29	0.48
17:X:69:ASN:O	17:X:70:PHE:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:226:LYS:O	6:F:227:PRO:C	2.56	0.48
7:G:49:VAL:HG13	7:G:102:ILE:HD13	1.94	0.48
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.48
8:H:138:GLN:HG3	8:H:285:LEU:HD21	1.94	0.48
10:P:375:VAL:C	10:P:377:TYR:N	2.69	0.48
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.48
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.48
3:C:203:LEU:HD21	4:D:123:LEU:HD23	1.93	0.48
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.48
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.78	0.48
6:F:394:LYS:HB2	7:G:155:GLU:HG2	1.95	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
8:H:85:LEU:HD23	8:H:105:ILE:HA	1.93	0.48
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.48
9:I:105:ARG:HH12	12:R:58:ASN:HB2	1.78	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
10:P:328:MET:HE1	10:P:377:TYR:C	2.39	0.48
15:V:35:LEU:HD13	15:V:48:THR:HG23	1.95	0.48
21:q:56:PHE:O	21:q:59:HIS:CD2	2.67	0.48
34:q:201:CDL:OB9	34:q:201:CDL:H311	2.13	0.48
1:A:65:PHE:CZ	8:H:294:LEU:HD21	2.49	0.48
2:B:97:LEU:HD21	2:B:141:MET:HG2	1.96	0.48
5:E:45:GLU:CD	5:E:45:GLU:H	2.21	0.48
6:F:261:TRP:CE2	6:F:265:PHE:HE2	2.31	0.48
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.48
7:G:638:THR:O	7:G:639:LEU:C	2.56	0.48
9:I:107:PRO:HG3	21:q:106:ARG:HH11	1.75	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.95	0.48
19:a:37:ARG:CB	19:a:48:MET:HE2	2.43	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
21:q:64:TYR:CD2	21:q:81:MET:HB2	2.48	0.48
3:C:98:PHE:HB2	15:V:94:MET:HE3	1.96	0.48
5:E:147:ILE:O	5:E:151:LEU:HD13	2.14	0.48
6:F:106:SER:HB2	6:F:111:LYS:HZ2	1.79	0.48
7:G:33:GLU:OE2	7:G:40:SER:HA	2.14	0.48
7:G:572:HIS:HB2	7:G:699:SER:OG	2.13	0.48
8:H:196:ALA:C	8:H:198:PHE:N	2.70	0.48
8:H:199:ASP:HB3	8:H:279:ARG:HD2	1.95	0.48
8:H:316:PRO:HA	18:Z:58:ARG:NH1	2.22	0.48
9:I:72:MET:CE	22:r:16:SER:HB2	2.43	0.48
14:T:93:ILE:HD13	14:T:108:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:80:GLU:O	17:X:81:PRO:C	2.55	0.48
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.48	0.48
1:A:50:PRO:HA	4:D:80:MET:HE2	1.96	0.48
2:B:170:TYR:O	2:B:171:TYR:HB2	2.14	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
5:E:142:ARG:HG3	5:E:182:ALA:CB	2.44	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
9:I:35:THR:CG2	22:r:107:SER:HA	2.44	0.48
9:I:89:GLU:OE1	21:q:58:ARG:HD2	2.14	0.48
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.43	0.48
16:W:42:TRP:O	16:W:46:VAL:HG23	2.14	0.48
16:W:87:ILE:O	16:W:91:MET:HG3	2.12	0.48
18:Z:58:ARG:NH2	20:b:46:ASN:HA	2.29	0.48
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.48	0.48
2:B:112:TYR:CE1	9:I:84:ILE:HD11	2.48	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.14	0.48
8:H:17:MET:SD	8:H:225:MET:HA	2.54	0.48
10:P:81:ILE:HD11	12:R:46:VAL:HG11	1.96	0.48
18:Z:114:THR:O	18:Z:114:THR:CG2	2.60	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
5:E:109:MET:HE2	7:G:196:GLY:HA3	1.96	0.48
6:F:102:MET:CG	6:F:149:MET:HB2	2.43	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
7:G:140:GLN:HG3	7:G:141:ASP:N	2.28	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
8:H:200:LEU:CD2	8:H:282:TYR:HA	2.38	0.48
9:I:123:CYS:SG	25:I:302:SF4:S3	3.12	0.48
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.14	0.48
12:R:60:ALA:O	12:R:61:ILE:C	2.56	0.48
13:S:27:SER:H	13:S:34:ARG:HH22	1.62	0.48
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.48
6:F:50:ASP:CG	6:F:52:ARG:HB2	2.39	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.95	0.48
16:W:120:ASP:OD1	16:W:121:PHE:N	2.46	0.48
17:X:80:GLU:HB3	17:X:81:PRO:HD3	1.96	0.48
4:D:300:TRP:HE1	4:D:302:LEU:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:293:SER:CA	6:F:338:ASP:HB3	2.42	0.47
6:F:297:LYS:HB2	6:F:333:GLU:CA	2.44	0.47
8:H:3:PHE:O	8:H:4:ILE:C	2.58	0.47
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.47
22:r:32:ALA:HB1	22:r:36:GLN:HE21	1.78	0.47
22:r:54:TYR:HA	22:r:57:ARG:HG2	1.96	0.47
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.79	0.47
4:D:142:VAL:HG11	4:D:185:MET:CG	2.44	0.47
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.47
6:F:261:TRP:CE2	6:F:265:PHE:CE2	3.02	0.47
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.47
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.47
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.47
8:H:187:ILE:CD1	24:H:402:3PE:H242	2.44	0.47
9:I:54:THR:HA	20:b:13:TRP:HE1	1.79	0.47
10:P:335:LEU:O	10:P:336:GLU:HB2	2.14	0.47
12:R:46:VAL:HA	12:R:49:VAL:HG23	1.96	0.47
14:T:100:VAL:O	14:T:141:PRO:HD2	2.15	0.47
14:T:104:PHE:CD1	14:T:110:LEU:CB	2.94	0.47
18:Z:129:THR:HB	18:Z:132:GLU:CG	2.43	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.47
1:A:113:TRP:CH2	8:H:287:HIS:CD2	3.02	0.47
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.28	0.47
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
10:P:311:GLU:O	10:P:312:PRO:C	2.57	0.47
13:S:50:ASN:O	13:S:51:LEU:C	2.57	0.47
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.39	0.47
5:E:81:VAL:HG21	5:E:104:LEU:HD21	1.95	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.96	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.96	0.47
10:P:170:LEU:HG	10:P:171:ASN:N	2.28	0.47
10:P:237:LYS:HZ2	10:P:322:ILE:HG23	1.79	0.47
2:B:174:SER:HA	3:C:203:LEU:CD2	2.45	0.47
3:C:221:GLU:OE1	16:W:114:GLU:HB2	2.14	0.47
4:D:240:LEU:HG	4:D:244:ILE:HD11	1.96	0.47
6:F:61:ASP:O	6:F:140:GLU:OE1	2.32	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:150:ARG:NE	10:P:190:GLU:HG2	2.27	0.47
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.47
17:X:137:LEU:HA	20:b:58:ARG:NH2	2.30	0.47
22:r:25:GLN:H	22:r:25:GLN:CD	2.21	0.47
1:A:106:TRP:HZ3	20:b:19:LEU:HD21	1.78	0.47
4:D:185:MET:SD	4:D:204:PHE:HZ	2.37	0.47
4:D:362:LYS:HG3	22:r:54:TYR:CZ	2.50	0.47
26:D:501:UQ1:O1	26:D:501:UQ1:C8	2.50	0.47
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.45	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:217:GLU:CD	6:F:224:ARG:HH22	2.23	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:341:ILE:HG13	7:G:545:LEU:HD11	1.95	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.74	0.47
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.47
7:G:642:VAL:O	7:G:645:ARG:HB3	2.14	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
11:Q:129:SER:HB2	15:V:116:ILE:HD12	1.97	0.47
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.29	0.47
16:W:46:VAL:O	16:W:50:VAL:HG23	2.14	0.47
23:s:55:PHE:O	23:s:56:ARG:C	2.57	0.47
2:B:75:VAL:HG13	2:B:218:LEU:HB3	1.95	0.47
3:C:66:GLU:O	3:C:69:PRO:HD3	2.14	0.47
3:C:67:ILE:CD1	15:V:47:TYR:HD2	2.24	0.47
4:D:320:ILE:HD11	9:I:36:TYR:CE2	2.49	0.47
5:E:114:VAL:HG13	5:E:118:TYR:CE2	2.50	0.47
5:E:180:VAL:CG1	5:E:181:ASN:N	2.78	0.47
5:E:190:ASN:HB3	5:E:215:PRO:HB3	1.96	0.47
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.47
6:F:254:ILE:O	6:F:258:GLY:N	2.48	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.47	0.47
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.47
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.47
7:G:106:SER:O	7:G:107:GLU:C	2.57	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
8:H:94:PRO:CG	8:H:97:ASN:HB3	2.39	0.47
8:H:142:TYR:HE1	8:H:285:LEU:CD2	2.27	0.47
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:212:ARG:O	10:P:213:PHE:C	2.55	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
13:S:48:HIS:HE1	13:S:95:LEU:CD2	2.25	0.47
13:S:58:CYS:HB2	13:S:61:VAL:CG1	2.43	0.47
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.49	0.47
14:T:134:ASP:O	14:T:138:LEU:HG	2.14	0.47
15:V:116:ILE:HG23	15:V:116:ILE:O	2.15	0.47
16:W:32:LYS:O	16:W:36:ARG:HG3	2.15	0.47
16:W:97:ILE:HG13	16:W:98:LYS:H	1.78	0.47
17:X:39:THR:CG2	17:X:40:ASN:N	2.77	0.47
17:X:82:PHE:HB2	17:X:107:PHE:CE1	2.50	0.47
18:Z:97:ILE:HG13	18:Z:98:MET:HE3	1.95	0.47
18:Z:125:TYR:HA	18:Z:128:ARG:HB2	1.95	0.47
19:a:22:SER:O	19:a:23:THR:C	2.57	0.47
3:C:203:LEU:CD2	4:D:123:LEU:HD21	2.32	0.47
5:E:153:ARG:HG3	5:E:154:LYS:N	2.29	0.47
5:E:153:ARG:NH2	5:E:154:LYS:HE2	2.29	0.47
6:F:297:LYS:HB2	6:F:333:GLU:HB2	1.94	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:292:ASN:O	20:b:18:VAL:HG11	2.14	0.47
10:P:272:LEU:CG	10:P:375:VAL:HG21	2.25	0.47
17:X:25:LEU:O	17:X:29:ALA:N	2.48	0.47
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.15	0.47
18:Z:58:ARG:HH21	20:b:46:ASN:HA	1.78	0.47
1:A:65:PHE:O	1:A:69:ILE:HG13	2.14	0.47
2:B:98:ALA:HB3	2:B:135:GLY:HA2	1.96	0.47
4:D:159:LEU:HD22	22:r:60:ARG:HG3	1.97	0.47
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
9:I:54:THR:HA	20:b:13:TRP:NE1	2.30	0.47
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.96	0.47
10:P:245:VAL:HA	10:P:265:PHE:CD2	2.49	0.47
10:P:318:LYS:O	10:P:319:VAL:C	2.58	0.47
10:P:333:PRO:HB2	10:P:337:ASP:CB	2.36	0.47
19:a:2:TRP:O	19:a:5:ILE:HG12	2.14	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
9:I:93:LEU:O	21:q:93:MET:CG	2.63	0.47
10:P:55:VAL:HG12	10:P:123:SER:HA	1.96	0.47
10:P:192:ARG:HH21	10:P:200:ILE:HG12	1.80	0.47
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:276:LEU:O	10:P:280:ILE:HG13	2.15	0.47
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.44	0.47
13:S:27:SER:O	13:S:34:ARG:NH2	2.48	0.47
13:S:40:ARG:HH12	13:S:84:ALA:HB1	1.79	0.47
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.50	0.47
16:W:94:GLN:HG3	16:W:98:LYS:NZ	2.29	0.47
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.47
1:A:104:TYR:CZ	1:A:108:GLN:HG3	2.50	0.46
6:F:424:ILE:HG13	7:G:76:ARG:HD3	1.97	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.46
8:H:186:PHE:CZ	8:H:270:PHE:HD1	2.32	0.46
8:H:210:GLY:CA	8:H:213:VAL:HG23	2.46	0.46
9:I:188:GLU:OE2	12:R:33:HIS:NE2	2.47	0.46
10:P:76:MET:HE1	10:P:254:LYS:CE	2.45	0.46
16:W:97:ILE:CG1	16:W:98:LYS:N	2.75	0.46
19:a:49:GLU:CD	19:a:52:ARG:HH11	2.22	0.46
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.43	0.46
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.46
7:G:75:CYS:SG	27:G:803:FES:S1	3.13	0.46
7:G:639:LEU:O	7:G:640:ASP:C	2.58	0.46
10:P:209:ARG:O	10:P:210:GLU:HB2	2.15	0.46
17:X:41:LYS:O	17:X:42:GLU:C	2.59	0.46
21:q:137:TRP:CH2	21:q:140:PRO:HD3	2.51	0.46
22:r:50:SER:O	22:r:51:ASN:C	2.58	0.46
5:E:163:THR:HB	5:E:164:PRO:HD2	1.97	0.46
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.97	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
7:G:544:MET:HE3	7:G:565:PHE:CE2	2.42	0.46
8:H:312:ALA:HB2	20:b:41:TYR:HB2	1.98	0.46
10:P:207:PHE:CD2	10:P:241:TYR:HD1	2.33	0.46
12:R:38:TYR:OH	12:R:47:ARG:NH2	2.48	0.46
15:V:22:GLU:O	15:V:26:ILE:HG12	2.15	0.46
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.44	0.46
3:C:73:GLN:HG2	15:V:103:LEU:HD21	1.96	0.46
4:D:92:HIS:HB2	4:D:458:PHE:CE2	2.49	0.46
6:F:122:PRO:HG3	6:F:373:PHE:CZ	2.50	0.46
17:X:35:GLN:HG3	17:X:70:PHE:HE1	1.80	0.46
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.81	0.46
23:s:52:LEU:HB3	23:s:56:ARG:HH11	1.81	0.46
2:B:100:CYS:HB2	2:B:134:ALA:CB	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
7:G:462:PHE:CD1	7:G:465:VAL:HB	2.50	0.46
10:P:331:ASP:O	10:P:332:LEU:C	2.59	0.46
15:V:72:LEU:CD1	15:V:72:LEU:C	2.89	0.46
16:W:50:VAL:HA	16:W:55:LEU:HD12	1.97	0.46
17:X:54:ARG:NH2	18:Z:116:TRP:HB2	2.31	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.59	0.46
21:q:117:VAL:HB	21:q:122:GLU:HB3	1.96	0.46
2:B:82:ILE:CA	8:H:57:MET:HE1	2.41	0.46
4:D:137:ASP:O	4:D:223:HIS:CE1	2.68	0.46
4:D:278:VAL:O	15:V:12:VAL:HG11	2.15	0.46
4:D:356:ILE:HD11	4:D:357:LYS:HE3	1.98	0.46
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.15	0.46
6:F:270:ASN:HD21	6:F:340:ASP:N	2.13	0.46
8:H:14:LEU:O	8:H:17:MET:HB3	2.15	0.46
2:B:194:CYS:CB	2:B:195:PRO:HD3	2.42	0.46
3:C:217:ARG:HH12	16:W:112:GLU:CB	2.27	0.46
4:D:139:LEU:HD13	4:D:424:ILE:HG21	1.98	0.46
6:F:50:ASP:OD2	6:F:52:ARG:HB2	2.15	0.46
6:F:224:ARG:HD3	11:Q:164:PHE:CE1	2.51	0.46
7:G:648:GLU:HG2	13:S:66:TRP:CZ2	2.50	0.46
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.46
8:H:89:LEU:CD1	8:H:233:LEU:CD1	2.77	0.46
10:P:288:PHE:CZ	10:P:290:PRO:HB3	2.51	0.46
12:R:38:TYR:CD2	12:R:48:PHE:HE2	2.33	0.46
17:X:46:CYS:HB3	17:X:56:CYS:SG	2.56	0.46
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.97	0.46
4:D:259:GLU:HB3	18:Z:25:LEU:HD21	1.97	0.46
6:F:77:LEU:O	6:F:81:LYS:HG2	2.16	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
6:F:318:ILE:HG22	6:F:326:LEU:CA	2.45	0.46
9:I:155:CYS:SG	25:I:302:SF4:S2	3.14	0.46
12:R:51:ARG:HD2	21:q:125:VAL:CG1	2.46	0.46
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.46
1:A:73:LEU:N	1:A:74:PRO:HD2	2.31	0.46
3:C:70:LYS:O	15:V:104:VAL:N	2.47	0.46
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.46
7:G:643:ARG:HA	7:G:646:LEU:HD12	1.98	0.46
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.46
8:H:200:LEU:HD12	8:H:201:THR:N	2.31	0.46
10:P:66:GLY:O	10:P:69:VAL:N	2.49	0.46
18:Z:36:PHE:O	18:Z:40:ILE:HG12	2.16	0.46
18:Z:54:ASN:HA	18:Z:57:ARG:HD3	1.96	0.46
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.28	0.46
2:B:166:ASN:O	2:B:166:ASN:CG	2.59	0.46
5:E:176:LEU:HD13	5:E:186:GLN:HB2	1.98	0.46
6:F:88:ARG:HB2	6:F:247:THR:OG1	2.16	0.46
6:F:93:PHE:O	6:F:94:PRO:C	2.58	0.46
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.46
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.50	0.46
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.81	0.46
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.46
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.97	0.46
15:V:50:GLN:HE22	22:r:93:LYS:HG3	1.80	0.46
17:X:5:VAL:CG1	17:X:7:LEU:HG	2.46	0.46
17:X:78:CYS:SG	17:X:114:LYS:HD2	2.56	0.46
18:Z:70:ALA:O	18:Z:73:PRO:HD2	2.16	0.46
19:a:58:ASN:HB2	19:a:61:TYR:CE2	2.51	0.46
21:q:59:HIS:HE1	21:q:60:ARG:NE	2.14	0.46
22:r:91:GLU:OE1	22:r:91:GLU:HA	2.15	0.46
6:F:120:GLY:O	6:F:121:GLU:C	2.59	0.45
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.99	0.45
7:G:301:ARG:HA	7:G:572:HIS:CD2	2.52	0.45
7:G:593:SER:O	7:G:643:ARG:NH2	2.46	0.45
9:I:178:GLU:OE2	21:q:119:ALA:HB2	2.15	0.45
10:P:157:LYS:O	10:P:160:GLY:N	2.49	0.45
10:P:220:TYR:HA	10:P:223:PHE:CD2	2.51	0.45
10:P:261:LYS:HB2	10:P:263:PHE:CE1	2.51	0.45
12:R:104:CYS:C	12:R:106:TYR:N	2.73	0.45
17:X:131:VAL:N	20:b:59:ASP:OD1	2.49	0.45
20:b:19:LEU:HD22	24:b:201:3PE:H221	1.98	0.45
20:b:28:LEU:O	20:b:32:MET:HG2	2.15	0.45
20:b:38:TYR:O	20:b:39:THR:C	2.58	0.45
20:b:45:ILE:N	20:b:80:TRP:HH2	2.14	0.45
4:D:194:ILE:HD12	4:D:268:TRP:CZ3	2.51	0.45
4:D:293:LEU:CD2	4:D:300:TRP:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:222:PHE:H	5:E:225:GLU:CD	2.24	0.45
6:F:261:TRP:CD2	6:F:265:PHE:HE2	2.34	0.45
7:G:165:ILE:O	7:G:213:MET:HA	2.16	0.45
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	0.45
8:H:137:ALA:HA	8:H:140:ILE:HG12	1.98	0.45
9:I:107:PRO:HB3	21:q:106:ARG:HD2	1.98	0.45
14:T:144:ILE:O	14:T:148:ILE:HG12	2.15	0.45
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.45
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.50	0.45
16:W:83:ASP:O	16:W:87:ILE:HG12	2.17	0.45
22:r:20:LEU:HD12	22:r:21:GLN:N	2.31	0.45
1:A:22:PHE:HA	8:H:60:PRO:HG3	1.98	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.97	0.45
4:D:292:MET:HA	4:D:329:ARG:HD3	1.97	0.45
5:E:73:HIS:ND1	6:F:236:PHE:CD1	2.85	0.45
6:F:394:LYS:HD3	7:G:155:GLU:HB3	1.98	0.45
7:G:43:VAL:HB	7:G:47:THR:HG21	1.99	0.45
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.45
8:H:194:ASN:ND2	8:H:201:THR:HG21	2.31	0.45
10:P:295:LEU:O	10:P:296:PHE:C	2.59	0.45
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.45
12:R:72:VAL:HG21	12:R:77:ILE:CD1	2.46	0.45
12:R:101:THR:HG22	12:R:112:LYS:HB2	1.99	0.45
16:W:71:MET:C	16:W:73:ASN:N	2.70	0.45
2:B:95:PHE:HE1	2:B:131:MET:CE	2.28	0.45
3:C:85:ILE:HD11	3:C:140:ILE:HD11	1.98	0.45
4:D:88:HIS:CE1	4:D:90:ALA:HB3	2.52	0.45
4:D:201:PHE:HB2	8:H:32:GLN:HB3	1.98	0.45
4:D:301:ASP:HB2	4:D:318:VAL:HG21	1.98	0.45
5:E:192:TYR:OH	5:E:213:PRO:HD2	2.16	0.45
6:F:45:LEU:O	6:F:46:TYR:HB2	2.16	0.45
6:F:270:ASN:HD22	6:F:338:ASP:CB	2.29	0.45
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
14:T:99:SER:O	14:T:141:PRO:HG2	2.16	0.45
14:T:123:GLU:HG2	14:T:130:ILE:CD1	2.47	0.45
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.45
3:C:70:LYS:O	15:V:103:LEU:HA	2.16	0.45
3:C:186:ILE:HD12	4:D:429:PHE:CZ	2.52	0.45
4:D:243:ASP:OD2	22:r:31:ILE:HG13	2.16	0.45
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:362:LYS:O	4:D:384:LEU:HD21	2.17	0.45
6:F:47:GLY:O	6:F:48:ARG:HB2	2.17	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.31	0.45
6:F:274:LYS:HZ2	6:F:352:ALA:HB3	1.81	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.45
10:P:259:VAL:H	10:P:261:LYS:HG2	1.82	0.45
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.45
21:q:68:MET:O	21:q:69:ASN:C	2.57	0.45
34:q:201:CDL:H341	34:q:201:CDL:H171	1.99	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.46	0.45
4:D:460:GLU:O	4:D:463:ARG:HG2	2.16	0.45
5:E:58:ASN:O	5:E:62:ILE:HG12	2.16	0.45
5:E:226:PRO:HB2	5:E:229:GLY:O	2.17	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.45
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.52	0.45
15:V:99:PRO:HD2	15:V:100:TRP:CE3	2.51	0.45
21:q:55:PHE:HD1	21:q:55:PHE:H	1.64	0.45
2:B:96:GLY:O	4:D:93:GLY:HA3	2.16	0.45
2:B:98:ALA:HA	4:D:116:LEU:HD21	1.99	0.45
2:B:197:THR:O	2:B:200:ALA:HB3	2.17	0.45
3:C:203:LEU:CD1	4:D:123:LEU:CD2	2.84	0.45
5:E:87:ARG:NH2	6:F:163:TYR:CD1	2.85	0.45
6:F:72:GLY:O	6:F:76:ILE:HG13	2.17	0.45
6:F:87:GLY:H	6:F:92:GLY:CA	2.29	0.45
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.98	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.98	0.45
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
10:P:218:ALA:HB2	10:P:280:ILE:CG2	2.47	0.45
12:R:70:ASN:HB2	12:R:111:PHE:HD2	1.81	0.45
13:S:40:ARG:HD2	13:S:88:THR:OG1	2.16	0.45
14:T:100:VAL:O	14:T:142:GLN:HB2	2.15	0.45
16:W:23:ILE:CD1	16:W:84:LEU:HD21	2.47	0.45
16:W:67:ARG:HD2	16:W:71:MET:SD	2.57	0.45
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.45
21:q:68:MET:HG2	21:q:115:PHE:HE2	1.82	0.45
1:A:102:LEU:HD11	1:A:106:TRP:HE1	1.82	0.45
4:D:179:ARG:HH22	4:D:303:ARG:HD3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.45
8:H:224:PHE:CZ	29:H:401:UQ9:H12A	2.52	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
10:P:238:GLN:HB3	10:P:326:ASP:OD2	2.17	0.45
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.31	0.45
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.16	0.45
21:q:4:VAL:HA	21:q:7:LEU:HD12	1.99	0.45
2:B:92:PRO:HA	2:B:130:VAL:O	2.16	0.45
4:D:174:PHE:O	4:D:178:THR:HG23	2.17	0.45
6:F:61:ASP:O	6:F:256:ARG:NH2	2.50	0.45
6:F:227:PRO:HB3	7:G:95:PRO:HD2	1.98	0.45
7:G:160:VAL:O	7:G:174:THR:HG22	2.17	0.45
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.45
7:G:401:LEU:CD1	7:G:462:PHE:CE2	2.88	0.45
8:H:17:MET:CE	8:H:225:MET:CG	2.94	0.45
8:H:63:PRO:O	8:H:66:THR:HG22	2.17	0.45
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.45
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.45
9:I:67:ILE:HG13	30:I:301:PC1:H231	1.98	0.45
9:I:88:PHE:CE2	21:q:30:ALA:HA	2.51	0.45
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.45
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.45
14:T:87:LEU:HA	14:T:87:LEU:HD23	1.72	0.45
18:Z:66:GLU:HA	18:Z:69:ILE:CG1	2.46	0.45
19:a:1:MET:HG3	34:q:201:CDL:HB21	1.99	0.45
22:r:54:TYR:CE2	22:r:58:ASP:HB3	2.51	0.45
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.96	0.45
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.45
4:D:163:PRO:HG2	4:D:168:GLN:HG2	1.96	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.17	0.45
7:G:341:ILE:HD12	7:G:555:ILE:CG1	2.47	0.45
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.45
7:G:649:VAL:HA	13:S:20:ARG:NE	2.31	0.45
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.45
8:H:30:TYR:CE1	19:a:1:MET:C	2.95	0.45
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.45
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:184:LEU:HD23	11:Q:114:TRP:CH2	2.51	0.45
9:I:188:GLU:OE1	12:R:56:ASN:CB	2.65	0.45
10:P:170:LEU:HD12	10:P:171:ASN:H	1.81	0.45
10:P:315:THR:O	10:P:316:LYS:C	2.58	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
17:X:28:ALA:HB2	17:X:82:PHE:CZ	2.52	0.45
23:s:52:LEU:O	23:s:56:ARG:HG2	2.17	0.45
2:B:120:VAL:HG21	29:H:401:UQ9:H1M	1.99	0.44
3:C:98:PHE:HE1	15:V:44:TYR:CD1	2.34	0.44
3:C:203:LEU:CD2	4:D:123:LEU:CD2	2.88	0.44
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.44
4:D:301:ASP:OD2	4:D:318:VAL:HG22	2.16	0.44
5:E:55:THR:O	5:E:56:PRO:C	2.59	0.44
5:E:62:ILE:O	5:E:66:VAL:HG23	2.17	0.44
6:F:75:TRP:O	6:F:79:GLU:HG2	2.17	0.44
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.44
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.93	0.44
10:P:55:VAL:HA	10:P:79:GLN:O	2.18	0.44
10:P:209:ARG:CA	10:P:352:VAL:HG22	2.47	0.44
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.44
16:W:71:MET:O	16:W:72:LYS:C	2.59	0.44
18:Z:68:ARG:O	18:Z:69:ILE:C	2.60	0.44
20:b:59:ASP:OD1	20:b:59:ASP:N	2.49	0.44
5:E:242:PHE:O	6:F:257:ARG:NH1	2.50	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
8:H:113:VAL:HG21	8:H:136:VAL:HG23	1.99	0.44
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.52	0.44
8:H:196:ALA:O	8:H:198:PHE:N	2.51	0.44
10:P:225:ALA:HB1	10:P:291:TYR:CD1	2.52	0.44
13:S:51:LEU:HA	13:S:52:PRO:HD3	1.86	0.44
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.44
17:X:134:ASP:O	17:X:135:ARG:C	2.58	0.44
21:q:3:LEU:HD12	21:q:6:VAL:CG2	2.48	0.44
21:q:44:TYR:CD1	21:q:68:MET:HG3	2.52	0.44
2:B:97:LEU:HB2	2:B:134:ALA:O	2.17	0.44
2:B:114:MET:HE3	2:B:119:VAL:HG12	1.97	0.44
5:E:243:GLY:O	6:F:257:ARG:HD2	2.17	0.44
6:F:126:LYS:O	6:F:129:GLU:HG2	2.18	0.44
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.44
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:60:PRO:HG2	8:H:62:ARG:HH22	1.82	0.44
9:I:203:ALA:CB	21:q:88:ARG:NH1	2.80	0.44
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.44
1:A:65:PHE:HE2	8:H:294:LEU:HD21	1.76	0.44
2:B:167:GLY:HA3	9:I:150:THR:HB	1.99	0.44
2:B:199:GLU:O	2:B:200:ALA:C	2.60	0.44
4:D:159:LEU:O	4:D:161:ILE:HG23	2.17	0.44
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.44
6:F:48:ARG:HA	6:F:48:ARG:NH1	2.29	0.44
6:F:51:TRP:HB3	6:F:133:HIS:O	2.17	0.44
6:F:273:THR:HA	6:F:292:MET:H	1.82	0.44
6:F:292:MET:O	6:F:293:SER:HB2	2.17	0.44
6:F:379:CYS:SG	25:F:502:SF4:S2	3.16	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:144:MET:HG3	7:G:144:MET:O	2.17	0.44
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.47	0.44
8:H:196:ALA:CB	8:H:274:ARG:HA	2.45	0.44
10:P:82:ILE:HD12	10:P:105:PHE:CE1	2.52	0.44
13:S:42:VAL:O	13:S:46:LYS:HG3	2.18	0.44
16:W:45:GLU:O	16:W:46:VAL:C	2.58	0.44
21:q:23:LEU:HD11	21:q:33:ILE:HD13	1.99	0.44
21:q:44:TYR:CE1	21:q:68:MET:HE3	2.51	0.44
3:C:73:GLN:HE21	15:V:112:TRP:HE1	1.65	0.44
4:D:121:GLU:OE2	4:D:463:ARG:HD2	2.18	0.44
4:D:142:VAL:HG11	4:D:185:MET:CB	2.48	0.44
4:D:250:ASN:HA	22:r:23:LYS:HE3	1.99	0.44
5:E:62:ILE:HG23	5:E:81:VAL:HG22	2.00	0.44
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.46	0.44
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.44
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.98	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
7:G:593:SER:OG	7:G:639:LEU:HD22	2.18	0.44
8:H:17:MET:HE1	8:H:225:MET:CG	2.48	0.44
10:P:358:THR:O	10:P:359:TYR:C	2.60	0.44
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.44
17:X:26:LYS:HE2	17:X:26:LYS:HB3	1.74	0.44
21:q:86:TRP:CD2	21:q:98:PRO:HG2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:LEU:HD23	2:B:136:THR:O	2.18	0.44
4:D:304:LYS:HG3	4:D:316:PHE:CZ	2.53	0.44
5:E:181:ASN:OD1	5:E:221:ARG:HD2	2.17	0.44
6:F:297:LYS:CE	6:F:333:GLU:HB2	2.48	0.44
6:F:383:THR:HG23	7:G:120:LEU:HD23	1.98	0.44
7:G:68:ARG:O	7:G:189:ILE:HD11	2.18	0.44
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.44
8:H:184:MET:SD	8:H:296:LEU:HD23	2.58	0.44
9:I:79:ARG:NE	22:r:20:LEU:HD22	2.33	0.44
10:P:59:PHE:CD1	10:P:83:PRO:HG2	2.52	0.44
10:P:156:SER:HB2	10:P:161:VAL:CG2	2.47	0.44
10:P:275:HIS:CB	10:P:372:ALA:HB1	2.48	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.44
13:S:24:CYS:SG	13:S:61:VAL:O	2.75	0.44
14:T:132:ASP:O	14:T:133:ILE:C	2.60	0.44
17:X:58:LYS:O	17:X:59:GLU:C	2.59	0.44
19:a:37:ARG:HB2	19:a:48:MET:HE2	1.99	0.44
2:B:81:LEU:CD1	8:H:53:MET:HE1	2.47	0.44
2:B:138:THR:HG21	4:D:116:LEU:HA	2.00	0.44
2:B:170:TYR:O	2:B:171:TYR:CD2	2.71	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
7:G:621:LYS:NZ	16:W:131:PRO:HD3	2.33	0.44
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.48	0.44
8:H:303:TRP:CZ3	20:b:28:LEU:HG	2.52	0.44
10:P:245:VAL:HA	10:P:265:PHE:HD2	1.82	0.44
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.44
15:V:56:LEU:O	15:V:57:ASP:C	2.61	0.44
17:X:40:ASN:O	17:X:41:LYS:C	2.58	0.44
2:B:202:LEU:HD21	9:I:86:TYR:HB2	1.94	0.44
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.44
4:D:82:LEU:HD12	8:H:126:LYS:CD	2.44	0.44
4:D:158:LEU:O	4:D:392:PRO:HG2	2.18	0.44
7:G:36:VAL:HG22	7:G:102:ILE:HD12	1.98	0.44
7:G:127:ASP:OD1	7:G:127:ASP:C	2.59	0.44
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.77	0.44
8:H:307:LEU:HD11	18:Z:47:TYR:CD1	2.52	0.44
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.44
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.44
13:S:16:LEU:HD13	13:S:69:TYR:CE1	2.52	0.44
18:Z:69:ILE:CG2	20:b:54:PRO:CD	2.96	0.44
4:D:198:THR:HG21	8:H:275:ALA:HB1	2.00	0.44
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.40	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
6:F:231:ALA:O	6:F:239:PRO:HA	2.18	0.44
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.44
6:F:412:LEU:CD2	6:F:435:VAL:HG13	2.48	0.44
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.44
7:G:466:LEU:HD13	7:G:500:ILE:CG1	2.48	0.44
7:G:557:ARG:HD3	21:q:144:TYR:CZ	2.53	0.44
10:P:130:ILE:N	10:P:130:ILE:HD12	2.33	0.44
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.44
13:S:51:LEU:CD1	13:S:95:LEU:HD12	2.46	0.44
17:X:137:LEU:O	17:X:138:PRO:C	2.58	0.44
2:B:223:ARG:C	10:P:138:ASN:HD21	2.25	0.43
3:C:78:SER:C	3:C:80:LEU:H	2.26	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
4:D:267:ILE:HD13	8:H:280:PHE:CE1	2.53	0.43
4:D:390:GLN:OE1	7:G:145:MET:HE1	2.18	0.43
5:E:117:PHE:HB2	6:F:220:GLN:HE21	1.83	0.43
6:F:67:GLU:O	6:F:71:LYS:HG2	2.18	0.43
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.43
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.99	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
7:G:339:ALA:O	7:G:545:LEU:HD12	2.18	0.43
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.43
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.59	0.43
8:H:142:TYR:CD2	8:H:289:LEU:HD12	2.53	0.43
10:P:327:VAL:HG22	10:P:328:MET:N	2.32	0.43
13:S:19:ILE:CD1	13:S:94:VAL:HG11	2.48	0.43
14:T:140:CYS:SG	14:T:143:GLU:CB	3.03	0.43
17:X:140:ASN:HD21	17:X:144:SER:N	2.16	0.43
18:Z:98:MET:HB3	18:Z:104:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:92:CYS:O	22:r:34:ARG:HG3	2.18	0.43
1:A:63:LEU:O	1:A:64:LEU:C	2.61	0.43
3:C:70:LYS:HG2	15:V:104:VAL:HG23	2.00	0.43
4:D:95:LEU:HD21	4:D:97:LEU:HD11	1.99	0.43
4:D:133:LEU:O	4:D:134:PRO:C	2.60	0.43
4:D:232:VAL:O	4:D:356:ILE:HD12	2.19	0.43
4:D:268:TRP:CE2	4:D:272:THR:HG21	2.53	0.43
5:E:231:THR:CG2	6:F:303:HIS:HA	2.47	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.97	0.43
8:H:199:ASP:HB3	8:H:279:ARG:CD	2.48	0.43
8:H:287:HIS:CE1	24:H:402:3PE:N	2.81	0.43
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.43
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.82	0.43
12:R:104:CYS:C	12:R:106:TYR:H	2.26	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.43
16:W:71:MET:O	16:W:74:ALA:N	2.39	0.43
20:b:82:LYS:HB3	20:b:82:LYS:HE2	1.81	0.43
34:q:201:CDL:HB61	34:q:201:CDL:OA9	2.18	0.43
1:A:112:GLU:O	1:A:113:TRP:C	2.58	0.43
2:B:112:TYR:OH	9:I:91:GLY:HA3	2.19	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.43
8:H:97:ASN:OD1	8:H:97:ASN:O	2.36	0.43
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.43
2:B:170:TYR:OH	4:D:131:GLN:O	2.36	0.43
3:C:224:GLU:OE2	10:P:45:LYS:HD3	2.18	0.43
4:D:129:TYR:CE2	4:D:391:VAL:HG22	2.54	0.43
5:E:79:LEU:HB2	5:E:80:PRO:HD3	2.01	0.43
5:E:232:SER:HB2	6:F:37:ASP:OD1	2.18	0.43
6:F:317:VAL:HG22	6:F:356:VAL:HG22	2.00	0.43
7:G:462:PHE:CZ	7:G:466:LEU:HD21	2.54	0.43
10:P:168:SER:O	10:P:202:ARG:HA	2.17	0.43
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.43
17:X:37:ASP:OD2	20:b:70:PRO:HD2	2.17	0.43
1:A:95:VAL:HG11	8:H:302:MET:CG	2.48	0.43
2:B:99:CYS:HB3	4:D:141:TYR:HB2	2.00	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
4:D:220:ALA:HB3	4:D:224:ALA:HA	2.00	0.43
7:G:141:ASP:O	7:G:145:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
7:G:346:VAL:HG21	7:G:548:LEU:HD21	2.00	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
8:H:92:PRO:HG3	8:H:247:TYR:HE1	1.84	0.43
8:H:142:TYR:O	8:H:146:MET:HB2	2.18	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
17:X:46:CYS:SG	17:X:135:ARG:HD3	2.58	0.43
20:b:15:LYS:O	20:b:15:LYS:HG3	2.18	0.43
4:D:240:LEU:CG	4:D:244:ILE:HD11	2.49	0.43
5:E:247:GLY:O	6:F:64:LYS:CD	2.67	0.43
6:F:381:GLN:HG3	7:G:74:ASN:OD1	2.19	0.43
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.48	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
8:H:257:THR:O	8:H:260:MET:HB3	2.18	0.43
24:H:402:3PE:H331	24:H:402:3PE:H362	1.68	0.43
12:R:40:GLU:HG3	12:R:41:LYS:HG2	2.00	0.43
13:S:18:GLU:O	13:S:19:ILE:HD13	2.19	0.43
13:S:30:SER:O	13:S:31:GLN:C	2.59	0.43
1:A:10:ASN:ND2	8:H:84:SER:OG	2.51	0.43
2:B:172:HIS:CE1	2:B:179:ARG:HD3	2.54	0.43
3:C:70:LYS:HA	15:V:102:PRO:C	2.44	0.43
4:D:261:MET:HE3	4:D:261:MET:HB3	1.74	0.43
4:D:378:LEU:HD22	7:G:126:LEU:HD13	2.01	0.43
4:D:384:LEU:HD23	7:G:144:MET:HE1	2.00	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
7:G:639:LEU:HD21	7:G:643:ARG:NH2	2.34	0.43
8:H:132:ALA:O	8:H:136:VAL:HG12	2.18	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
10:P:170:LEU:O	10:P:171:ASN:CG	2.61	0.43
11:Q:55:VAL:HG21	16:W:78:ASP:OD1	2.18	0.43
16:W:120:ASP:HB3	16:W:123:SER:OG	2.18	0.43
18:Z:98:MET:HE2	18:Z:98:MET:HA	2.01	0.43
18:Z:121:ILE:HA	18:Z:124:MET:HE2	1.99	0.43
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.43
5:E:38:PHE:O	7:G:205:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:394:LYS:CB	7:G:155:GLU:HG2	2.48	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43
8:H:43:TYR:CE2	21:q:27:PHE:CZ	3.06	0.43
8:H:127:TYR:HD1	8:H:207:LEU:CD2	2.15	0.43
8:H:272:TRP:CZ2	9:I:74:LEU:HB2	2.54	0.43
9:I:50:MET:CE	20:b:10:LYS:HG2	2.49	0.43
10:P:76:MET:HE1	10:P:254:LYS:HE2	2.01	0.43
21:q:79:GLY:O	21:q:82:VAL:HG22	2.19	0.43
22:r:54:TYR:C	22:r:56:THR:N	2.76	0.43
2:B:92:PRO:HD2	2:B:120:VAL:O	2.19	0.43
3:C:97:THR:O	15:V:90:LEU:CD1	2.67	0.43
4:D:152:SER:HA	4:D:229:PRO:HA	2.00	0.43
6:F:46:TYR:O	6:F:48:ARG:HG2	2.19	0.43
6:F:410:ASP:OD1	6:F:410:ASP:C	2.62	0.43
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.43
10:P:316:LYS:O	10:P:320:GLU:HG2	2.19	0.43
11:Q:52:LEU:HD23	16:W:19:SER:O	2.19	0.43
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.43
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.43
16:W:38:LEU:HG	16:W:70:PHE:HZ	1.84	0.43
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.53	0.43
17:X:120:PRO:HG3	20:b:71:GLN:NE2	2.34	0.43
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.43
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.43
2:B:81:LEU:HD11	30:q:202:PC1:H361	2.00	0.43
2:B:114:MET:HB2	2:B:119:VAL:HB	2.01	0.43
2:B:166:ASN:HB2	2:B:190:TYR:CD2	2.45	0.43
4:D:91:ALA:HB1	4:D:95:LEU:HB3	2.01	0.43
4:D:203:MET:HE1	4:D:255:ILE:HA	2.01	0.43
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.50	0.43
4:D:303:ARG:CG	4:D:401:GLU:HB3	2.48	0.43
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.43
6:F:398:ARG:HH22	7:G:155:GLU:CD	2.26	0.43
7:G:401:LEU:HD21	7:G:466:LEU:HD11	2.01	0.43
10:P:197:GLU:HB3	10:P:259:VAL:HG22	1.99	0.43
18:Z:69:ILE:HG23	20:b:54:PRO:CD	2.46	0.43
18:Z:111:PHE:CE2	18:Z:117:VAL:HG21	2.52	0.43
19:a:55:SER:O	19:a:56:GLY:C	2.61	0.43
21:q:34:ARG:HD3	21:q:54:GLN:OE1	2.18	0.43
3:C:104:ASN:HD22	22:r:94:ALA:HB1	1.83	0.42
5:E:142:ARG:HG3	5:E:182:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:42:PHE:CD1	6:F:137:LYS:HD2	2.54	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.42
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.49	0.42
7:G:36:VAL:O	7:G:39:GLN:HG2	2.19	0.42
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	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
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.19	0.42
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.54	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
10:P:259:VAL:N	10:P:261:LYS:HG2	2.33	0.42
11:Q:51:GLN:HB3	16:W:26:ARG:HH22	1.84	0.42
12:R:43:TYR:C	12:R:45:ARG:H	2.27	0.42
17:X:69:ASN:O	17:X:73:GLN:HG3	2.19	0.42
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.42
21:q:125:VAL:O	21:q:125:VAL:CG2	2.67	0.42
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
1:A:109:LYS:HD2	1:A:112:GLU:HB2	2.00	0.42
2:B:93:MET:SD	2:B:125:PRO:HG3	2.59	0.42
2:B:194:CYS:HB2	9:I:153:ILE:C	2.43	0.42
3:C:55:LYS:HE2	3:C:55:LYS:HB3	1.82	0.42
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.54	0.42
5:E:162:THR:HG22	5:E:163:THR:N	2.34	0.42
5:E:180:VAL:HG11	5:E:224:CYS:CB	2.48	0.42
5:E:180:VAL:CG1	5:E:181:ASN:H	2.32	0.42
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.42
7:G:31:LEU:HA	7:G:31:LEU:HD23	1.79	0.42
8:H:136:VAL:O	8:H:140:ILE:HG23	2.19	0.42
29:H:401:UQ9:H1M	29:H:401:UQ9:H7A	1.83	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
10:P:64:PHE:CE1	10:P:209:ARG:O	2.69	0.42
10:P:235:THR:HG21	10:P:323:HIS:CD2	2.55	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.63	0.42
3:C:49:ARG:HH21	3:C:54:HIS:CG	2.37	0.42
4:D:79:ASN:O	4:D:80:MET:C	2.62	0.42
4:D:381:HIS:HE1	9:I:161:ALA:O	2.02	0.42
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.34	0.42
6:F:81:LYS:HD3	6:F:96:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
6:F:409:ILE:HG12	6:F:446:LEU:HD23	1.96	0.42
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.42
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
19:a:17:VAL:O	19:a:18:ILE:C	2.62	0.42
22:r:113:LEU:HD13	22:r:113:LEU:HA	1.92	0.42
1:A:92:PHE:HZ	8:H:306:SER:HB2	1.83	0.42
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.42
4:D:189:THR:CG2	26:D:501:UQ1:HM23	2.49	0.42
4:D:266:ARG:HH21	9:I:63:TRP:HA	1.85	0.42
4:D:280:ALA:HB1	15:V:11:LEU:CG	2.44	0.42
4:D:280:ALA:HB3	15:V:11:LEU:HD23	2.01	0.42
5:E:101:ALA:HA	5:E:106:VAL:HG22	2.01	0.42
5:E:110:ARG:HD3	5:E:110:ARG:HA	1.81	0.42
5:E:114:VAL:O	5:E:118:TYR:HD2	2.02	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
8:H:68:MET:HG3	8:H:68:MET:O	2.19	0.42
9:I:113:CYS:SG	25:I:303:SF4:S4	3.17	0.42
10:P:220:TYR:CG	10:P:226:VAL:HG13	2.55	0.42
12:R:76:ILE:HD11	12:R:92:TYR:CB	2.48	0.42
14:T:108:LEU:HD23	14:T:108:LEU:C	2.44	0.42
18:Z:98:MET:HA	18:Z:101:VAL:HG23	2.01	0.42
22:r:54:TYR:HA	22:r:57:ARG:CG	2.48	0.42
22:r:54:TYR:HD1	22:r:57:ARG:HG3	1.83	0.42
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.42	0.42
26:D:501:UQ1:HM23	26:D:501:UQ1:HM32	2.00	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
7:G:360:LYS:HE3	7:G:632:ILE:CB	2.38	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
8:H:49:PHE:HB3	30:q:202:PC1:H381	2.01	0.42
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.48	0.42
30:I:301:PC1:H221	18:Z:35:MET:HE2	2.00	0.42
10:P:242:VAL:HG13	10:P:243:ALA:N	2.35	0.42
10:P:265:PHE:CD1	10:P:334:GLY:HA3	2.55	0.42
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.01	0.42
12:R:77:ILE:HG12	12:R:78:ALA:N	2.34	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
16:W:120:ASP:OD1	16:W:120:ASP:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:65:LEU:CB	20:b:50:PRO:O	2.63	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42
1:A:52:SER:O	1:A:53:MET:C	2.61	0.42
2:B:81:LEU:HD11	8:H:53:MET:HE1	2.01	0.42
2:B:202:LEU:HD21	9:I:86:TYR:HB3	1.99	0.42
3:C:85:ILE:CD1	3:C:140:ILE:HD11	2.50	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.42
7:G:612:PRO:HG2	16:W:129:HIS:HD2	1.83	0.42
8:H:24:GLU:CD	8:H:195:ARG:HH22	2.27	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
9:I:135:ARG:NH1	12:R:61:ILE:HG23	2.27	0.42
12:R:81:GLY:CA	12:R:88:HIS:CD2	3.02	0.42
17:X:91:TYR:OH	19:a:28:LYS:HE2	2.19	0.42
17:X:143:HIS:ND1	18:Z:115:ARG:HA	2.35	0.42
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.42
2:B:92:PRO:HG3	2:B:119:VAL:CG1	2.49	0.42
2:B:104:MET:HE3	2:B:104:MET:HB2	1.61	0.42
3:C:64:VAL:HG21	3:C:85:ILE:HD11	2.01	0.42
3:C:232:PHE:CE1	7:G:244:GLU:HG3	2.55	0.42
4:D:420:TYR:CD2	15:V:114:TRP:HH2	2.37	0.42
5:E:64:ALA:HA	5:E:67:LYS:HD3	2.02	0.42
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.42
6:F:51:TRP:HB2	6:F:133:HIS:O	2.19	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.42
8:H:7:LEU:HD13	8:H:7:LEU:HA	1.93	0.42
8:H:113:VAL:HG22	8:H:136:VAL:HG23	2.02	0.42
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.42
10:P:263:PHE:CD2	10:P:333:PRO:O	2.66	0.42
10:P:283:MET:SD	10:P:369:THR:HG21	2.60	0.42
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.42
13:S:16:LEU:CD1	13:S:19:ILE:HD11	2.48	0.42
23:s:53:SER:HA	23:s:56:ARG:HG2	2.02	0.42
2:B:70:ARG:HG3	2:B:72:GLU:H	1.85	0.42
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.42
4:D:193:ASP:O	8:H:205:SER:CB	2.67	0.42
4:D:207:ARG:O	4:D:211:PHE:CD1	2.69	0.42
5:E:109:MET:HE2	7:G:196:GLY:CA	2.49	0.42
5:E:226:PRO:HA	6:F:286:CYS:HB3	2.02	0.42
6:F:102:MET:SD	6:F:241:THR:OG1	2.74	0.42
6:F:268:GLU:HG2	6:F:269:ARG:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.42
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.42
8:H:65:THR:HG22	10:P:359:TYR:CB	2.50	0.42
8:H:206:GLU:O	8:H:207:LEU:HB2	2.20	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
14:T:133:ILE:HG23	14:T:134:ASP:N	2.35	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
24:b:201:3PE:H2E1	24:b:201:3PE:H2B2	1.80	0.42
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.42
3:C:72:VAL:HG23	3:C:72:VAL:O	2.20	0.42
3:C:224:GLU:OE1	11:Q:118:ALA:HB2	2.20	0.42
4:D:184:ILE:HD12	4:D:210:MET:HE1	2.02	0.42
4:D:354:GLY:O	22:r:42:PRO:HG2	2.20	0.42
4:D:361:ALA:HB3	7:G:149:ASP:HB3	2.01	0.42
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.54	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.42
8:H:172:MET:HE3	8:H:176:LEU:CB	2.47	0.42
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.42
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.42
9:I:123:CYS:SG	25:I:302:SF4:S2	3.17	0.42
10:P:99:ASP:HB3	10:P:102:GLN:CD	2.45	0.42
10:P:207:PHE:O	10:P:241:TYR:HA	2.20	0.42
10:P:243:ALA:O	10:P:244:ASP:C	2.62	0.42
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.42
14:T:138:LEU:HD11	14:T:147:TYR:CD2	2.54	0.42
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.42
20:b:15:LYS:O	20:b:16:GLU:HB2	2.20	0.42
4:D:170:ILE:CD1	4:D:236:LEU:HD11	2.49	0.41
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.55	0.41
5:E:131:ILE:HD13	5:E:151:LEU:HD21	2.02	0.41
6:F:69:LEU:CD1	6:F:143:LEU:HD21	2.49	0.41
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.41
8:H:116:ILE:HA	8:H:211:PHE:CE1	2.54	0.41
8:H:196:ALA:O	8:H:279:ARG:HG2	2.19	0.41
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.41
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.41
16:W:23:ILE:CG2	16:W:83:ASP:HB2	2.50	0.41
16:W:53:MET:SD	16:W:106:VAL:HG21	2.60	0.41
16:W:78:ASP:HA	16:W:79:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:141:PRO:C	17:X:143:HIS:H	2.27	0.41
20:b:31:ILE:O	20:b:32:MET:C	2.63	0.41
20:b:69:HIS:HB3	20:b:72:ASP:CG	2.45	0.41
34:q:201:CDL:H511	22:r:8:ILE:HD11	2.01	0.41
3:C:160:ILE:HG13	4:D:285:ASN:ND2	2.34	0.41
4:D:159:LEU:CD2	22:r:60:ARG:HG3	2.50	0.41
4:D:211:PHE:O	4:D:212:GLU:C	2.62	0.41
5:E:62:ILE:HD13	5:E:84:LEU:HD13	2.01	0.41
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
7:G:360:LYS:HB3	7:G:632:ILE:HB	2.01	0.41
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.28	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.41
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.41
14:T:93:ILE:CD1	14:T:108:LEU:HD22	2.49	0.41
17:X:48:TRP:NE1	20:b:55:VAL:HG22	2.32	0.41
1:A:93:ILE:HD13	1:A:93:ILE:HA	1.90	0.41
3:C:52:VAL:O	3:C:56:GLN:HG3	2.20	0.41
4:D:144:MET:SD	4:D:144:MET:N	2.93	0.41
4:D:179:ARG:CG	4:D:183:HIS:CD2	3.04	0.41
5:E:183:PRO:O	5:E:194:ASP:N	2.53	0.41
6:F:102:MET:HG3	6:F:149:MET:HB2	2.02	0.41
6:F:268:GLU:CG	6:F:269:ARG:H	2.32	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.02	0.41
7:G:639:LEU:C	7:G:641:GLN:N	2.77	0.41
7:G:639:LEU:O	7:G:641:GLN:N	2.54	0.41
8:H:187:ILE:HG23	8:H:198:PHE:CZ	2.55	0.41
8:H:312:ALA:CB	20:b:41:TYR:HB2	2.50	0.41
9:I:48:VAL:CG1	9:I:53:ALA:HB2	2.50	0.41
9:I:184:LEU:CD2	11:Q:114:TRP:CH2	3.03	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41
10:P:230:SER:O	10:P:231:LEU:C	2.63	0.41
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.21	0.41
10:P:283:MET:HE3	10:P:357:ARG:NH1	2.35	0.41
18:Z:10:MET:HB3	18:Z:10:MET:HE2	1.75	0.41
19:a:49:GLU:OE2	19:a:49:GLU:HA	2.20	0.41
1:A:72:LEU:HB3	8:H:151:LEU:HD21	2.02	0.41
1:A:112:GLU:O	1:A:113:TRP:CD1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:179:ARG:HG3	4:D:183:HIS:NE2	2.34	0.41
4:D:267:ILE:CD1	8:H:280:PHE:CE1	3.03	0.41
4:D:353:PRO:HB3	18:Z:10:MET:SD	2.60	0.41
6:F:77:LEU:HD13	6:F:100:SER:HA	2.03	0.41
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.36	0.41
6:F:147:ARG:HD3	6:F:191:TYR:HD2	1.72	0.41
6:F:217:GLU:OE2	6:F:224:ARG:NH2	2.53	0.41
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.35	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:53:CYS:SG	7:G:102:ILE:HG21	2.60	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:282:ASN:HB2	7:G:285:TRP:O	2.20	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.41
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.56	0.41
9:I:79:ARG:NH2	22:r:20:LEU:HD22	2.34	0.41
13:S:23:LEU:O	13:S:57:GLU:HA	2.20	0.41
13:S:36:PHE:HZ	13:S:44:LEU:HD12	1.86	0.41
14:T:133:ILE:HG13	14:T:137:LYS:NZ	2.36	0.41
17:X:132:LYS:HB3	17:X:132:LYS:HE2	1.84	0.41
20:b:25:VAL:O	20:b:26:TRP:C	2.64	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
22:r:41:LEU:N	22:r:41:LEU:HD22	2.35	0.41
1:A:104:TYR:HA	1:A:107:THR:OG1	2.21	0.41
2:B:144:ALA:O	2:B:147:LYS:N	2.54	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.41
4:D:104:GLU:HG3	8:H:130:PHE:CZ	2.49	0.41
4:D:149:GLN:NE2	4:D:309:ASP:OD2	2.53	0.41
6:F:54:LYS:HG3	6:F:55:GLY:H	1.85	0.41
6:F:427:LEU:HB2	28:F:501:FMN:HM71	2.02	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
8:H:13:ILE:HD13	8:H:13:ILE:HA	1.87	0.41
8:H:23:VAL:HG11	19:a:9:LEU:HD21	2.02	0.41
8:H:75:PRO:HB2	8:H:222:LEU:HB2	2.03	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
9:I:41:LYS:HD3	22:r:112:TYR:HE2	1.85	0.41
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.41
9:I:140:ARG:O	9:I:141:ARG:HG2	2.21	0.41
10:P:295:LEU:O	10:P:298:TYR:N	2.53	0.41
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:38:TYR:CD2	12:R:48:PHE:CE2	3.08	0.41
14:T:93:ILE:HD13	14:T:108:LEU:CD2	2.51	0.41
16:W:86:VAL:O	16:W:87:ILE:C	2.61	0.41
17:X:17:GLU:HG3	17:X:64:ASN:ND2	2.34	0.41
17:X:41:LYS:HD2	20:b:56:PRO:HG3	2.01	0.41
17:X:90:ASP:OD2	19:a:62:VAL:HG11	2.21	0.41
19:a:49:GLU:O	19:a:50:ARG:C	2.62	0.41
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
21:q:110:TRP:HB2	21:q:113:HIS:CE1	2.55	0.41
1:A:113:TRP:CH2	8:H:287:HIS:HB2	2.55	0.41
3:C:232:PHE:HE2	9:I:126:GLN:OE1	2.04	0.41
4:D:268:TRP:O	4:D:269:ARG:C	2.63	0.41
5:E:167:LEU:HB3	5:E:168:PHE:CD1	2.56	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.41
7:G:126:LEU:HD11	12:R:89:PRO:CB	2.47	0.41
7:G:161:GLU:OE2	12:R:96:ASP:N	2.53	0.41
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.84	0.41
8:H:174:LEU:HD23	8:H:174:LEU:HA	1.81	0.41
8:H:197:PRO:HD3	8:H:273:ILE:HG22	2.03	0.41
9:I:82:ALA:CA	22:r:26:LEU:HD21	2.50	0.41
15:V:94:MET:SD	15:V:99:PRO:HG3	2.60	0.41
17:X:120:PRO:HG3	20:b:71:GLN:HE21	1.86	0.41
20:b:49:THR:HA	20:b:50:PRO:HD3	1.89	0.41
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.91	0.41
2:B:154:GLU:O	2:B:156:ARG:N	2.52	0.41
4:D:270:ASN:HB2	8:H:284:GLN:OE1	2.20	0.41
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.21	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:66:LYS:NZ	6:F:189:SER:CA	2.79	0.41
6:F:384:PRO:HA	7:G:119:PHE:CD2	2.54	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
7:G:667:GLN:HB3	13:S:42:VAL:HG13	2.01	0.41
8:H:14:LEU:HD13	8:H:83:LEU:HD21	2.03	0.41
8:H:17:MET:SD	8:H:225:MET:C	3.03	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
9:I:92:PRO:HB3	21:q:92:CYS:HB2	2.02	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
9:I:162:CYS:SG	25:I:303:SF4:S2	3.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:93:ILE:HG23	14:T:108:LEU:HD13	2.03	0.41
15:V:96:LYS:HE2	15:V:96:LYS:HB2	1.95	0.41
17:X:37:ASP:OD1	17:X:37:ASP:C	2.62	0.41
17:X:142:TYR:O	17:X:143:HIS:C	2.62	0.41
2:B:92:PRO:HG3	2:B:119:VAL:HG12	2.02	0.41
2:B:95:PHE:HD2	2:B:141:MET:HE3	1.86	0.41
4:D:154:ALA:HB2	4:D:398:THR:HG22	2.00	0.41
4:D:326:CYS:SG	4:D:453:THR:HG21	2.61	0.41
5:E:176:LEU:HB3	5:E:191:TYR:OH	2.20	0.41
5:E:221:ARG:HH21	5:E:227:ALA:HB2	1.86	0.41
6:F:69:LEU:HD11	6:F:143:LEU:HG	2.03	0.41
7:G:102:ILE:O	7:G:103:LEU:C	2.60	0.41
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.41
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
10:P:88:VAL:HG12	10:P:92:MET:HE2	2.02	0.41
12:R:44:ARG:O	12:R:47:ARG:HB2	2.21	0.41
17:X:45:LEU:HD21	20:b:58:ARG:HE	1.86	0.41
21:q:120:THR:HA	21:q:121:PRO:HD3	1.83	0.41
22:r:54:TYR:CD1	22:r:57:ARG:HG3	2.56	0.41
1:A:67:LEU:O	1:A:70:ALA:HB3	2.21	0.41
2:B:71:ALA:O	2:B:75:VAL:HG23	2.21	0.41
3:C:216:LYS:HG3	10:P:209:ARG:HH11	1.85	0.41
3:C:241:PHE:HB3	3:C:242:PRO:HD2	2.03	0.41
4:D:216:ARG:NH2	4:D:240:LEU:HA	2.36	0.41
4:D:253:LEU:HD23	4:D:254:ARG:HH22	1.86	0.41
4:D:322:SER:OG	4:D:323:ARG:HG3	2.20	0.41
5:E:182:ALA:O	5:E:183:PRO:C	2.59	0.41
6:F:226:LYS:HD3	6:F:226:LYS:HA	1.84	0.41
6:F:309:GLY:HA3	6:F:313:ASN:HD22	1.85	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	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:544:MET:HE2	7:G:546:PHE:CZ	2.55	0.41
7:G:674:LEU:HD11	13:S:46:LYS:HE2	2.03	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
8:H:102:ILE:CD1	8:H:154:LEU:HD21	2.49	0.41
8:H:130:PHE:HD2	8:H:207:LEU:HD11	1.86	0.41
8:H:264:LEU:HD23	8:H:264:LEU:HA	1.81	0.41
24:H:402:3PE:H342	9:I:63:TRP:CZ2	2.55	0.41
10:P:265:PHE:CD1	10:P:265:PHE:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:359:TYR:HA	10:P:362:LEU:HG	2.02	0.41
12:R:79:CYS:O	12:R:88:HIS:CE1	2.74	0.41
14:T:110:LEU:HG	14:T:114:ASP:HB3	1.98	0.41
17:X:20:VAL:CG1	17:X:24:VAL:HB	2.51	0.41
18:Z:142:TRP:C	18:Z:143:TYR:CD2	2.99	0.41
20:b:16:GLU:N	20:b:17:PRO:HD3	2.35	0.41
21:q:78:ASP:OD1	21:q:78:ASP:O	2.39	0.41
4:D:92:HIS:CD2	26:D:501:UQ1:C3	3.04	0.41
4:D:398:THR:O	4:D:398:THR:HG23	2.20	0.41
6:F:303:HIS:O	6:F:304:ALA:HB3	2.20	0.41
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.86	0.41
6:F:418:GLN:NE2	22:r:53:TYR:OH	2.53	0.41
7:G:44:GLU:O	7:G:47:THR:HG23	2.21	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.41
7:G:127:ASP:HA	12:R:106:TYR:OH	2.20	0.41
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.26	0.41
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.41
8:H:82:ALA:HA	8:H:85:LEU:HD12	2.02	0.41
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.41
8:H:295:PRO:HG3	24:b:201:3PE:H382	2.02	0.41
9:I:75:SER:O	22:r:12:ARG:HG2	2.22	0.41
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.41
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.51	0.41
17:X:136:PRO:O	17:X:137:LEU:C	2.63	0.41
18:Z:98:MET:HB3	18:Z:104:TRP:HD1	1.86	0.41
19:a:48:MET:HE3	19:a:48:MET:HB2	1.77	0.41
2:B:98:ALA:O	4:D:141:TYR:CE2	2.75	0.40
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.40
4:D:145:MET:HG2	4:D:148:GLU:OE2	2.22	0.40
5:E:109:MET:HE1	7:G:198:THR:CG2	2.51	0.40
5:E:184:MET:HE3	5:E:184:MET:HB3	1.95	0.40
6:F:80:MET:O	6:F:83:SER:HB3	2.20	0.40
6:F:335:VAL:HG12	6:F:336:LEU:N	2.36	0.40
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.55	0.40
7:G:176:CYS:SG	25:G:802:SF4:S1	3.19	0.40
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.40
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.40
8:H:182:ALA:HB1	24:H:402:3PE:H2H1	2.03	0.40
8:H:306:SER:CB	8:H:310:PHE:HE2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:H:402:3PE:H272	24:H:402:3PE:H241	1.58	0.40
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.40
10:P:135:GLU:HG3	10:P:140:ASP:HA	2.03	0.40
10:P:203:PRO:HG2	31:P:401:NDP:C6N	2.51	0.40
13:S:17:ARG:O	13:S:52:PRO:HD2	2.21	0.40
4:D:391:VAL:HG23	4:D:413:SER:OG	2.21	0.40
5:E:68:ASN:ND2	23:s:56:ARG:NH2	2.68	0.40
6:F:53:LEU:O	6:F:54:LYS:C	2.62	0.40
6:F:257:ARG:HG2	6:F:261:TRP:CE3	2.55	0.40
6:F:276:PHE:CE2	6:F:290:GLU:HB3	2.56	0.40
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.40
7:G:664:TYR:OH	13:S:23:LEU:HD21	2.21	0.40
8:H:142:TYR:CE1	8:H:285:LEU:HD21	2.55	0.40
9:I:105:ARG:HH12	12:R:58:ASN:CB	2.34	0.40
10:P:169:HIS:ND1	31:P:401:NDP:H5N	2.36	0.40
15:V:114:TRP:O	15:V:116:ILE:HG22	2.21	0.40
16:W:23:ILE:HG21	16:W:83:ASP:HB2	2.02	0.40
16:W:27:ASP:O	16:W:28:LEU:C	2.64	0.40
17:X:21:SER:O	17:X:22:SER:C	2.63	0.40
17:X:25:LEU:HD11	19:a:50:ARG:NH2	2.36	0.40
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.55	0.40
18:Z:55:GLN:O	18:Z:59:ARG:HG3	2.21	0.40
20:b:23:PHE:HE2	24:b:201:3PE:H252	1.85	0.40
21:q:17:HIS:HE1	21:q:34:ARG:N	2.19	0.40
21:q:44:TYR:HE1	21:q:69:ASN:OD1	2.05	0.40
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.86	0.40
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.51	0.40
2:B:91:TRP:CD1	2:B:120:VAL:HG23	2.56	0.40
3:C:66:GLU:OE1	15:V:47:TYR:CE2	2.74	0.40
3:C:97:THR:HG21	15:V:97:TRP:HH2	1.86	0.40
7:G:32:ILE:HG22	7:G:33:GLU:N	2.36	0.40
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.40
8:H:95:LEU:HG	8:H:96:ILE:HG13	2.03	0.40
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.40
11:Q:57:GLU:O	11:Q:58:LYS:C	2.65	0.40
14:T:97:LYS:NZ	14:T:108:LEU:N	2.66	0.40
14:T:104:PHE:CE1	14:T:105:MET:HG2	2.56	0.40
17:X:48:TRP:CZ2	20:b:55:VAL:CG2	2.98	0.40
18:Z:104:TRP:O	18:Z:105:LYS:C	2.64	0.40
22:r:28:TYR:O	22:r:30:GLU:HG3	2.21	0.40
2:B:120:VAL:HG11	29:H:401:UQ9:C1M	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
3:C:141:ARG:HE	3:C:141:ARG:HB2	1.42	0.40
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.40
6:F:281:HIS:HB2	6:F:356:VAL:O	2.21	0.40
7:G:114:GLU:OE2	22:r:53:TYR:CA	2.60	0.40
7:G:355:LYS:HB2	7:G:366:LEU:CD2	2.52	0.40
8:H:114:TYR:O	8:H:117:LEU:N	2.55	0.40
8:H:316:PRO:HG3	18:Z:57:ARG:CB	2.49	0.40
10:P:80:VAL:HB	10:P:103:LEU:HD22	2.04	0.40
10:P:120:VAL:O	10:P:121:GLN:C	2.64	0.40
10:P:140:ASP:O	10:P:141:PHE:C	2.65	0.40
12:R:36:GLN:O	12:R:36:GLN:HG3	2.22	0.40
23:s:41:ASN:HD21	23:s:43:TYR:HB2	1.87	0.40
1:A:87:MET:HB3	1:A:87:MET:HE3	1.84	0.40
2:B:146:ARG:NH2	3:C:211:TYR:CZ	2.90	0.40
3:C:68:LEU:HD13	3:C:95:THR:HA	2.03	0.40
4:D:182:ASN:O	4:D:185:MET:HB3	2.22	0.40
4:D:255:ILE:CG1	4:D:337:MET:HE2	2.47	0.40
5:E:192:TYR:CD2	5:E:203:ILE:HD13	2.57	0.40
6:F:114:VAL:CG1	6:F:212:LEU:HD23	2.52	0.40
6:F:297:LYS:CB	6:F:333:GLU:HB2	2.51	0.40
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.03	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:302:LEU:N	7:G:571:HIS:O	2.45	0.40
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.42	0.40
8:H:251:LEU:HD11	8:H:254:LEU:HB2	2.03	0.40
10:P:56:ALA:HA	10:P:125:VAL:O	2.21	0.40
10:P:146:VAL:HG13	10:P:147:ASN:OD1	2.21	0.40
10:P:227:PRO:O	10:P:228:LEU:HD23	2.21	0.40
10:P:302:GLY:HA2	10:P:314:THR:CG2	2.50	0.40
11:Q:129:SER:HB2	15:V:116:ILE:CD1	2.52	0.40
13:S:59:SER:O	13:S:60:GLU:C	2.63	0.40
21:q:64:TYR:CE2	21:q:82:VAL:HG13	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/115 (76%)	83 (94%)	5 (6%)	0	100	100
2	B	155/224 (69%)	146 (94%)	7 (4%)	2 (1%)	9	40
3	C	196/263 (74%)	186 (95%)	10 (5%)	0	100	100
4	D	383/463 (83%)	365 (95%)	18 (5%)	0	100	100
5	E	208/248 (84%)	203 (98%)	5 (2%)	0	100	100
6	F	424/464 (91%)	409 (96%)	15 (4%)	0	100	100
7	G	685/727 (94%)	633 (92%)	52 (8%)	0	100	100
8	H	313/318 (98%)	298 (95%)	14 (4%)	1 (0%)	36	68
9	I	176/212 (83%)	175 (99%)	1 (1%)	0	100	100
10	P	337/377 (89%)	308 (91%)	28 (8%)	1 (0%)	36	68
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	78 (96%)	3 (4%)	0	100	100
13	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
14	T	73/156 (47%)	69 (94%)	4 (6%)	0	100	100
15	V	110/116 (95%)	106 (96%)	4 (4%)	0	100	100
16	W	112/131 (86%)	110 (98%)	2 (2%)	0	100	100
17	X	140/172 (81%)	129 (92%)	11 (8%)	0	100	100
18	Z	137/144 (95%)	133 (97%)	4 (3%)	0	100	100
19	a	65/70 (93%)	62 (95%)	3 (5%)	0	100	100
20	b	77/84 (92%)	72 (94%)	5 (6%)	0	100	100
21	q	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
22	r	91/113 (80%)	81 (89%)	9 (10%)	1 (1%)	11	43
23	s	20/104 (19%)	20 (100%)	0	0	100	100
All	All	4209/5036 (84%)	3995 (95%)	209 (5%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	88	PRO
10	P	329	PRO
2	B	171	TYR
22	r	39	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	84/104 (81%)	84 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	73	82
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	332/395 (84%)	330 (99%)	2 (1%)	78	84
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	85
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	89
8	H	279/280 (100%)	279 (100%)	0	100	100
9	I	152/178 (85%)	152 (100%)	0	100	100
10	P	296/325 (91%)	295 (100%)	1 (0%)	86	88
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68	80
12	R	70/96 (73%)	69 (99%)	1 (1%)	59	77
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	77
14	T	69/135 (51%)	69 (100%)	0	100	100
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	128 (99%)	1 (1%)	73	82
18	Z	120/123 (98%)	119 (99%)	1 (1%)	73	82
19	a	57/60 (95%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	b	70/73 (96%)	70 (100%)	0	100	100
21	q	129/131 (98%)	129 (100%)	0	100	100
22	r	85/96 (88%)	84 (99%)	1 (1%)	63	79
23	s	22/95 (23%)	22 (100%)	0	100	100
All	All	3696/4292 (86%)	3684 (100%)	12 (0%)	84	88

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

Mol	Chain	Res	Type
2	B	170	TYR
4	D	127	LYS
4	D	142	VAL
5	E	124	LYS
7	G	271	MET
10	P	316	LYS
11	Q	96	LYS
12	R	76	ILE
13	S	68	ARG
17	X	57	LEU
18	Z	6	VAL
22	r	92	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) 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	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	79	ASN
4	D	83	ASN
4	D	88	HIS
4	D	92	HIS

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Mol	Chain	Res	Type
4	D	112	HIS
4	D	117	HIS
4	D	147	ASN
4	D	160	ASN
4	D	168	GLN
4	D	182	ASN
4	D	270	ASN
4	D	381	HIS
4	D	454	GLN
5	E	68	ASN
5	E	132	GLN
5	E	245	GLN
6	F	44	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	281	HIS
6	F	303	HIS
6	F	313	ASN
6	F	346	GLN
6	F	418	GLN
7	G	74	ASN
7	G	205	GLN
7	G	260	ASN
7	G	444	HIS
7	G	495	ASN
7	G	498	GLN
7	G	514	ASN
7	G	571	HIS
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	124	ASN
8	H	169	GLN
8	H	258	ASN
8	H	287	HIS
8	H	292	ASN
10	P	43	HIS
10	P	79	GLN

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Mol	Chain	Res	Type
10	P	102	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
10	P	356	HIS
11	Q	51	GLN
11	Q	86	ASN
11	Q	88	GLN
12	R	58	ASN
13	S	25	GLN
13	S	48	HIS
15	V	41	HIS
16	W	54	GLN
16	W	94	GLN
16	W	105	HIS
17	X	77	HIS
17	X	140	ASN
18	Z	135	ASN
19	a	31	ASN
20	b	83	ASN
21	q	31	ASN
21	q	52	ASN
21	q	87	HIS
21	q	91	HIS
21	q	113	HIS
21	q	116	ASN
22	r	21	GLN
22	r	29	GLN
22	r	52	ASN
22	r	110	GLN
23	s	59	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
25	SF4	G	802	7	0,12,12	-	-	-		
24	3PE	b	201	-	45,45,50	0.97	2 (4%)	48,50,55	1.10	3 (6%)
25	SF4	I	303	9	0,12,12	-	-	-		
25	SF4	G	801	7	0,12,12	-	-	-		
31	NDP	P	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.67	11 (16%)
26	UQ1	D	501	-	18,18,18	1.32	3 (16%)	22,25,25	1.61	5 (22%)
27	FES	E	301	5	0,4,4	-	-	-		
30	PC1	I	301	-	46,46,53	0.99	2 (4%)	52,54,61	1.10	3 (5%)
33	EHZ	W	201	-	27,31,37	1.73	5 (18%)	37,41,47	1.55	5 (13%)
28	FMN	F	501	-	33,33,33	1.38	5 (15%)	48,50,50	1.23	7 (14%)
25	SF4	B	301	2	0,12,12	-	-	-		
34	CDL	q	201	-	56,56,99	1.19	4 (7%)	62,68,111	1.26	6 (9%)
27	FES	G	803	7	0,4,4	-	-	-		
30	PC1	q	202	-	34,34,53	1.14	2 (5%)	40,42,61	1.20	4 (10%)
24	3PE	A	401	-	45,45,50	1.11	5 (11%)	48,50,55	1.27	3 (6%)
24	3PE	H	402	-	45,45,50	0.92	2 (4%)	48,50,55	1.33	5 (10%)
25	SF4	F	502	6	0,12,12	-	-	-		
25	SF4	I	302	9	0,12,12	-	-	-		
29	UQ9	H	401	-	35,35,58	0.84	3 (8%)	42,45,73	0.63	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SF4	G	802	7	-	-	0/6/5/5
24	3PE	b	201	-	-	10/49/49/54	-
25	SF4	I	303	9	-	-	0/6/5/5
25	SF4	G	801	7	-	-	0/6/5/5
31	NDP	P	401	-	-	2/34/77/77	0/5/5/5
26	UQ1	D	501	-	-	6/9/33/33	0/1/1/1
27	FES	E	301	5	-	-	0/1/1/1
30	PC1	I	301	-	-	10/50/50/57	-
33	EHZ	W	201	-	-	12/39/39/45	-
28	FMN	F	501	-	-	0/18/18/18	0/3/3/3
25	SF4	B	301	2	-	-	0/6/5/5
34	CDL	q	201	-	-	15/67/67/110	-
27	FES	G	803	7	-	-	0/1/1/1
30	PC1	q	202	-	-	14/38/38/57	-
24	3PE	A	401	-	-	18/49/49/54	-
24	3PE	H	402	-	-	11/49/49/54	-
25	SF4	F	502	6	-	-	0/6/5/5
25	SF4	I	302	9	-	-	0/6/5/5
29	UQ9	H	401	-	-	15/30/54/81	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	W	201	EHZ	C15-N2	5.15	1.44	1.33
33	W	201	EHZ	C12-N1	5.03	1.44	1.33
28	F	501	FMN	C9A-C5A	4.80	1.49	1.41
24	b	201	3PE	O31-C31	4.26	1.45	1.33
31	P	401	NDP	C5A-C4A	4.22	1.46	1.39
30	I	301	PC1	O31-C31	4.17	1.45	1.33
34	q	201	CDL	OB8-CB7	4.15	1.45	1.33
34	q	201	CDL	OA8-CA7	4.11	1.45	1.33
30	q	202	PC1	O31-C31	4.06	1.45	1.33
34	q	201	CDL	OA6-CA5	4.06	1.45	1.34
30	q	202	PC1	O21-C21	4.05	1.45	1.34
24	b	201	3PE	O21-C21	4.04	1.45	1.34
30	I	301	PC1	O21-C21	4.02	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	q	201	CDL	OB6-CB5	4.00	1.45	1.34
26	D	501	UQ1	C2-C1	-3.91	1.37	1.48
24	H	402	3PE	O21-C21	3.84	1.45	1.34
24	H	402	3PE	O31-C31	3.71	1.44	1.33
24	A	401	3PE	O21-C21	3.26	1.43	1.34
31	P	401	NDP	C6N-C5N	3.23	1.39	1.33
24	A	401	3PE	O31-C31	3.00	1.42	1.33
28	F	501	FMN	C8-C7	2.99	1.48	1.40
29	H	401	UQ9	C3-C2	-2.80	1.40	1.48
31	P	401	NDP	C5A-C6A	2.60	1.48	1.41
28	F	501	FMN	C4-N3	-2.59	1.34	1.38
29	H	401	UQ9	C4-C5	-2.52	1.41	1.48
26	D	501	UQ1	C3-C4	-2.46	1.41	1.48
33	W	201	EHZ	O4-C15	-2.44	1.18	1.23
31	P	401	NDP	C8A-N7A	2.41	1.36	1.31
33	W	201	EHZ	O3-C12	-2.38	1.18	1.23
31	P	401	NDP	C5A-N7A	-2.34	1.34	1.39
26	D	501	UQ1	C3-C2	2.33	1.45	1.36
29	H	401	UQ9	C6-C5	-2.28	1.40	1.46
28	F	501	FMN	C4A-N5	2.20	1.35	1.30
33	W	201	EHZ	C9-S1	2.20	1.81	1.76
24	A	401	3PE	P-O12	-2.12	1.45	1.55
28	F	501	FMN	C5A-N5	-2.08	1.35	1.39
24	A	401	3PE	O21-C2	-2.06	1.41	1.46
24	A	401	3PE	O31-C3	-2.06	1.40	1.45

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	P	401	NDP	C5A-C4A-N3A	-6.13	118.75	126.75
33	W	201	EHZ	C8-C9-S1	6.05	121.11	113.63
31	P	401	NDP	N3A-C4A-N9A	4.75	134.91	127.08
24	A	401	3PE	O21-C21-C22	4.72	121.67	111.50
26	D	501	UQ1	O1-C1-C2	-4.70	110.95	120.93
24	H	402	3PE	O21-C21-C22	4.64	121.50	111.50
30	I	301	PC1	O21-C21-C22	4.37	120.91	111.50
34	q	201	CDL	OA6-CA5-C11	4.36	120.90	111.50
24	b	201	3PE	O21-C21-C22	4.13	120.41	111.50
30	q	202	PC1	O21-C21-C22	4.02	120.17	111.50
31	P	401	NDP	PN-O3-PA	-3.90	119.43	132.83
31	P	401	NDP	C2A-N3A-C4A	3.84	120.82	111.75
34	q	201	CDL	OB6-CB5-C51	3.63	119.32	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	501	UQ1	C3-C2-C1	-3.31	114.18	120.68
31	P	401	NDP	C4A-C5A-N7A	-3.29	106.61	110.62
24	H	402	3PE	C3-C2-C1	-3.20	104.22	111.79
30	q	202	PC1	O31-C31-C32	3.08	121.56	111.91
31	P	401	NDP	N3A-C2A-N1A	-3.08	123.79	128.60
30	I	301	PC1	O31-C31-C32	2.84	120.83	111.91
30	I	301	PC1	C2-O21-C21	-2.80	110.89	117.79
31	P	401	NDP	C5A-N7A-C8A	2.80	107.49	103.51
24	A	401	3PE	O31-C31-C32	2.79	120.66	111.91
31	P	401	NDP	C4A-N9A-C8A	2.71	108.67	105.73
28	F	501	FMN	C4-C4A-N5	2.71	122.09	118.23
34	q	201	CDL	OB8-CB7-C71	2.70	120.38	111.91
34	q	201	CDL	OA8-CA7-C31	2.63	120.16	111.91
29	H	401	UQ9	C1M-C1-C6	-2.63	120.11	124.40
33	W	201	EHZ	C10-S1-C9	2.62	110.03	101.87
24	b	201	3PE	C2-O21-C21	-2.58	111.43	117.79
24	b	201	3PE	O31-C31-C32	2.57	119.99	111.91
28	F	501	FMN	C4A-C10-N1	-2.55	118.81	124.73
24	H	402	3PE	O31-C31-C32	2.54	119.88	111.91
33	W	201	EHZ	C13-C12-N1	2.47	120.58	116.42
34	q	201	CDL	CA4-OA6-CA5	-2.44	111.77	117.79
33	W	201	EHZ	C14-N2-C15	-2.43	118.25	122.59
24	H	402	3PE	C24-C23-C22	-2.36	104.70	113.19
33	W	201	EHZ	O2-C9-S1	-2.35	119.56	122.61
30	q	202	PC1	C2-O21-C21	-2.35	112.01	117.79
34	q	201	CDL	CB4-OB6-CB5	-2.27	112.19	117.79
24	A	401	3PE	O12-P-O14	-2.26	101.08	112.24
28	F	501	FMN	O2-C2-N1	-2.21	118.16	121.83
31	P	401	NDP	C6A-C5A-N7A	2.21	136.13	132.02
31	P	401	NDP	N9A-C8A-N7A	-2.20	110.91	113.91
28	F	501	FMN	C4A-C10-N10	2.19	119.67	116.48
28	F	501	FMN	O4-C4-C4A	-2.18	120.82	126.60
26	D	501	UQ1	O1-C1-C6	-2.18	117.73	121.55
30	q	202	PC1	O31-C31-O32	-2.14	118.18	123.59
26	D	501	UQ1	CM2-O2-C2	2.11	123.93	116.47
28	F	501	FMN	C10-N1-C2	2.10	121.10	116.90
24	H	402	3PE	C26-C25-C24	-2.09	103.80	114.42
31	P	401	NDP	C3D-C2D-C1D	2.05	105.31	101.43
26	D	501	UQ1	O2-C2-C3	2.04	131.31	123.64
28	F	501	FMN	C4A-C4-N3	2.03	118.35	113.19

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	401	3PE	O22-C21-O21-C2
24	H	402	3PE	C11-O13-P-O11
24	H	402	3PE	C11-O13-P-O12
24	H	402	3PE	C11-O13-P-O14
24	H	402	3PE	O13-C11-C12-N
24	b	201	3PE	C1-O11-P-O14
24	b	201	3PE	O22-C21-O21-C2
26	D	501	UQ1	C1-C6-C7-C8
26	D	501	UQ1	C5-C6-C7-C8
29	H	401	UQ9	C24-C26-C27-C28
29	H	401	UQ9	C22-C23-C24-C26
29	H	401	UQ9	C22-C23-C24-C25
29	H	401	UQ9	C21-C22-C23-C24
29	H	401	UQ9	C19-C21-C22-C23
29	H	401	UQ9	C17-C18-C19-C21
29	H	401	UQ9	C17-C18-C19-C20
30	I	301	PC1	C11-O13-P-O12
30	I	301	PC1	C11-O13-P-O14
30	I	301	PC1	C11-O13-P-O11
30	q	202	PC1	C11-O13-P-O14
30	q	202	PC1	C1-O11-P-O12
30	q	202	PC1	C1-O11-P-O14
30	q	202	PC1	C1-O11-P-O13
33	W	201	EHZ	O1-C7-C8-C9
33	W	201	EHZ	C6-C7-C8-C9
33	W	201	EHZ	C16-C17-C20-O6
33	W	201	EHZ	O2-C9-S1-C10
33	W	201	EHZ	C8-C9-S1-C10
34	q	201	CDL	CA3-OA5-PA1-OA3
34	q	201	CDL	CA3-OA5-PA1-OA4
24	H	402	3PE	O32-C31-O31-C3
24	b	201	3PE	C32-C31-O31-C3
26	D	501	UQ1	C7-C8-C9-C10
26	D	501	UQ1	C7-C8-C9-C11
24	b	201	3PE	O32-C31-O31-C3
24	H	402	3PE	C32-C31-O31-C3
24	A	401	3PE	C22-C21-O21-C2
24	b	201	3PE	C22-C21-O21-C2
29	H	401	UQ9	C7-C8-C9-C10
30	I	301	PC1	C32-C31-O31-C3
30	I	301	PC1	O32-C31-O31-C3
29	H	401	UQ9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	H	402	3PE	C24-C25-C26-C27
24	A	401	3PE	C32-C31-O31-C3
30	q	202	PC1	C2-C1-O11-P
24	A	401	3PE	O32-C31-O31-C3
34	q	201	CDL	C12-C13-C14-C15
30	q	202	PC1	C11-O13-P-O11
34	q	201	CDL	CA3-OA5-PA1-OA2
33	W	201	EHZ	C18-C17-C20-O6
33	W	201	EHZ	C19-C17-C20-O6
24	A	401	3PE	C3-C2-O21-C21
24	A	401	3PE	O13-C11-C12-N
29	H	401	UQ9	C7-C8-C9-C11
24	H	402	3PE	C39-C3A-C3B-C3C
33	W	201	EHZ	C3-C4-C5-C6
34	q	201	CDL	C11-CA5-OA6-CA4
24	A	401	3PE	C27-C28-C29-C2A
33	W	201	EHZ	C5-C6-C7-O1
24	A	401	3PE	O21-C2-C3-O31
33	W	201	EHZ	C5-C6-C7-C8
34	q	201	CDL	C31-CA7-OA8-CA6
30	q	202	PC1	C32-C31-O31-C3
31	P	401	NDP	O4D-C1D-N1N-C6N
24	A	401	3PE	C37-C38-C39-C3A
34	q	201	CDL	OB6-CB4-CB6-OB8
24	H	402	3PE	C34-C35-C36-C37
34	q	201	CDL	OA7-CA5-OA6-CA4
30	I	301	PC1	C11-C12-N-C15
24	A	401	3PE	C2B-C2C-C2D-C2E
34	q	201	CDL	OA9-CA7-OA8-CA6
34	q	201	CDL	CB3-CB4-CB6-OB8
30	q	202	PC1	O32-C31-O31-C3
30	I	301	PC1	C11-C12-N-C13
30	q	202	PC1	C32-C33-C34-C35
24	A	401	3PE	C22-C23-C24-C25
24	H	402	3PE	C1-O11-P-O13
24	b	201	3PE	C1-O11-P-O13
30	I	301	PC1	C1-O11-P-O13
34	q	201	CDL	CA4-CA3-OA5-PA1
24	b	201	3PE	C1-O11-P-O12
30	q	202	PC1	C11-O13-P-O12
26	D	501	UQ1	C1-C2-O2-CM2
33	W	201	EHZ	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
30	q	202	PC1	O13-C11-C12-N
34	q	201	CDL	C1-CB2-OB2-PB2
33	W	201	EHZ	O4-C15-C16-O5
30	I	301	PC1	C11-C12-N-C14
29	H	401	UQ9	C12-C11-C9-C10
34	q	201	CDL	C1-CA2-OA2-PA1
24	A	401	3PE	O11-C1-C2-O21
34	q	201	CDL	CB2-OB2-PB2-OB5
24	A	401	3PE	C1-C2-C3-O31
24	A	401	3PE	C25-C26-C27-C28
31	P	401	NDP	PN-O3-PA-O2A
30	q	202	PC1	O11-C1-C2-C3
29	H	401	UQ9	C14-C16-C17-C18
24	b	201	3PE	C25-C26-C27-C28
24	A	401	3PE	C21-C22-C23-C24
30	q	202	PC1	C34-C35-C36-C37
29	H	401	UQ9	C12-C11-C9-C8
24	b	201	3PE	C2B-C2C-C2D-C2E
24	A	401	3PE	C39-C3A-C3B-C3C
24	H	402	3PE	C2F-C2G-C2H-C2I
30	q	202	PC1	C11-C12-N-C15
29	H	401	UQ9	C23-C24-C26-C27
24	A	401	3PE	C1-O11-P-O14
24	A	401	3PE	O11-C1-C2-C3
24	b	201	3PE	C37-C38-C39-C3A
34	q	201	CDL	C18-C19-C20-C21
29	H	401	UQ9	C25-C24-C26-C27
30	I	301	PC1	C2C-C2D-C2E-C2F
26	D	501	UQ1	C2-C3-O3-CM3

There are no ring outliers.

17 monomers are involved in 121 short contacts:

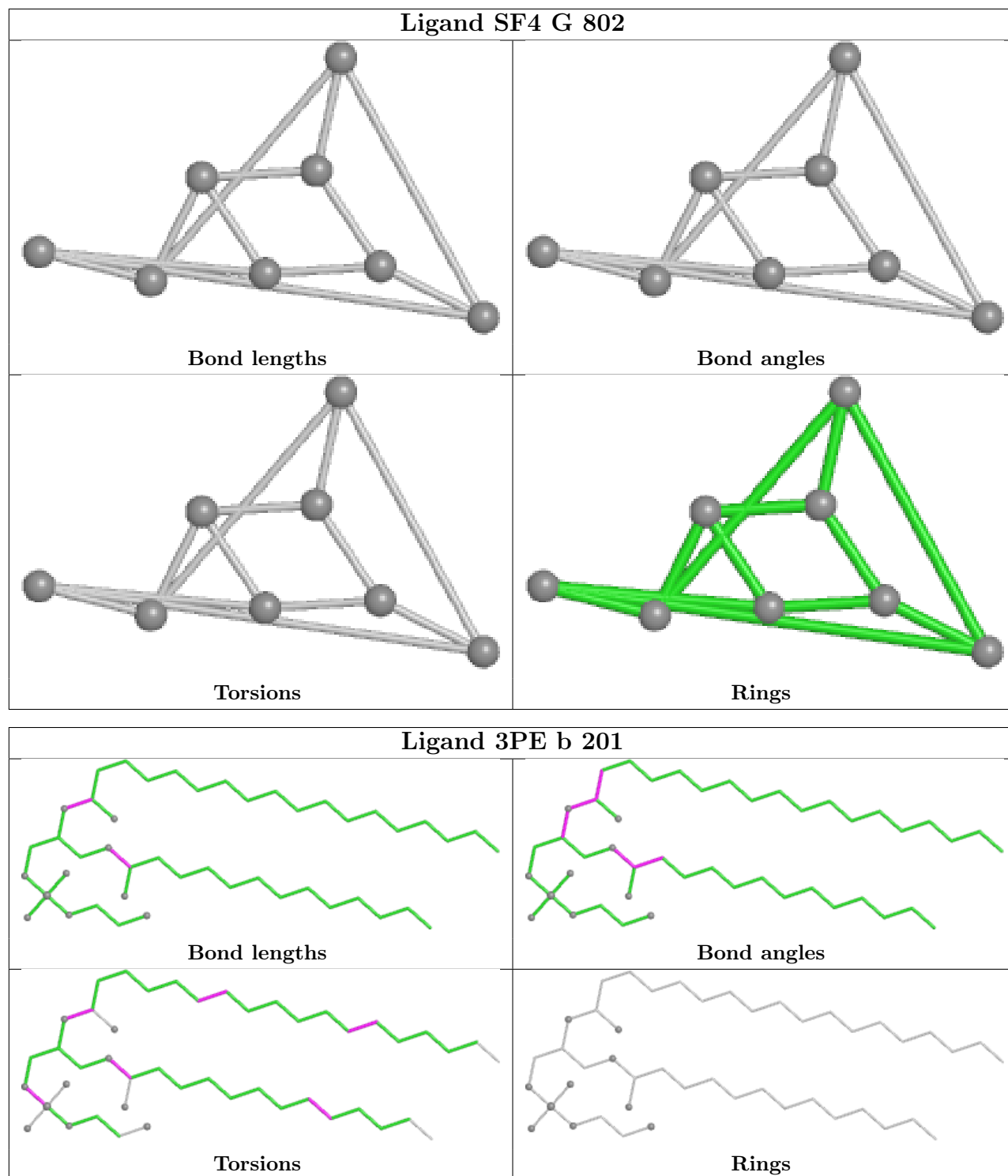
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	G	802	SF4	3	0
24	b	201	3PE	13	0
25	I	303	SF4	6	0
31	P	401	NDP	2	0
26	D	501	UQ1	14	0
27	E	301	FES	3	0
30	I	301	PC1	9	0
28	F	501	FMN	2	0

Continued on next page...

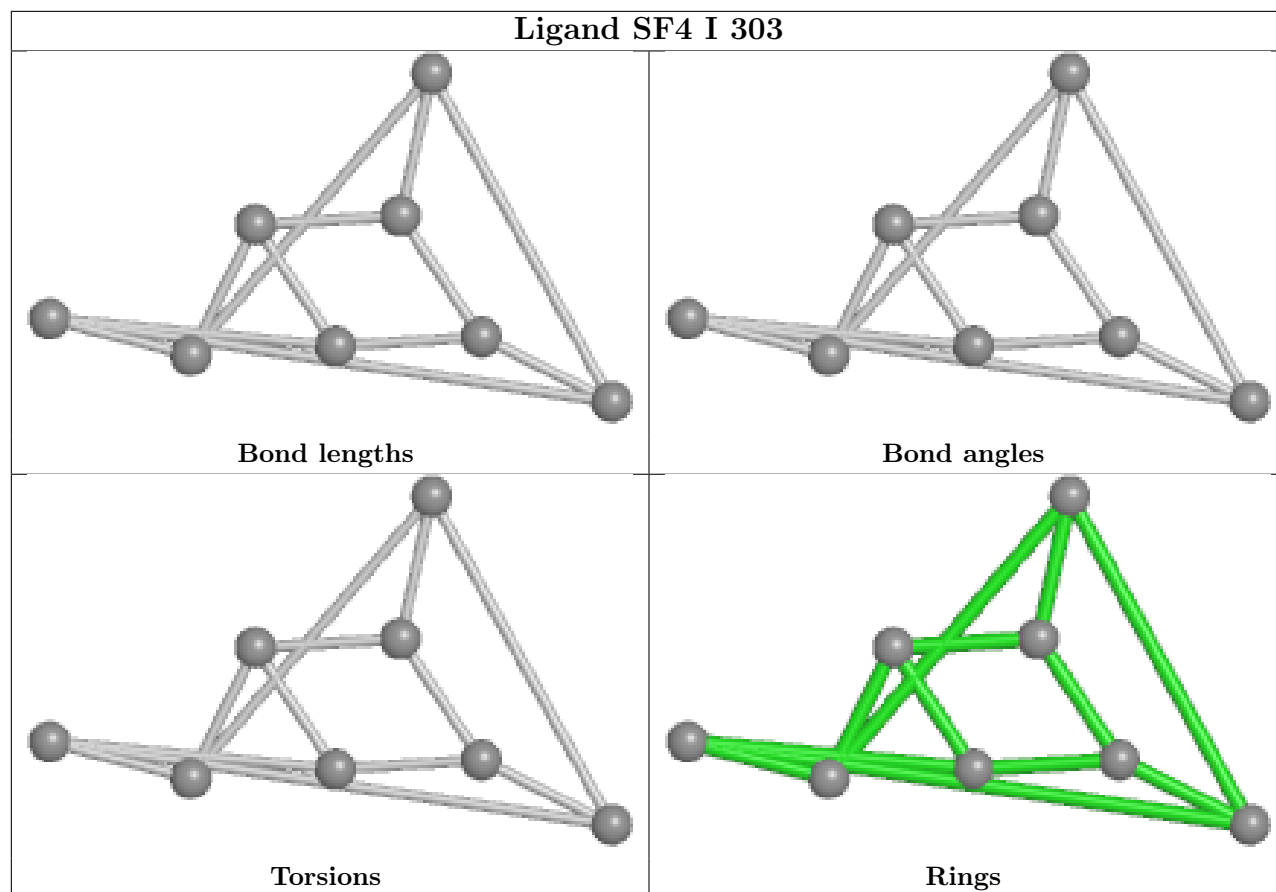
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	301	SF4	2	0
34	q	201	CDL	8	0
27	G	803	FES	6	0
30	q	202	PC1	6	0
24	A	401	3PE	3	0
24	H	402	3PE	16	0
25	F	502	SF4	9	0
25	I	302	SF4	10	0
29	H	401	UQ9	10	0

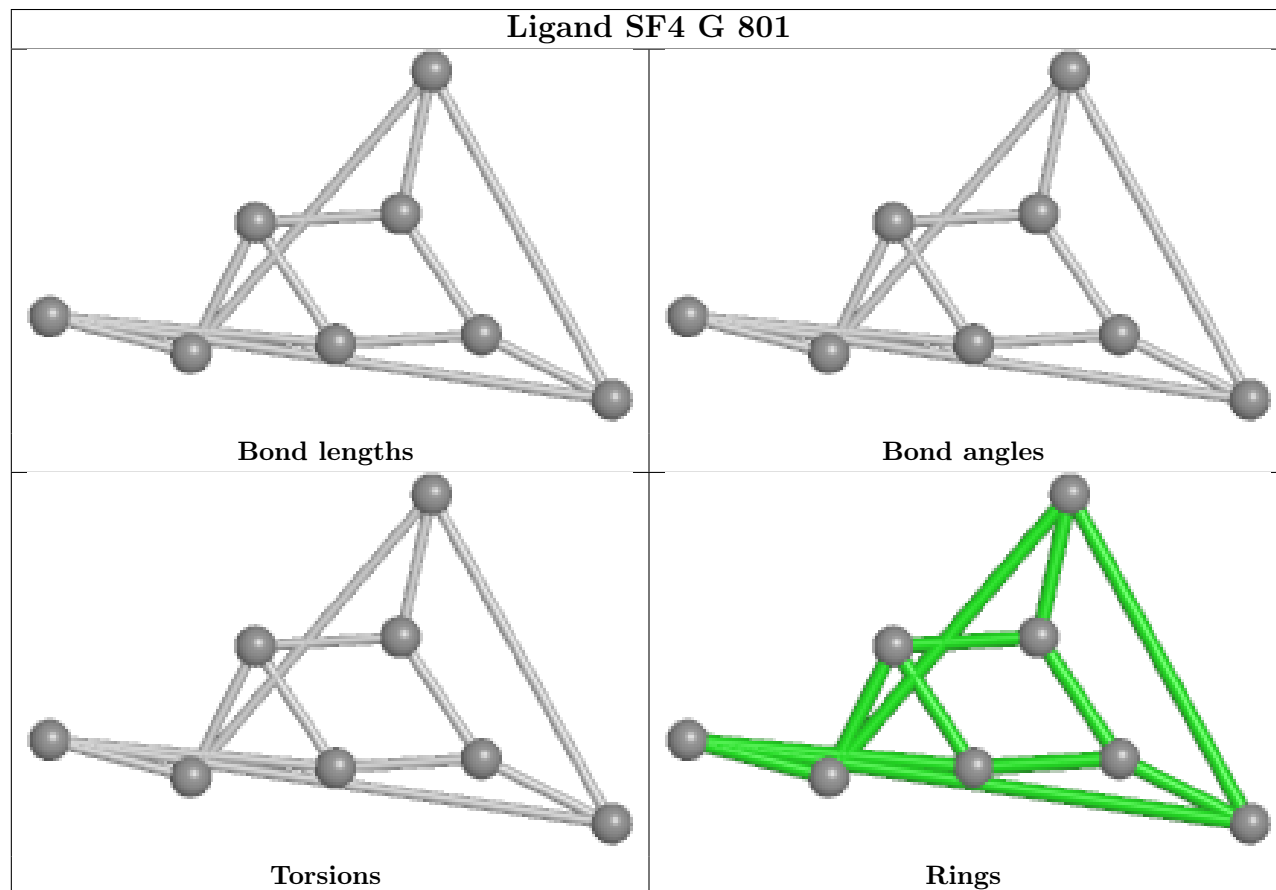
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

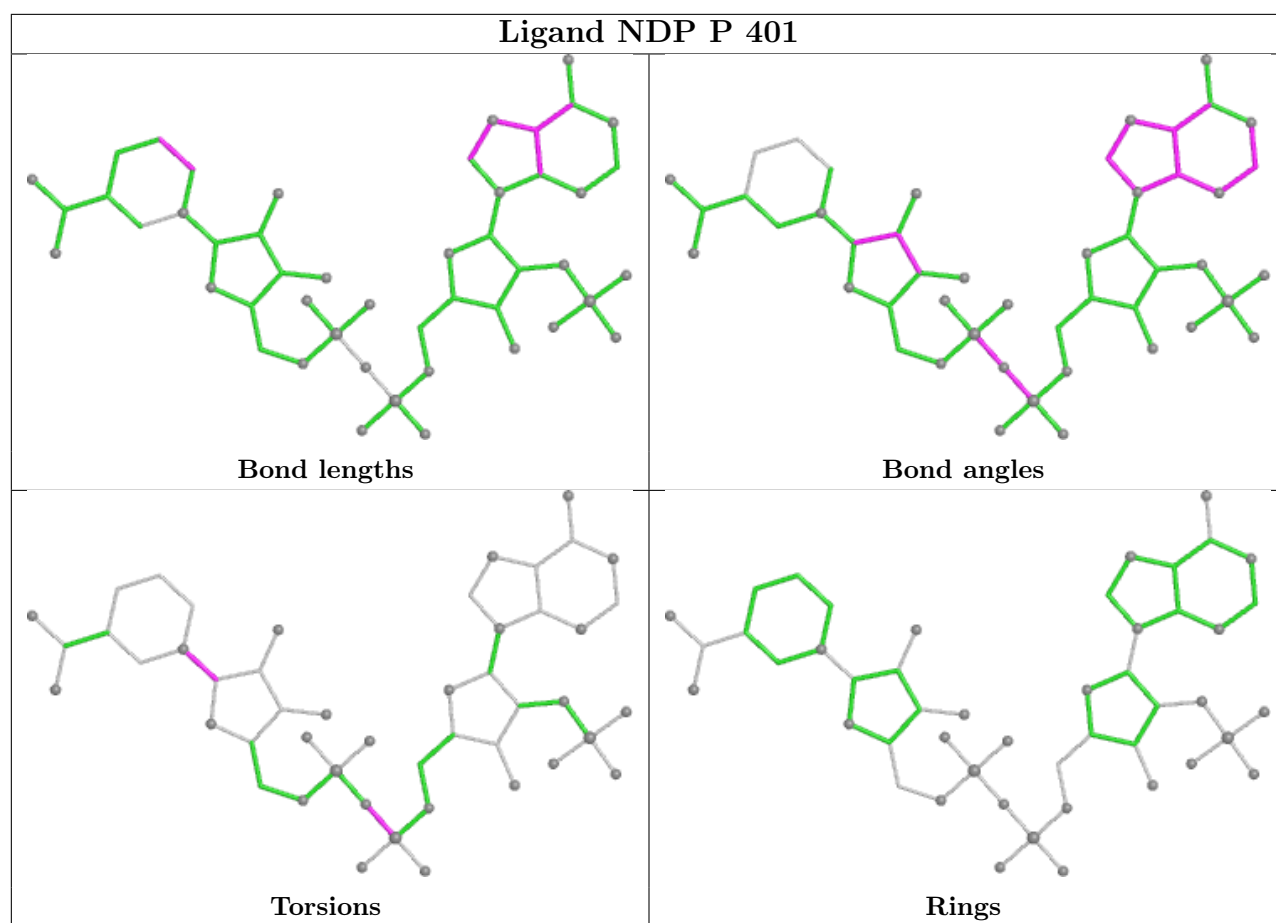


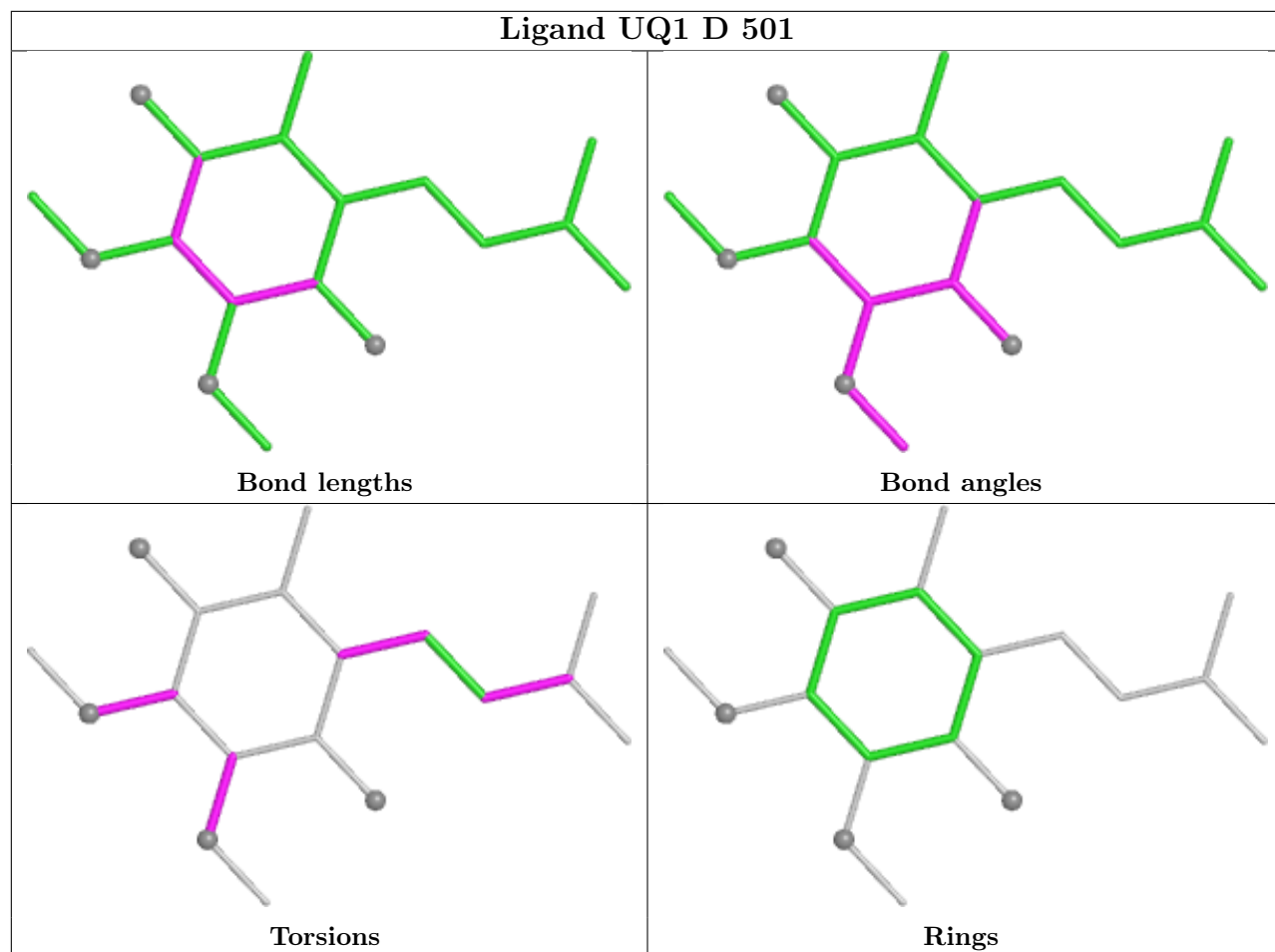
Ligand SF4 I 303

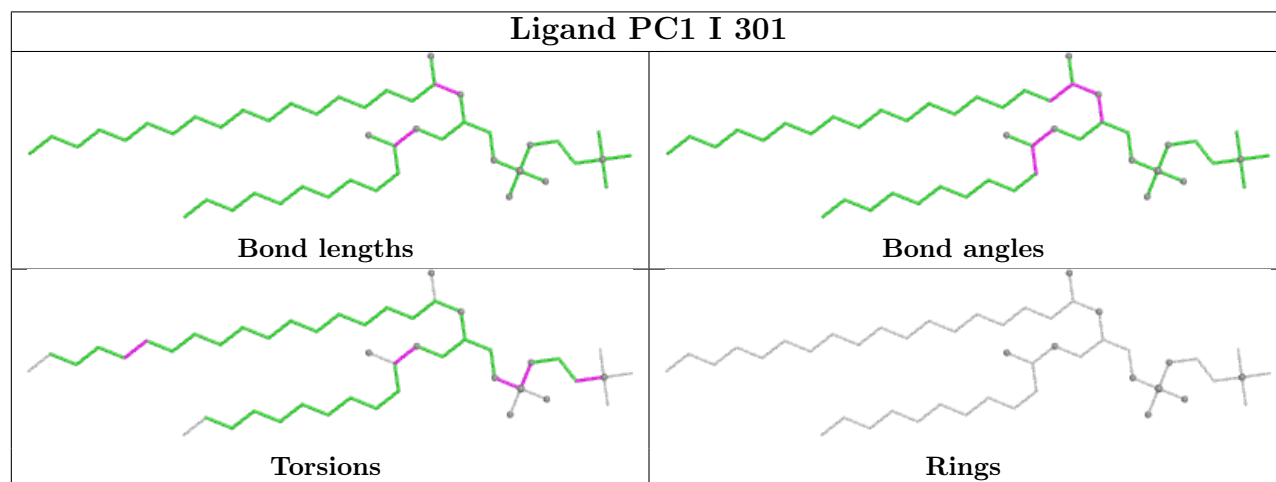
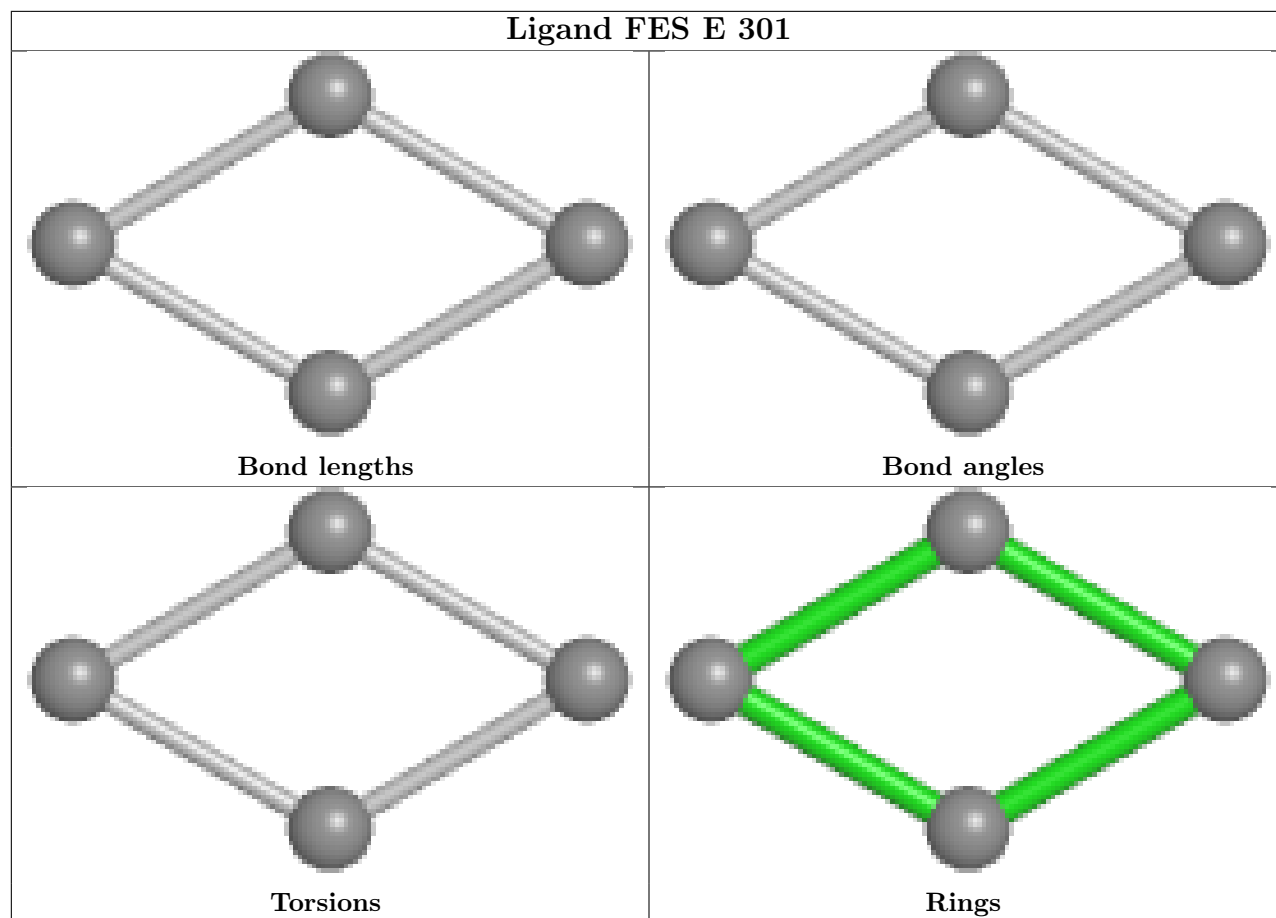


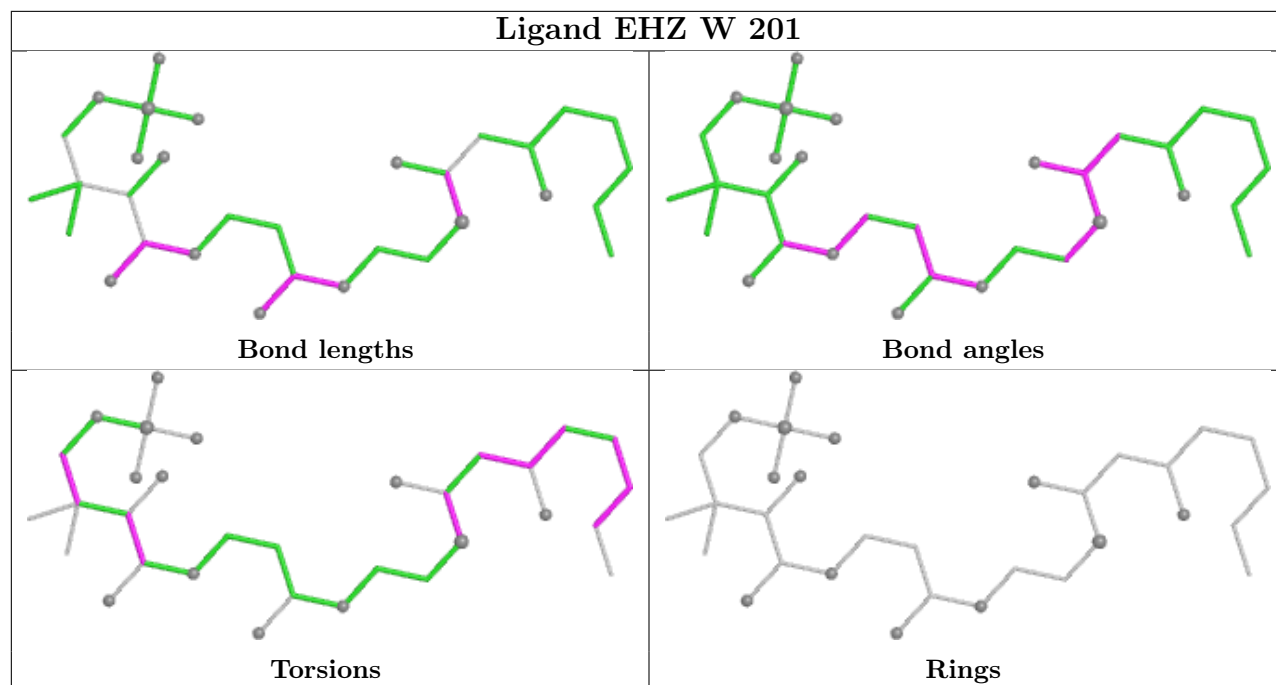
Ligand SF4 G 801

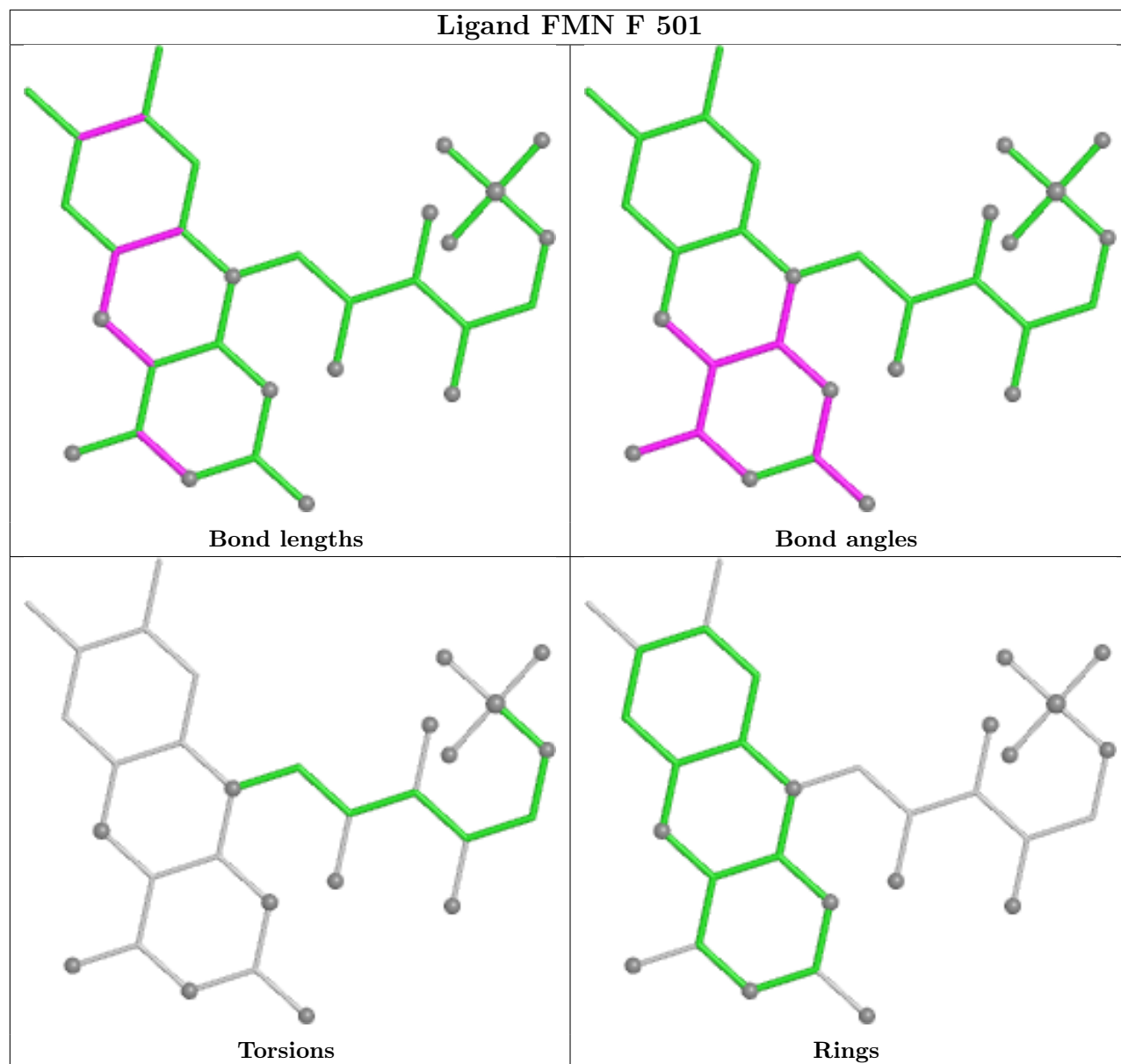


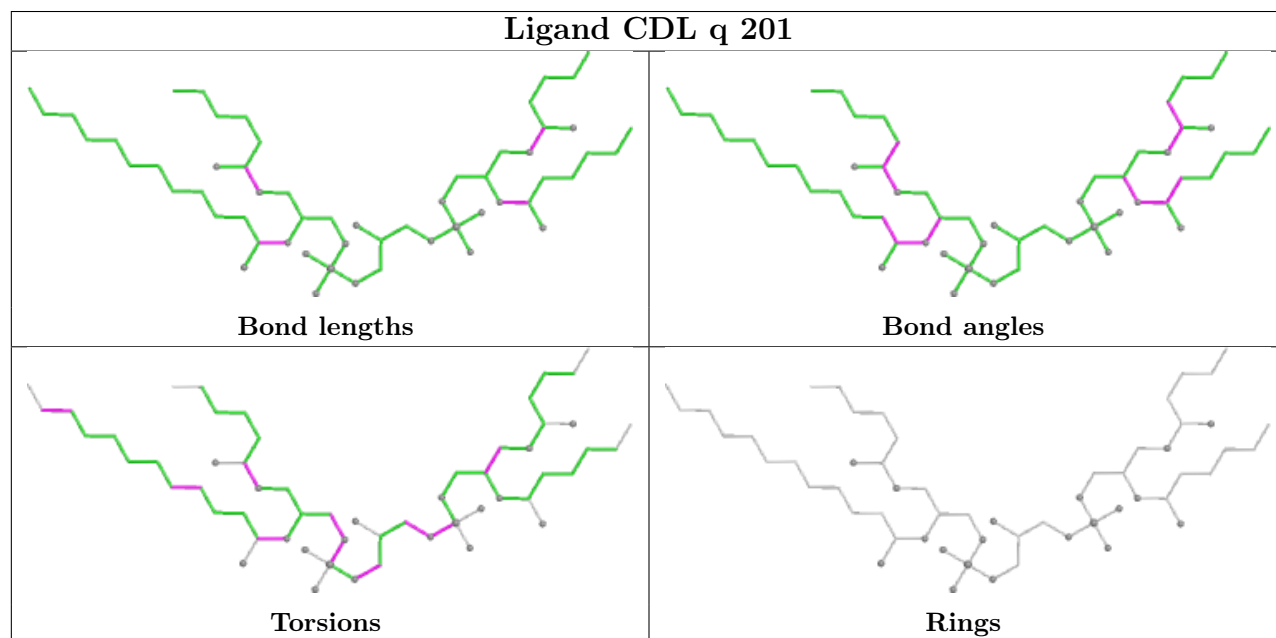
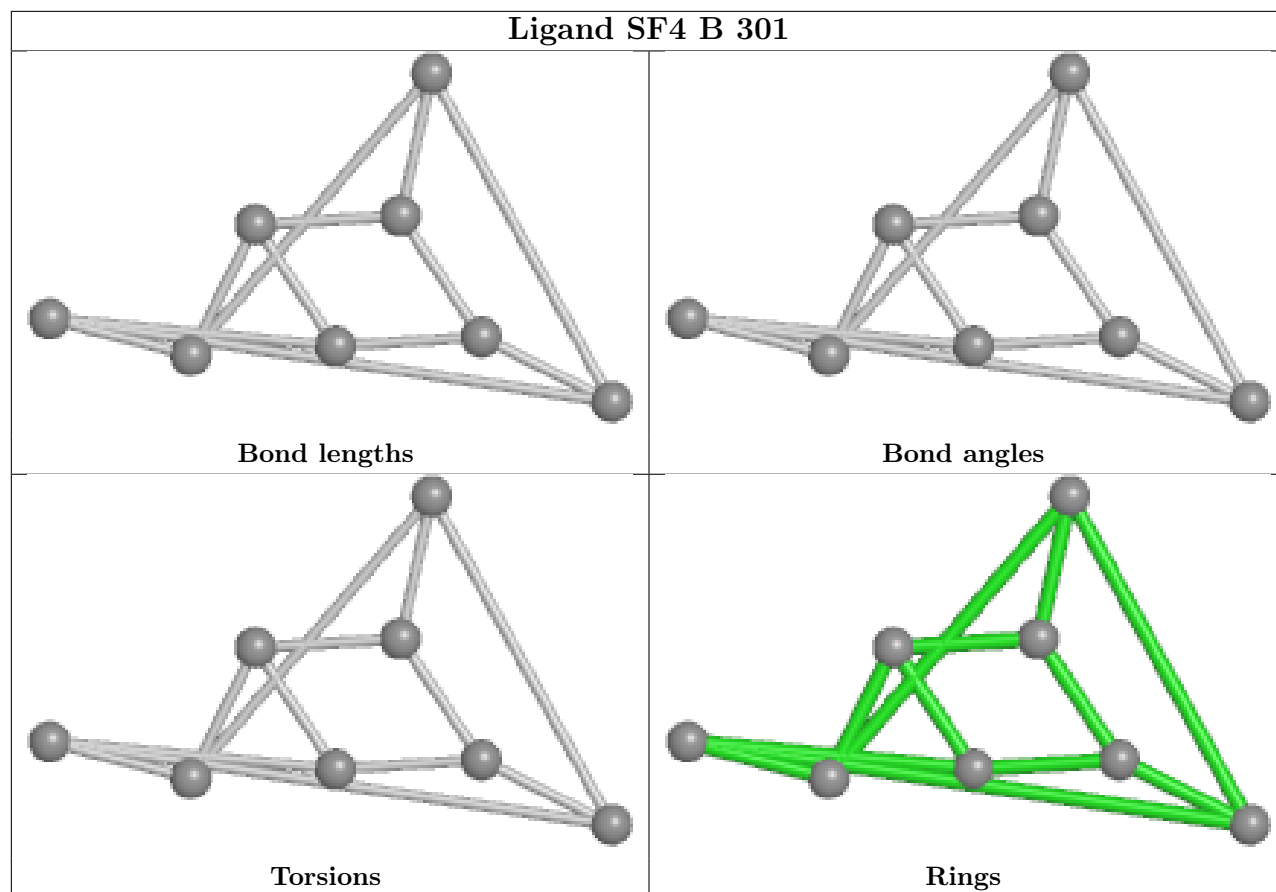


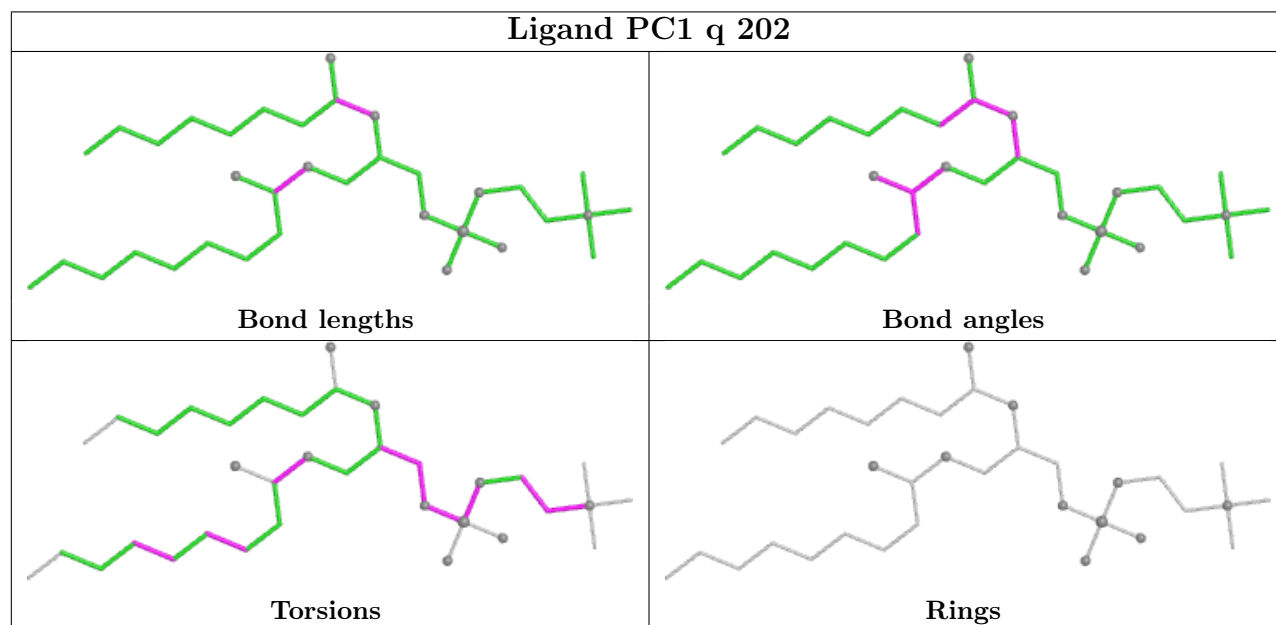
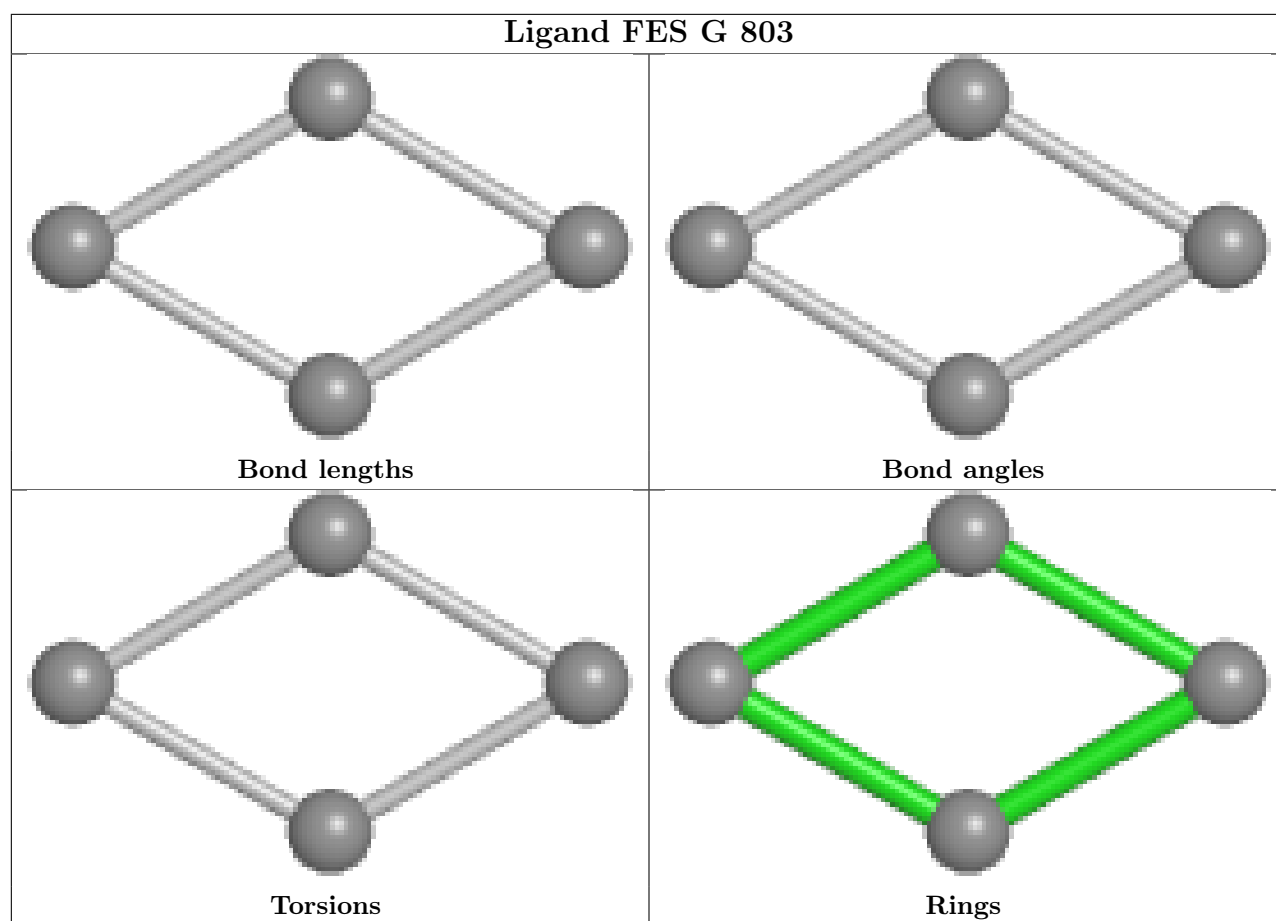


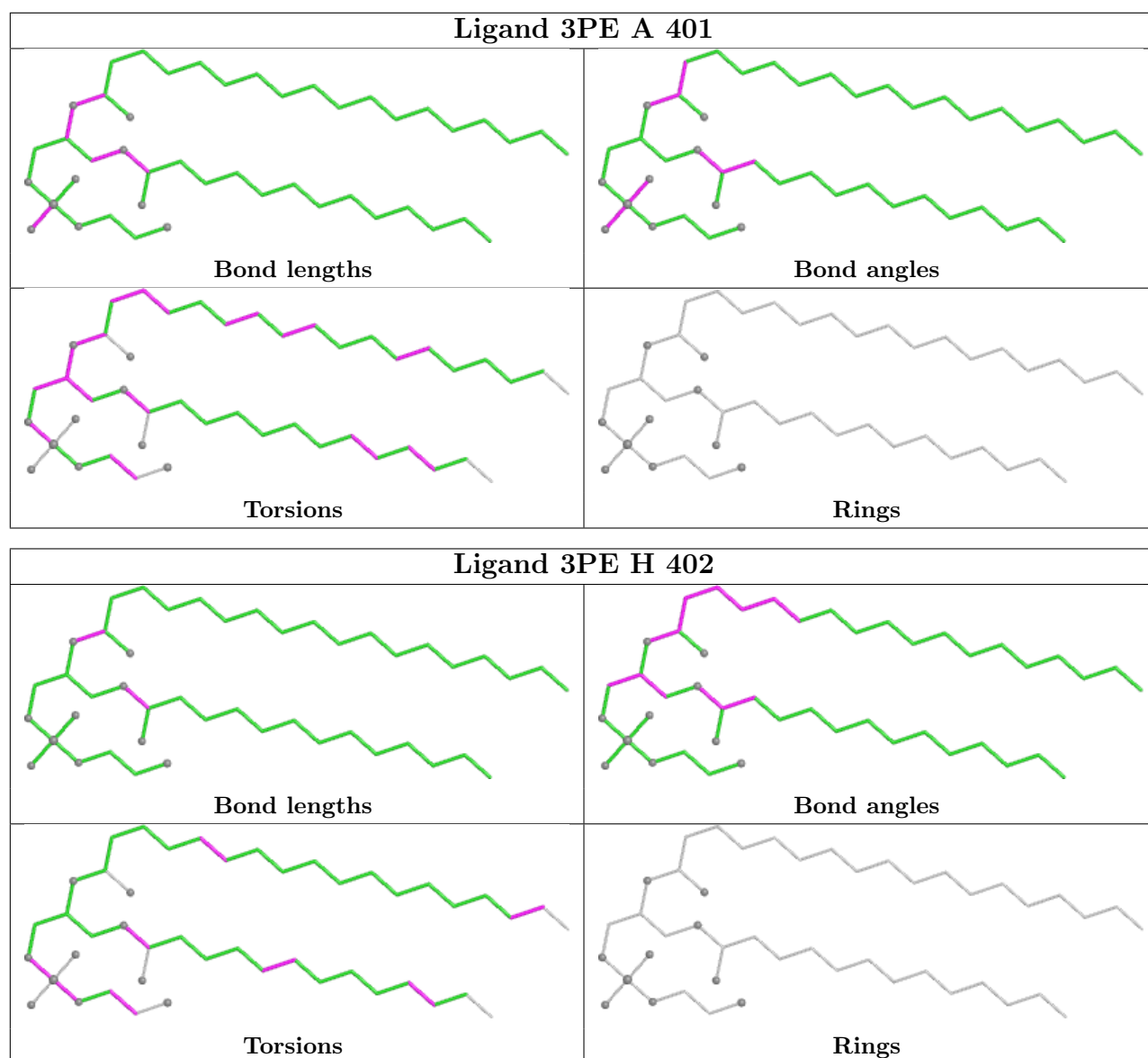


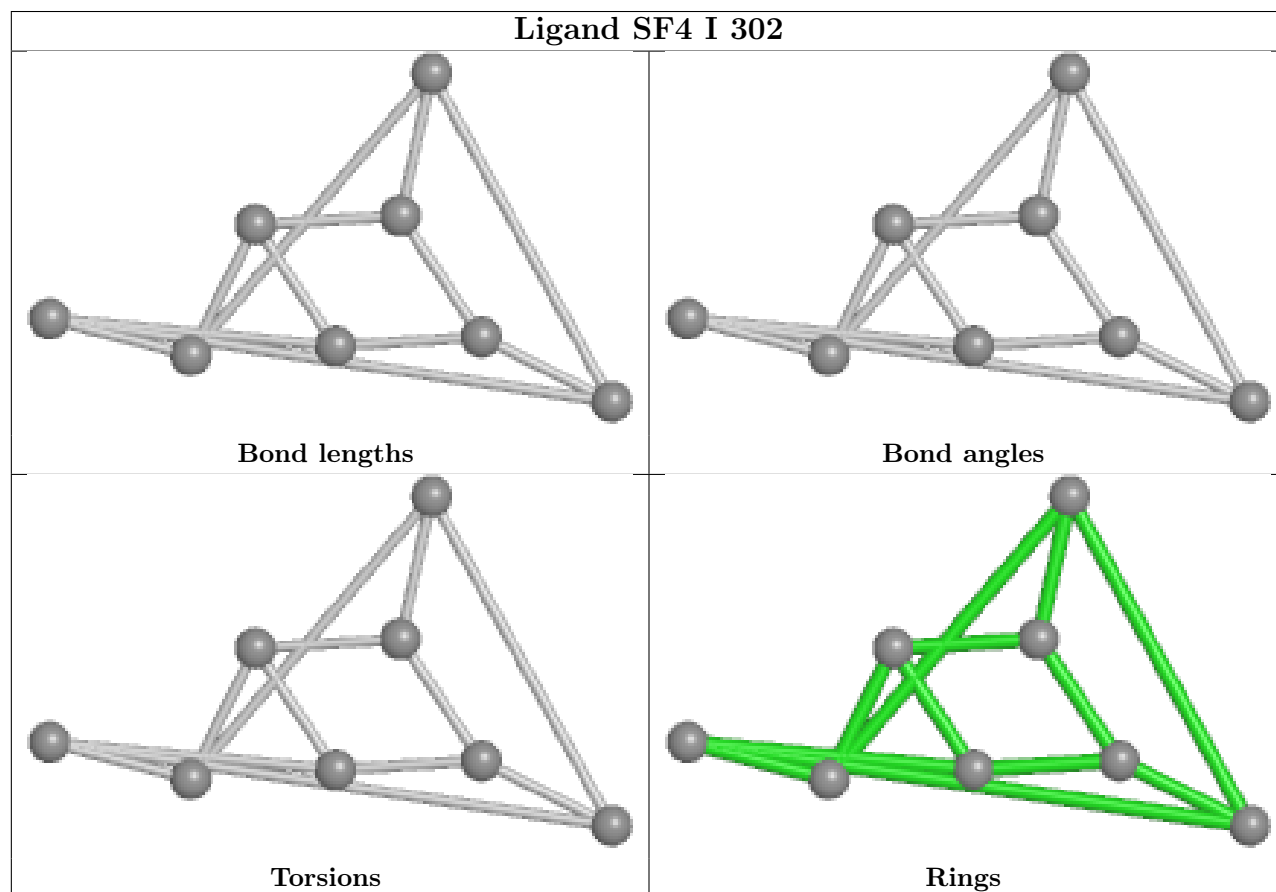
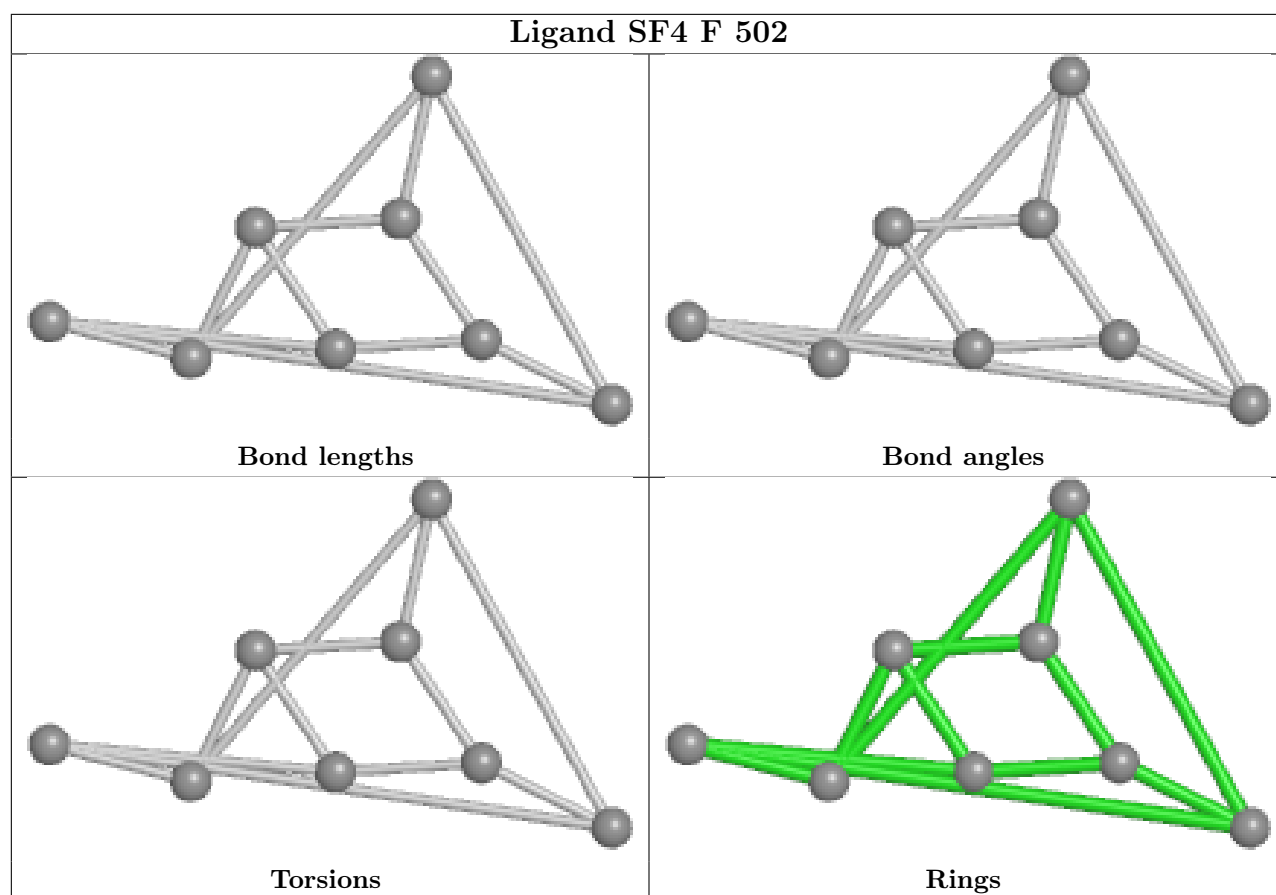


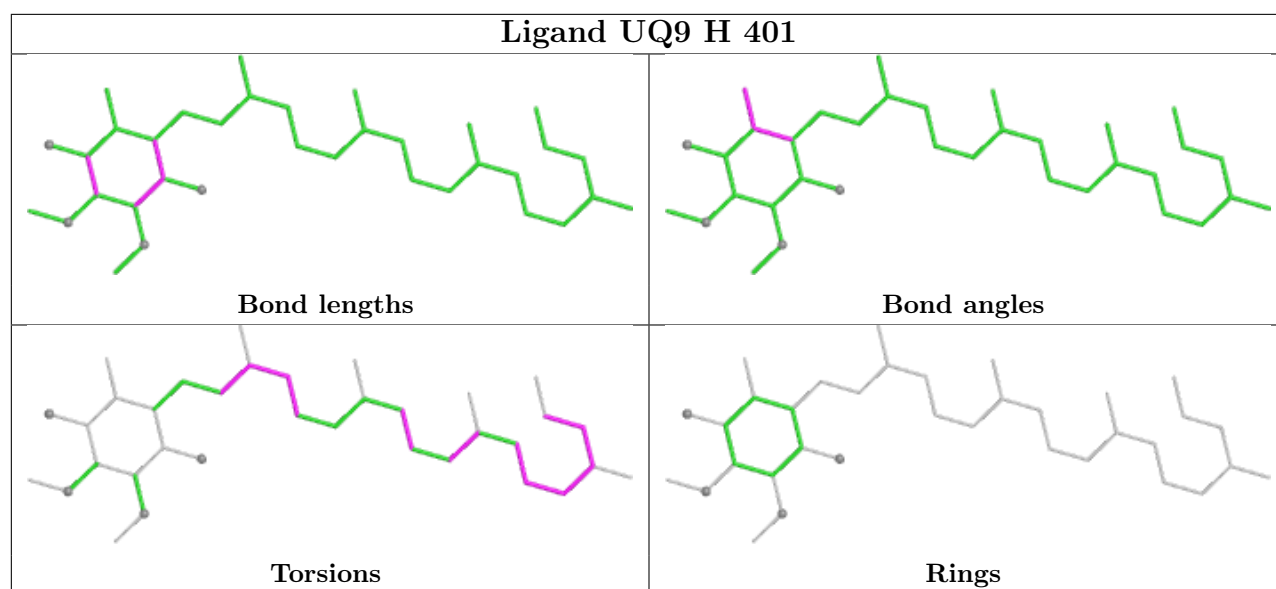












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

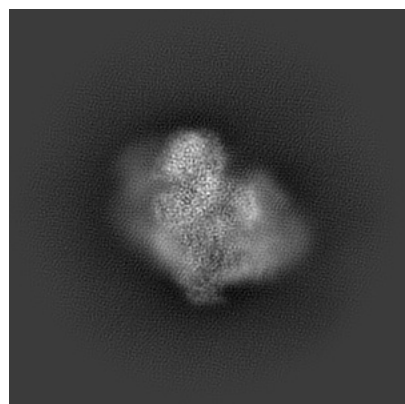
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35314. These allow visual inspection of the internal detail of the map and identification of artifacts.

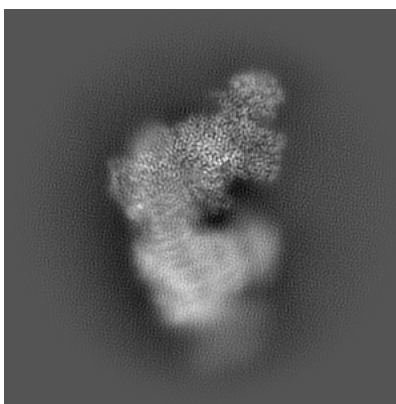
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

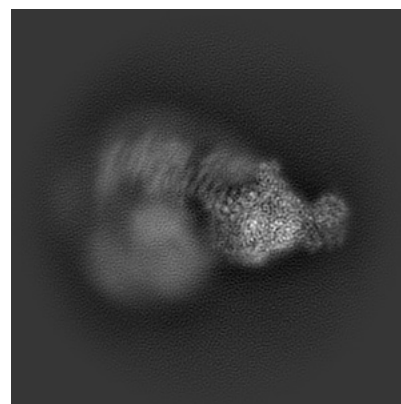
6.1.1 Primary map



X

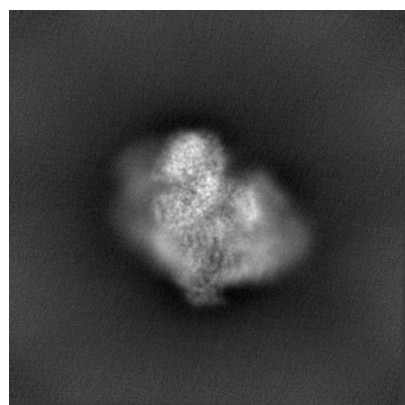


Y

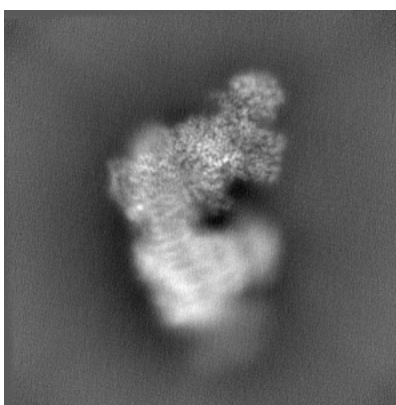


Z

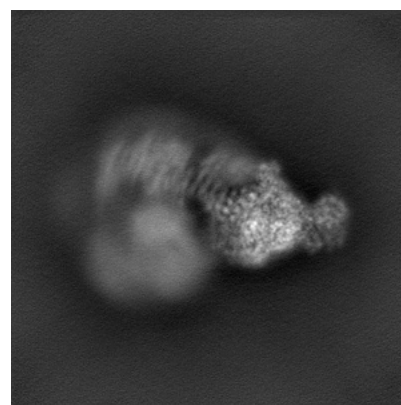
6.1.2 Raw map



X



Y

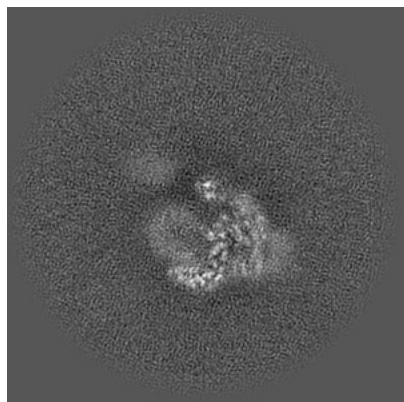


Z

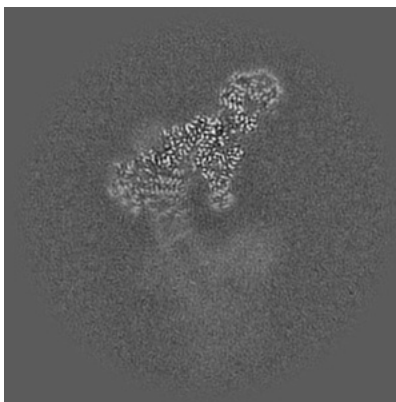
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

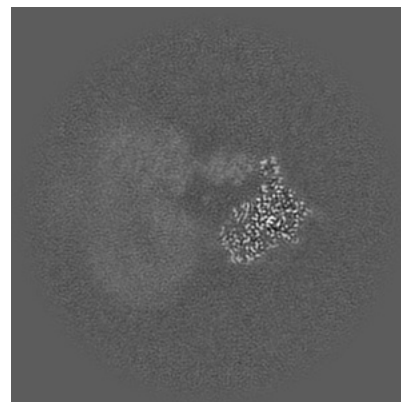
6.2.1 Primary map



X Index: 192

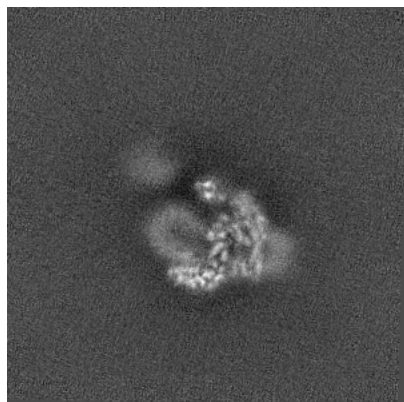


Y Index: 192

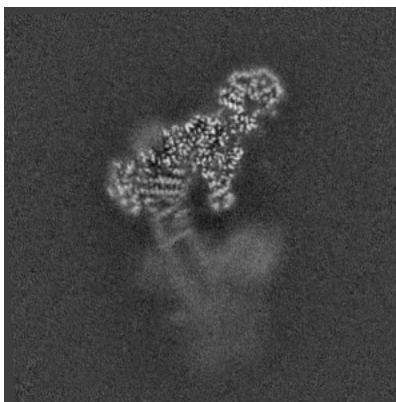


Z Index: 192

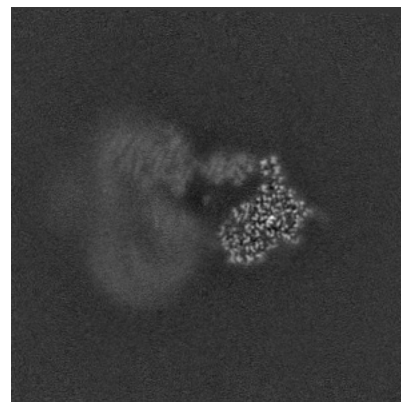
6.2.2 Raw map



X Index: 192



Y Index: 192

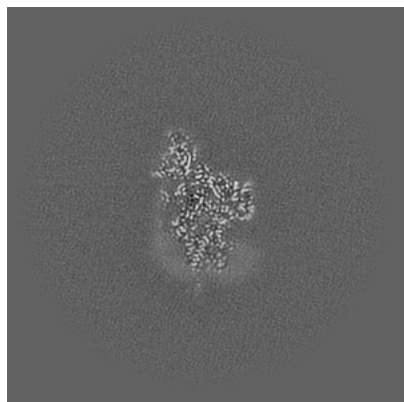


Z Index: 192

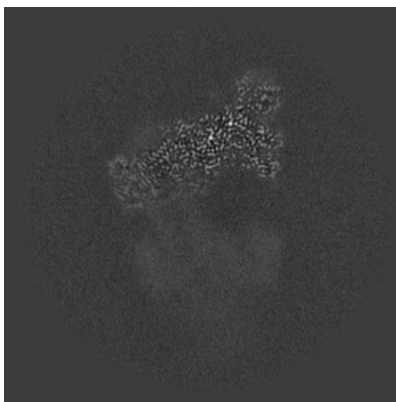
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

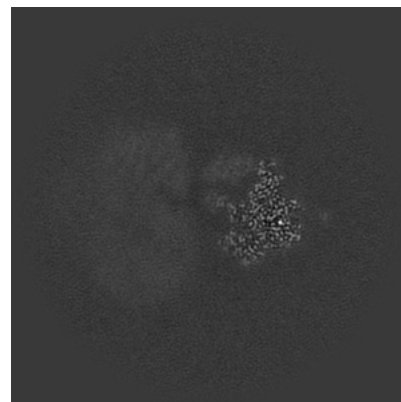
6.3.1 Primary map



X Index: 244

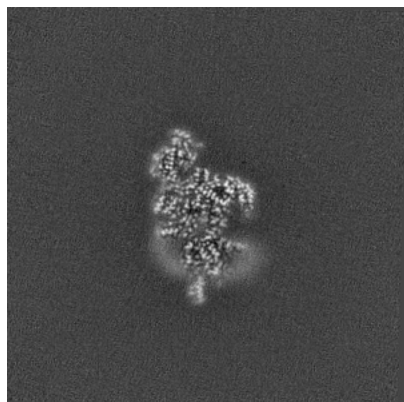


Y Index: 176

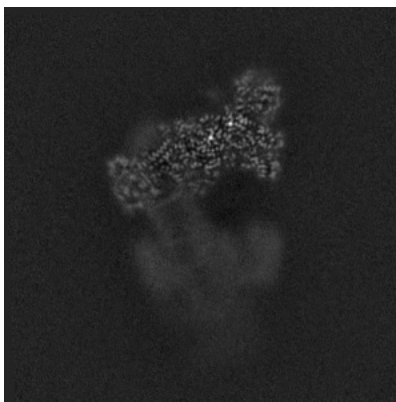


Z Index: 198

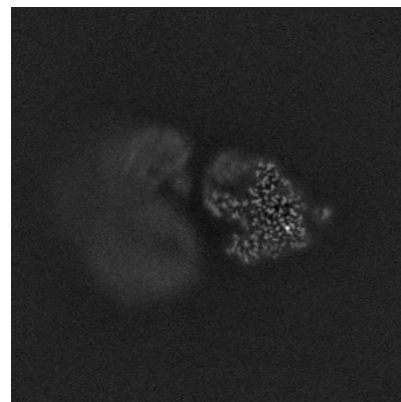
6.3.2 Raw map



X Index: 239



Y Index: 176

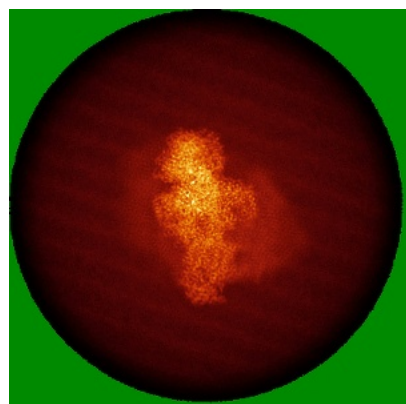


Z Index: 204

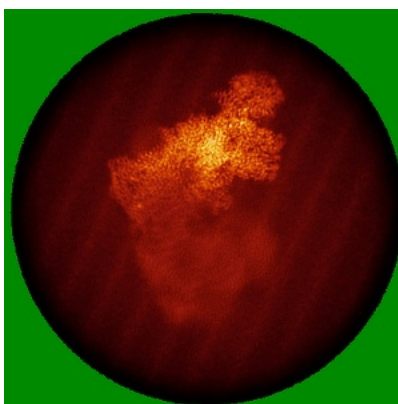
The images above show the largest variance slices of the map in three orthogonal directions.

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

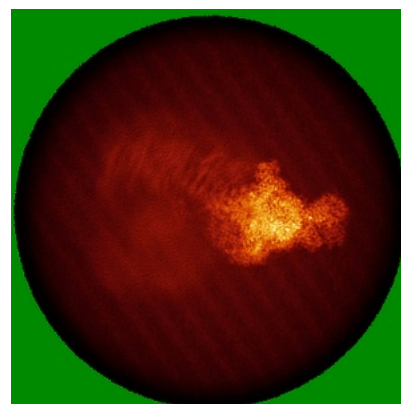
6.4.1 Primary map



X

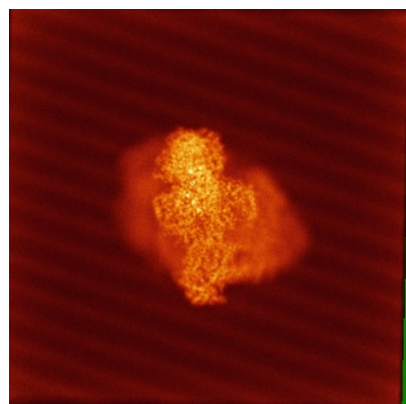


Y

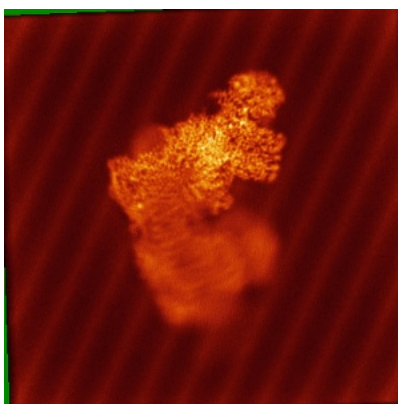


Z

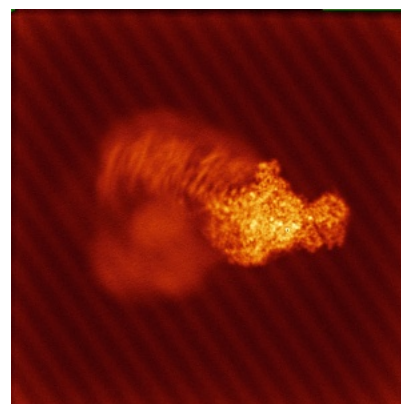
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



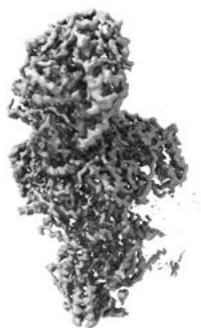
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

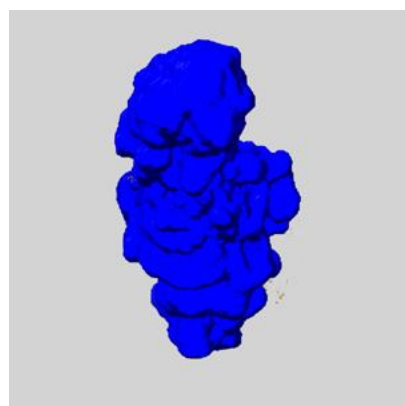
6.6 Mask visualisation [i](#)

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

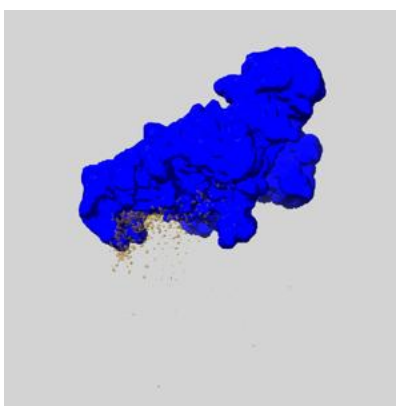
A mask typically either:

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

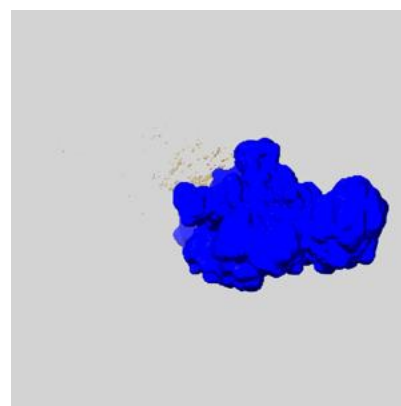
6.6.1 emd_35314_msk_1.map [i](#)



X



Y

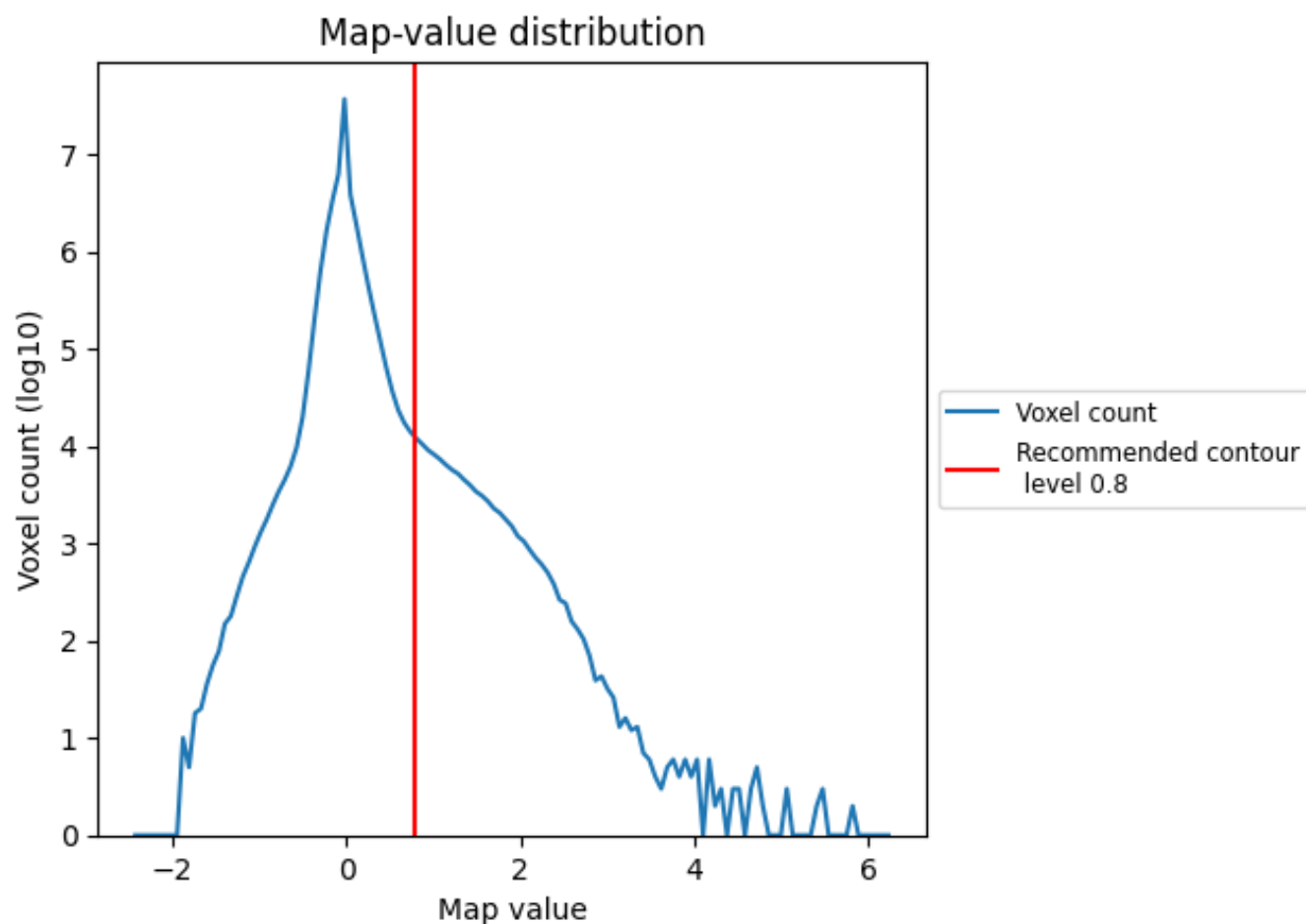


Z

7 Map analysis [i](#)

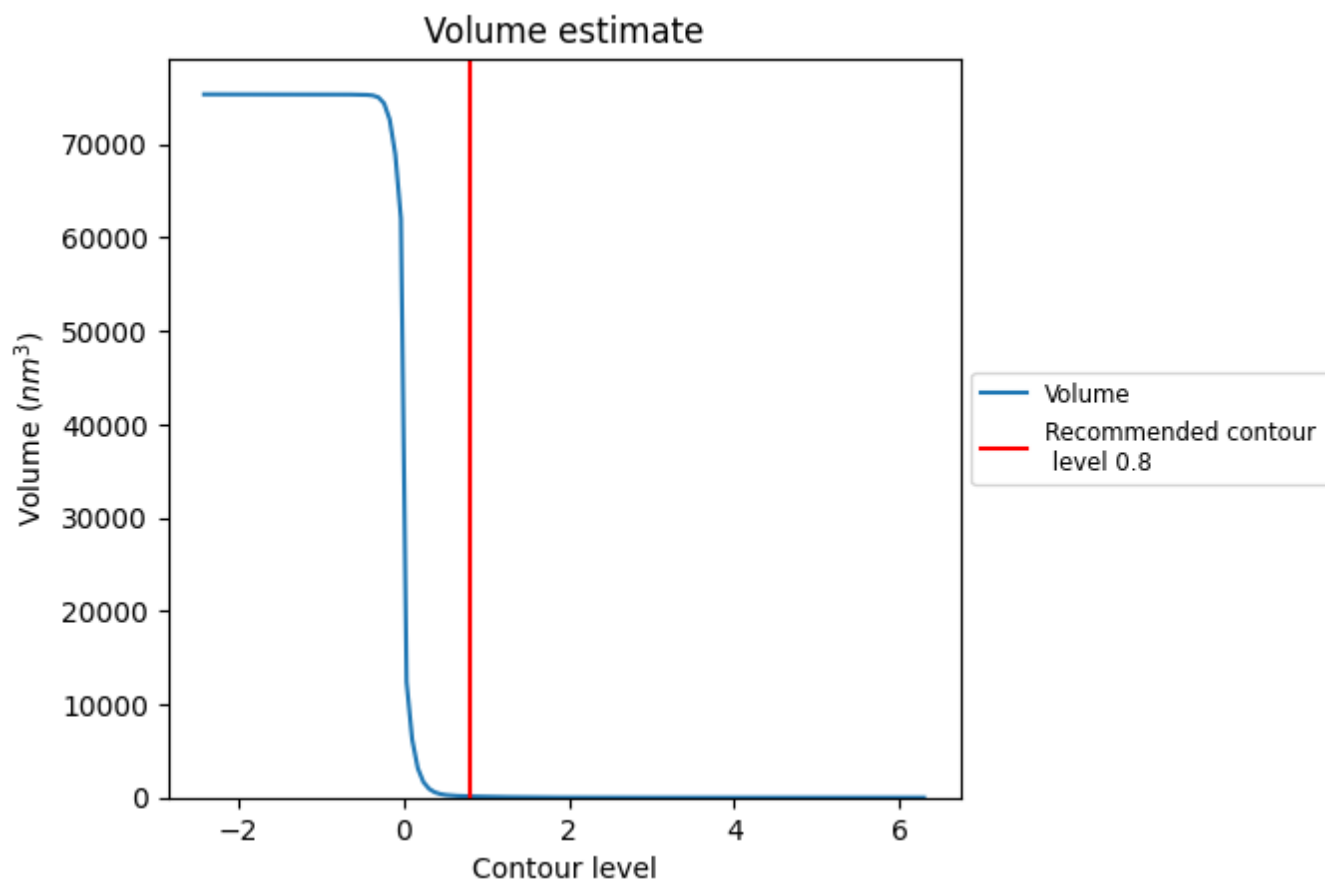
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

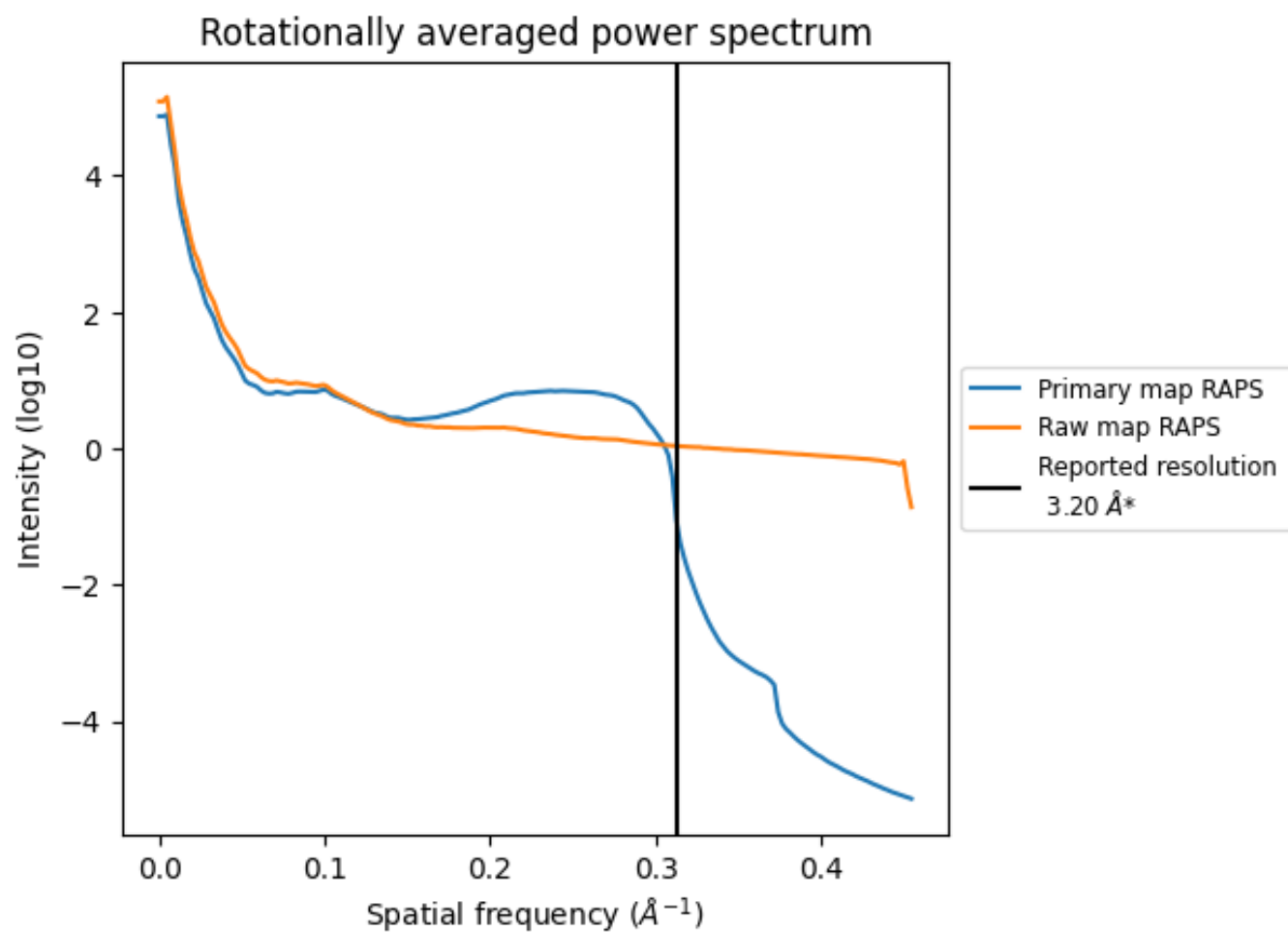
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm^3 ; this corresponds to an approximate mass of 117 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 ⓘ

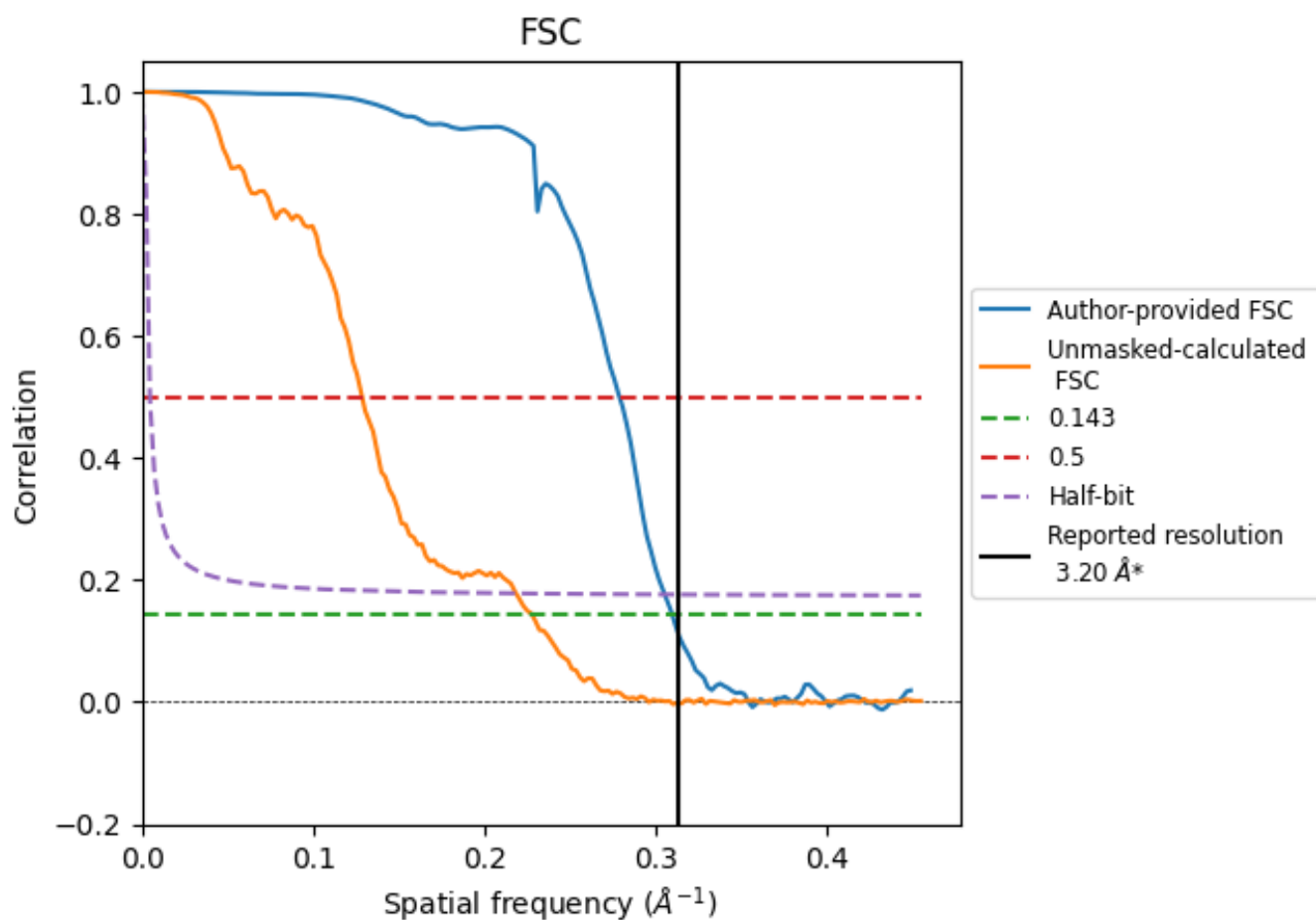


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

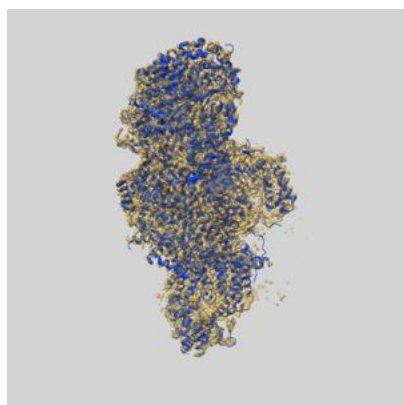
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.59	3.28
Unmasked-calculated*	4.39	7.78	4.58

*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 4.39 differs from the reported value 3.2 by more than 10 %

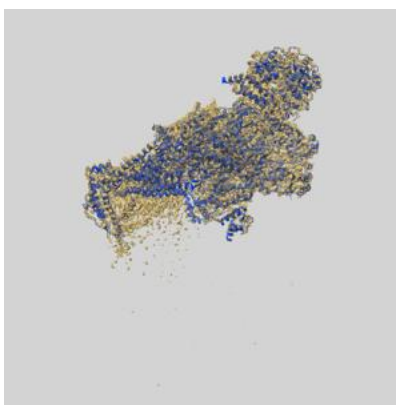
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35314 and PDB model 8IAP. Per-residue inclusion information can be found in section [3](#) on page [15](#).

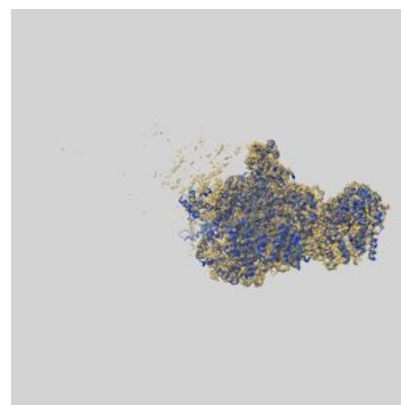
9.1 Map-model overlay [i](#)



X



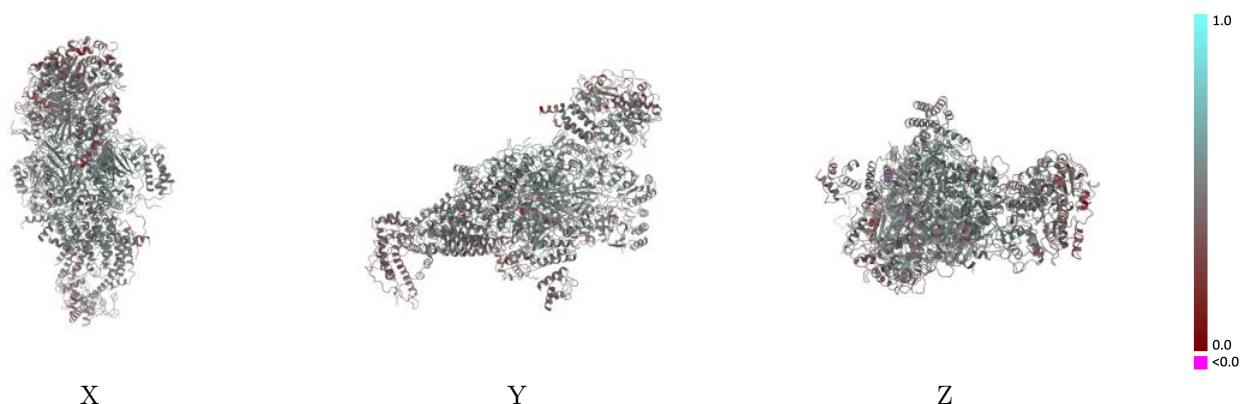
Y



Z

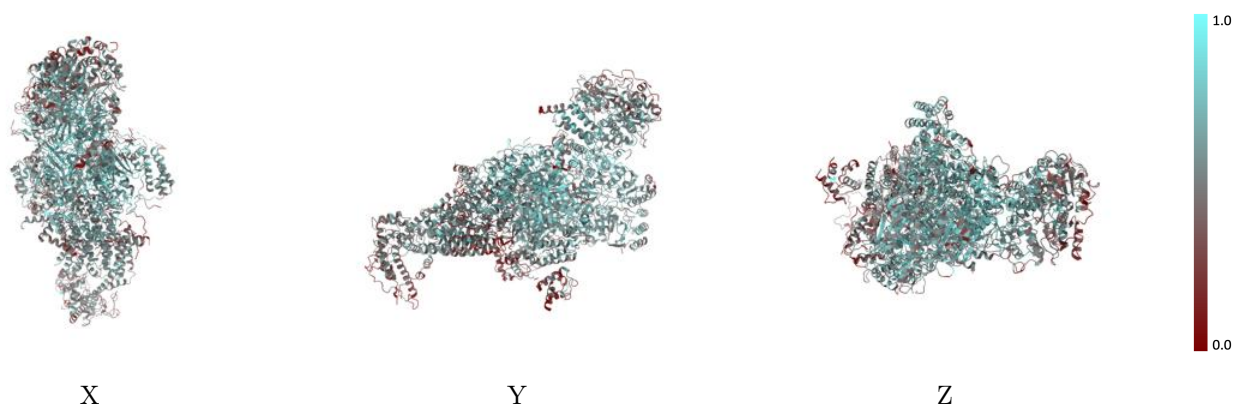
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



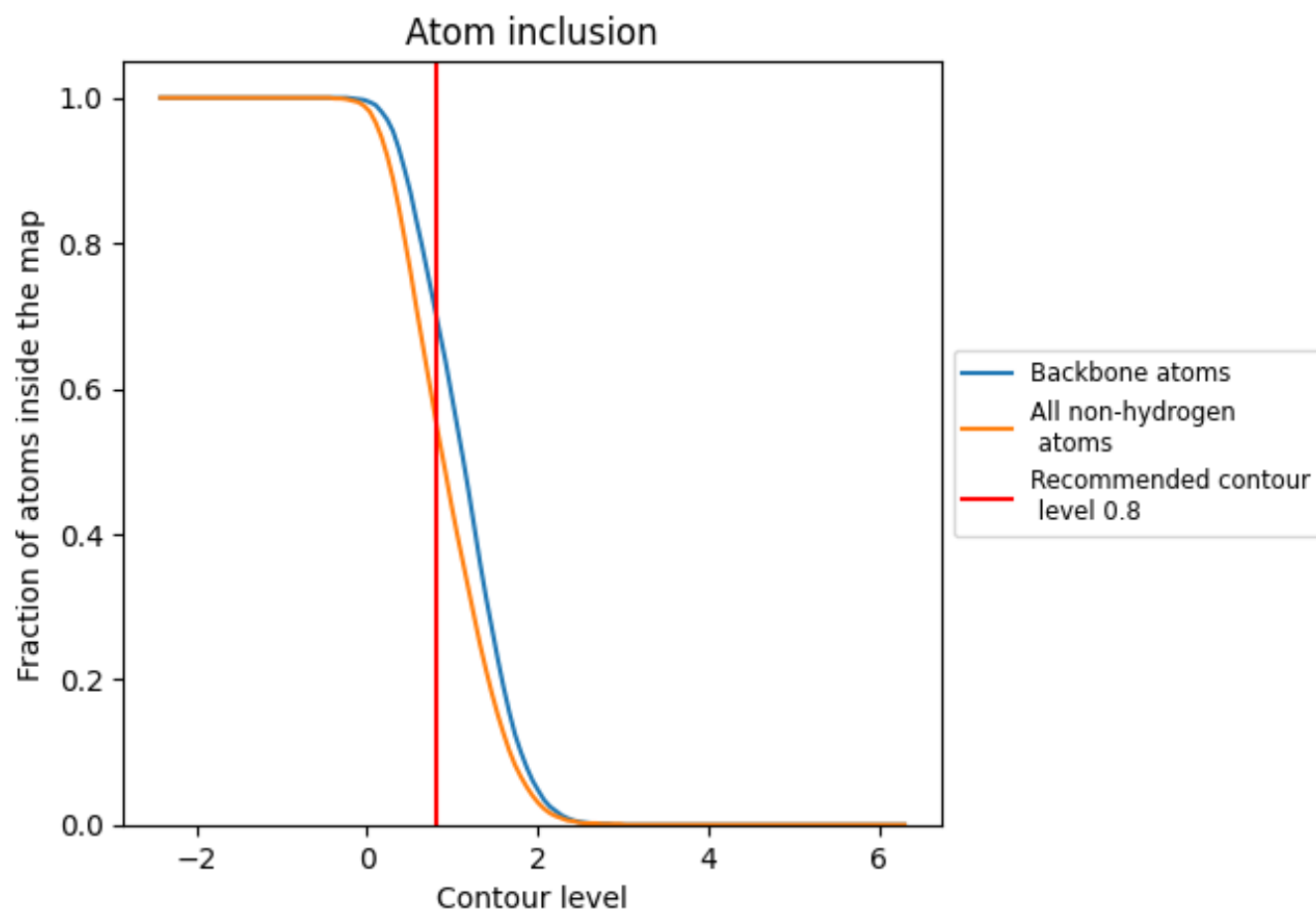
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 56% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5600	 0.4730
A	 0.4000	 0.4540
B	 0.6690	 0.5230
C	 0.6980	 0.5270
D	 0.6710	 0.5250
E	 0.4630	 0.4460
F	 0.5450	 0.4450
G	 0.6480	 0.4840
H	 0.5420	 0.4830
I	 0.6670	 0.5040
P	 0.4830	 0.4430
Q	 0.6090	 0.4940
R	 0.5500	 0.4890
S	 0.5800	 0.4580
T	 0.2920	 0.4100
V	 0.5950	 0.4580
W	 0.5570	 0.4840
X	 0.3800	 0.3770
Z	 0.4410	 0.4310
a	 0.5710	 0.4610
b	 0.3860	 0.4250
q	 0.5070	 0.4840
r	 0.4620	 0.5030
s	 0.2700	 0.3720

