



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 06:59 PM JST

PDB ID : 8IBA / pdb_00008iba
EMDB ID : EMD-35337
Title : Respiratory complex Peripheral Arm of CI, focus-refined map of type IB, Wild type mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
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:

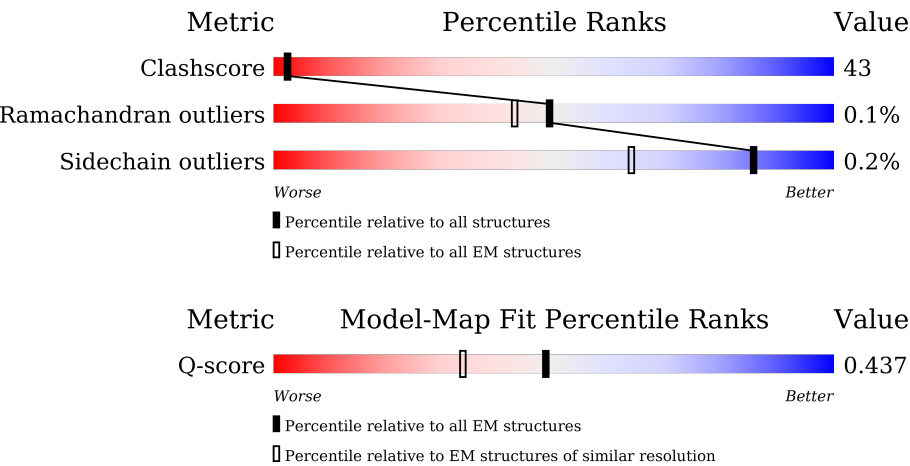
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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	10% 32% 47% 19%
2	B	224	28% 36% 5% 30%
3	C	263	38% 33% 25%
4	D	463	35% 44% 17%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	SF4	B	301	-	-	X	-
25	SF4	F	502	-	-	X	-
25	SF4	G	802	-	-	X	-
25	SF4	I	303	-	-	X	-
25	SF4	I	304	-	-	X	-

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

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 34006 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	93	Total	C	N	O	S	0	0
			762	528	108	120	6		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	386	Total	C	N	O	S	0	0
			3095	1974	534	564	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	316	Total	C	N	O	S	0	0
			2525	1698	382	423	22		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

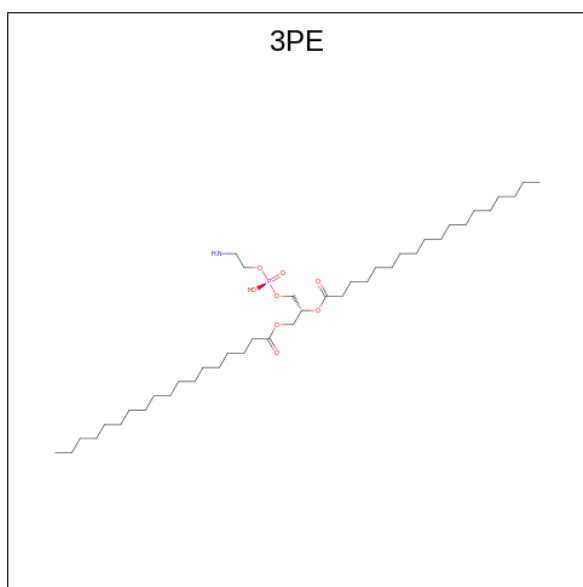
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

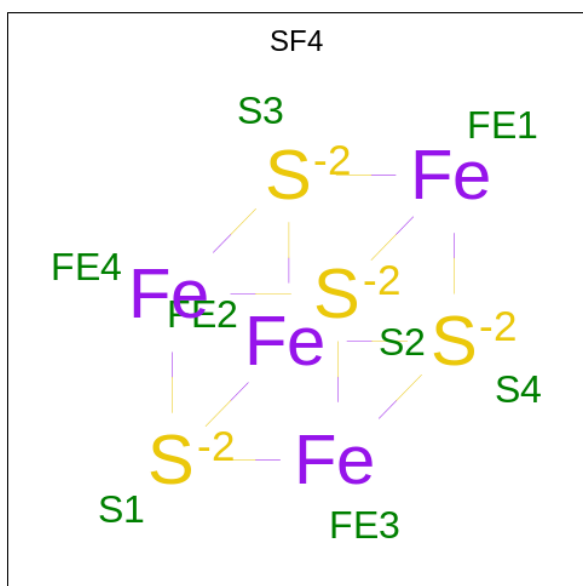
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	26	Total	C	N	O	0	0
			226	147	38	41		

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



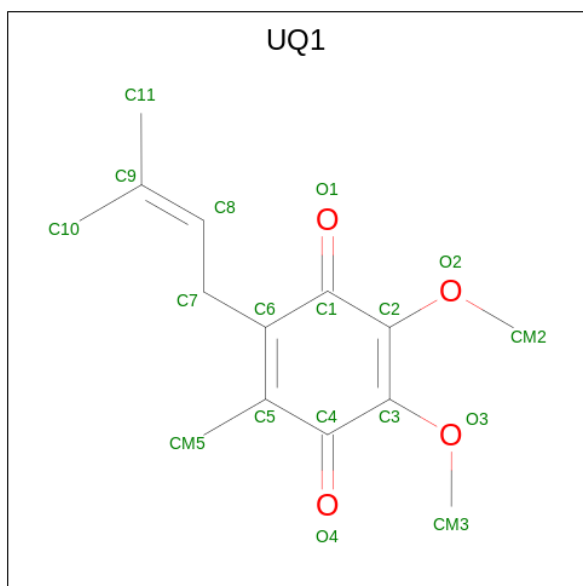
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	I	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	b	1	Total	C	N	O	P	0
			46	36	1	8	1	

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



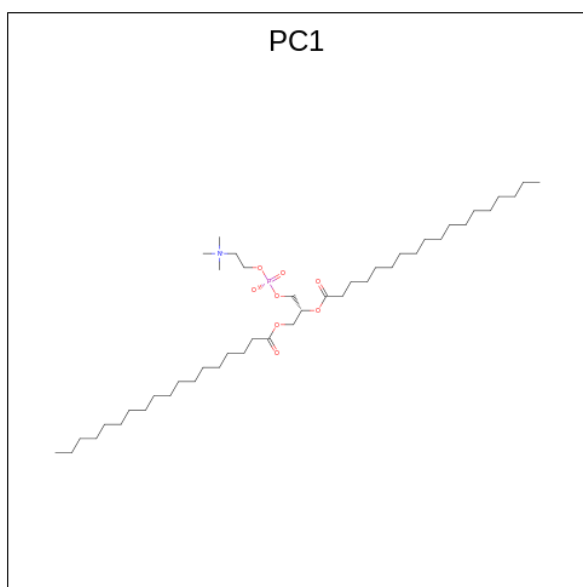
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	Fe	S	0
			8	4	4	
25	F	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	

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



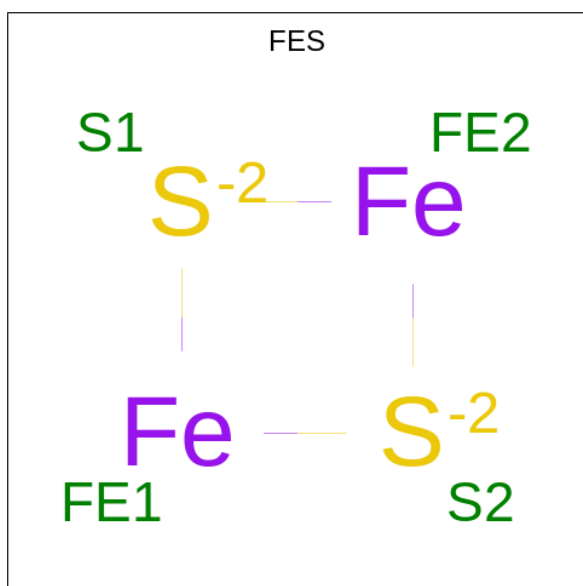
Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total	C	O	0
			18	14	4	

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
27	I	1	Total	C	N	O	P	0
			47	37	1	8	1	

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



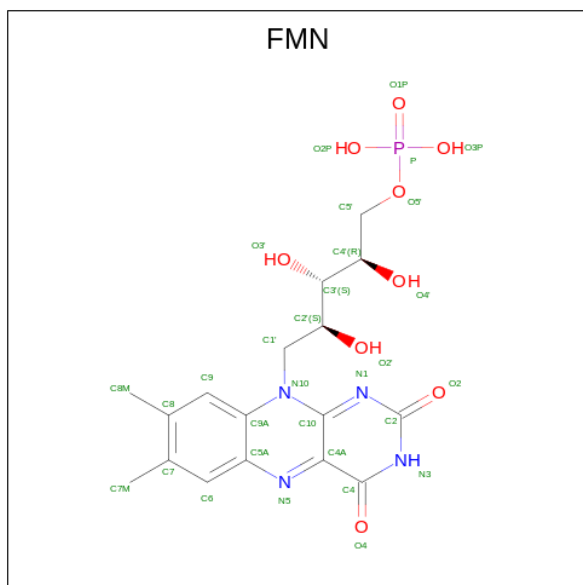
Mol	Chain	Residues	Atoms			AltConf
28	E	1	Total	Fe	S	0
			4	2	2	

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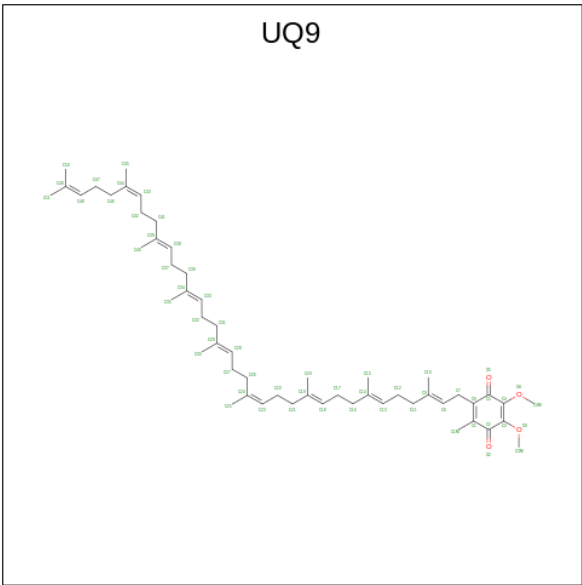
Mol	Chain	Residues	Atoms			AltConf
28	G	1	Total	Fe	S	0
			4	2	2	

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



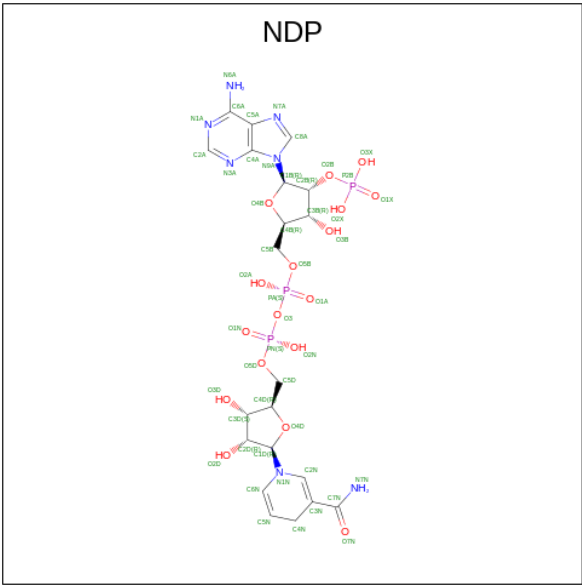
Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 30 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



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

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



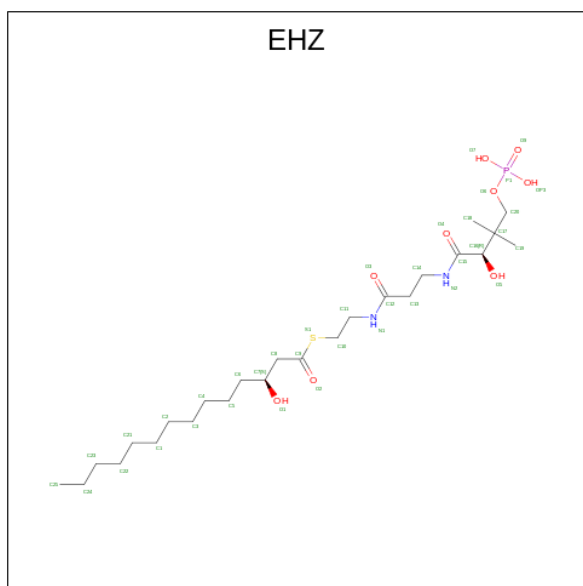
Mol	Chain	Residues	Atoms					AltConf
31	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

depositor).

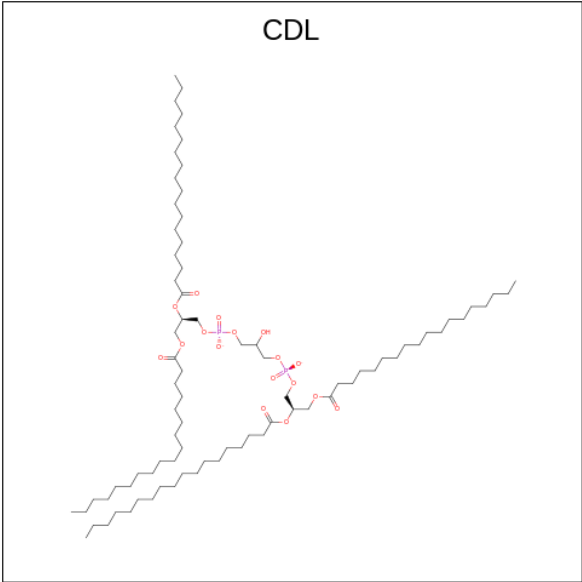
Mol	Chain	Residues	Atoms		AltConf
32	R	1	Total	Zn	0
			1	1	

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



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

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

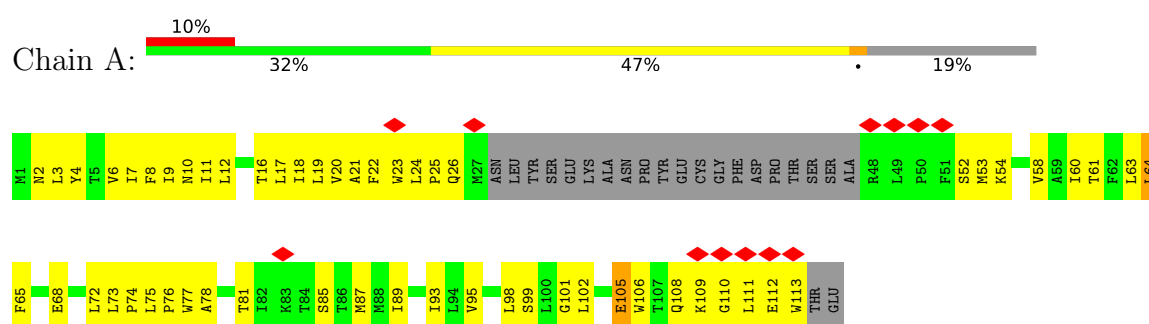


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
34	a	1	57	38	17	2	0

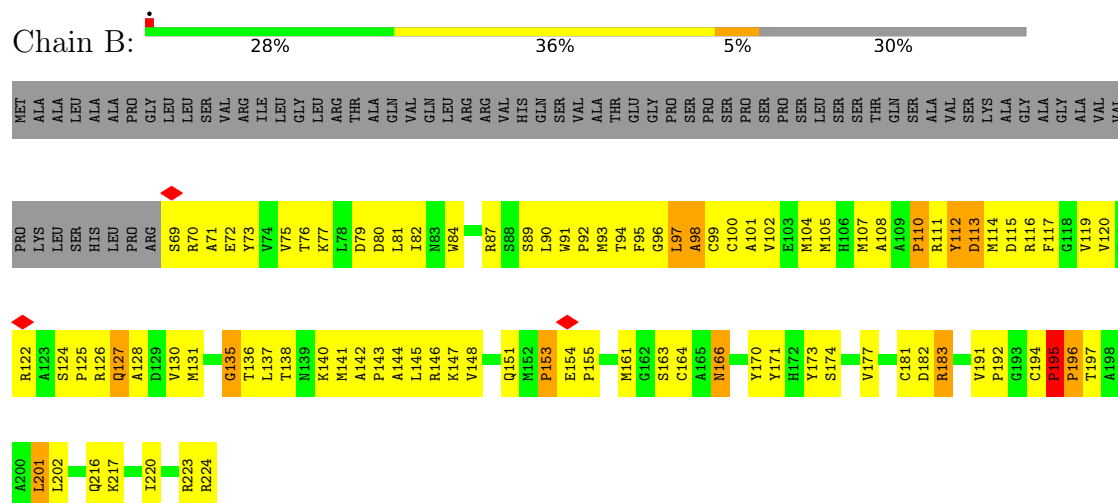
3 Residue-property plots [i](#)

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.

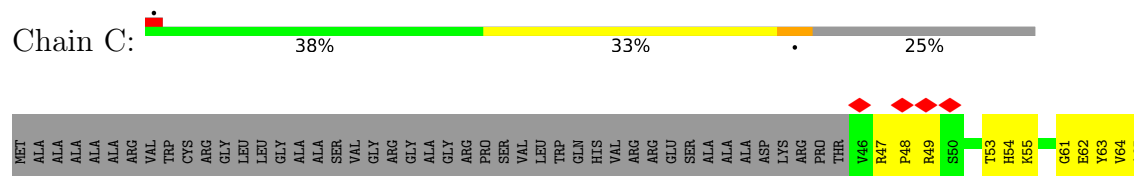
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



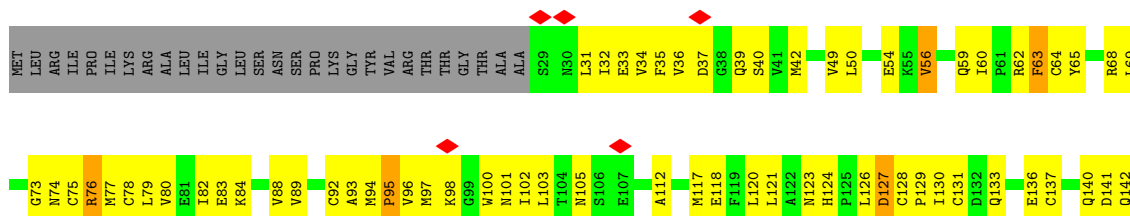
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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

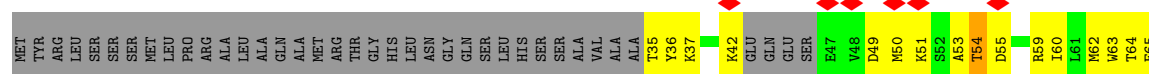




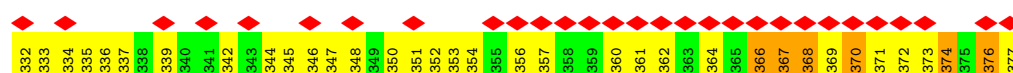
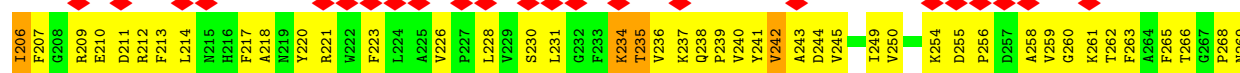
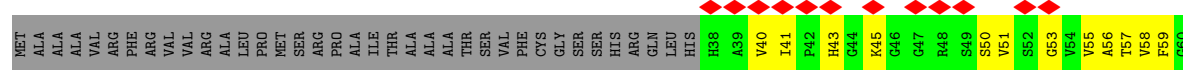




- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

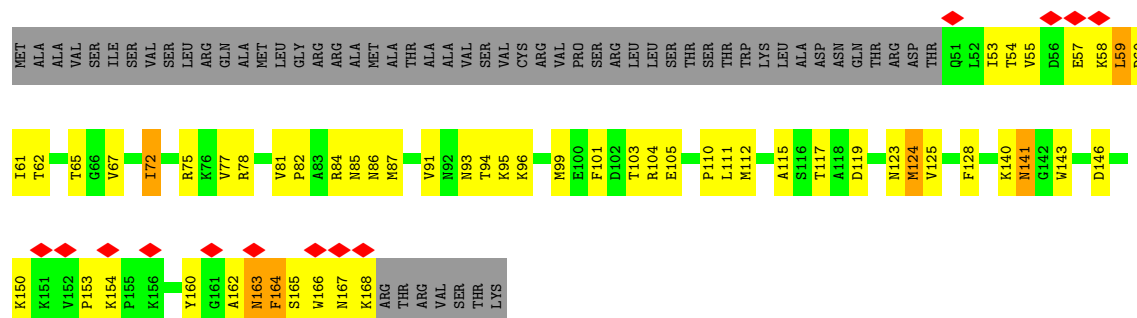


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

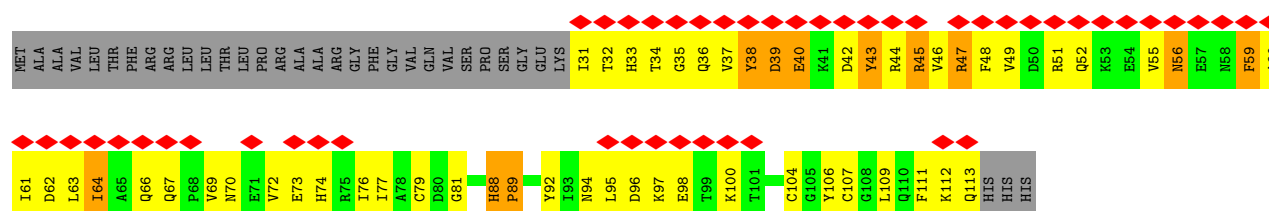
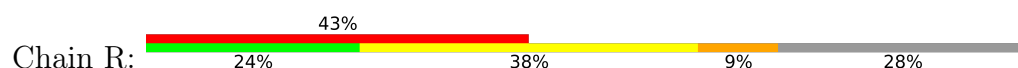


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

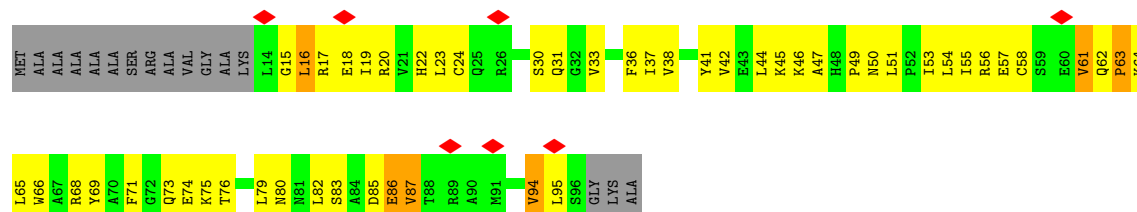




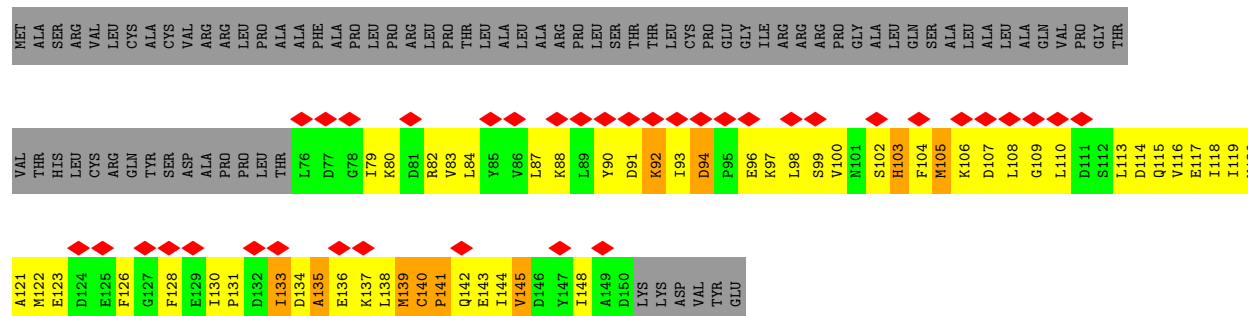
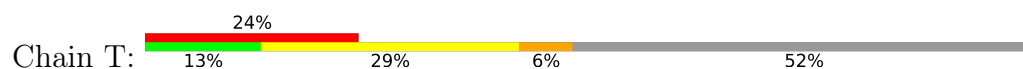
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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

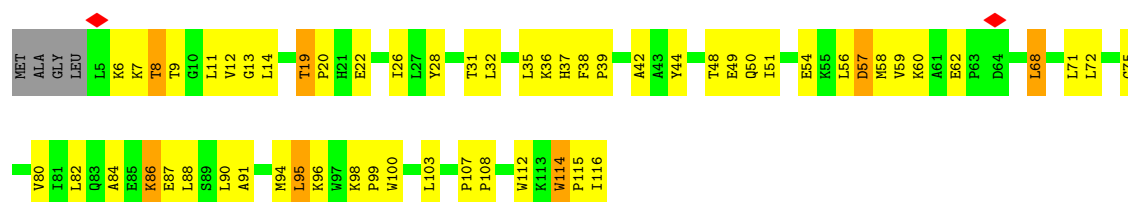


- Molecule 14: Acyl carrier protein, mitochondrial

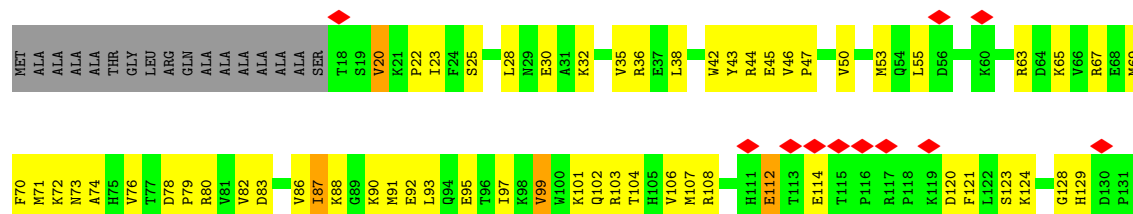


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

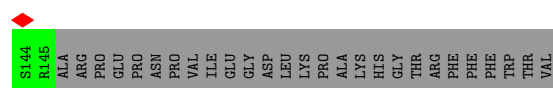
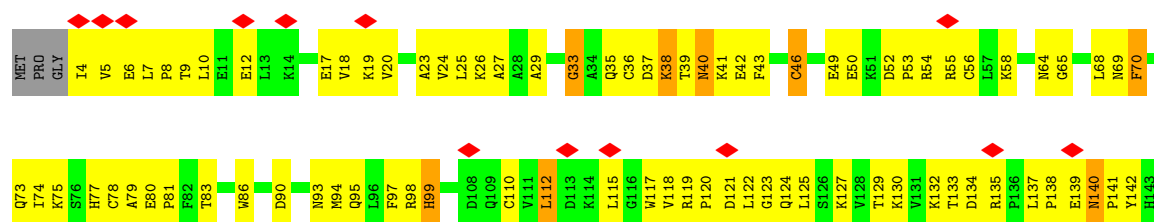




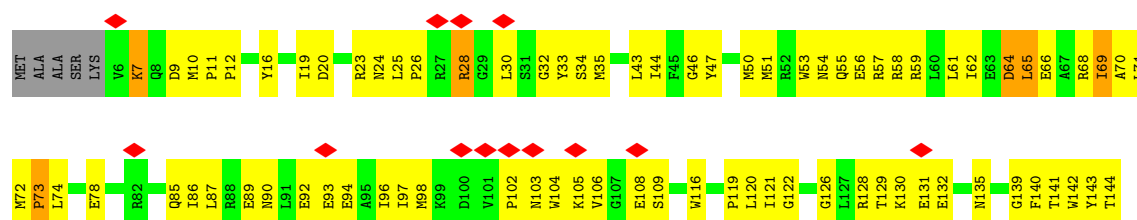
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



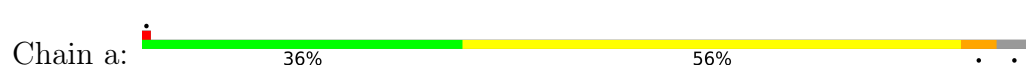
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



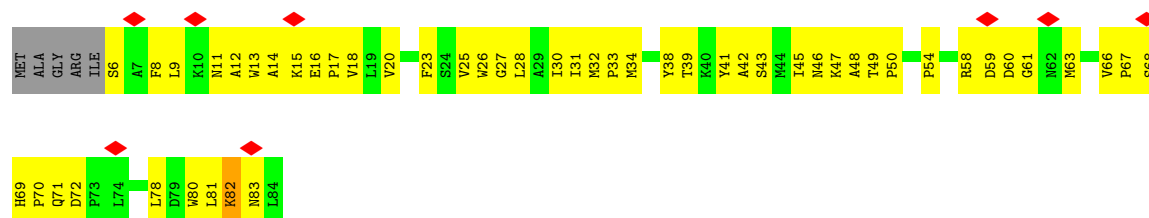
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



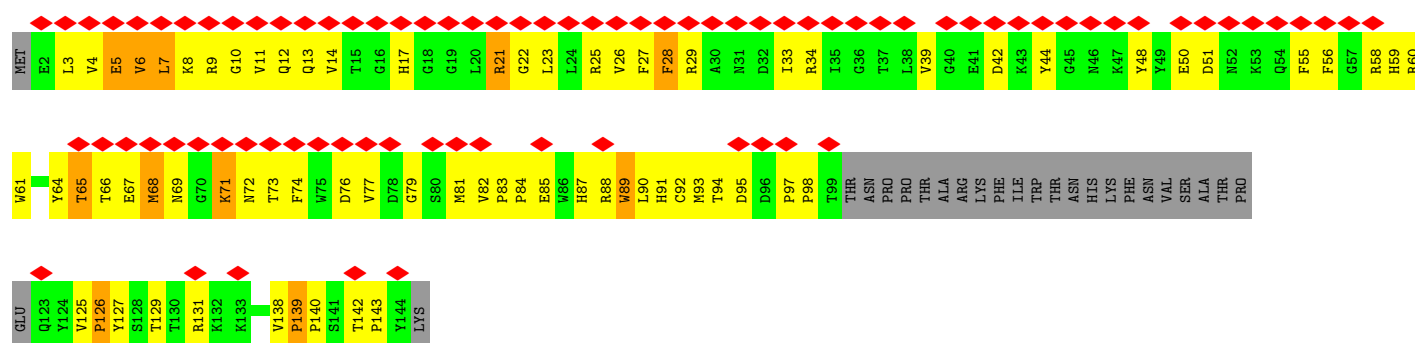
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



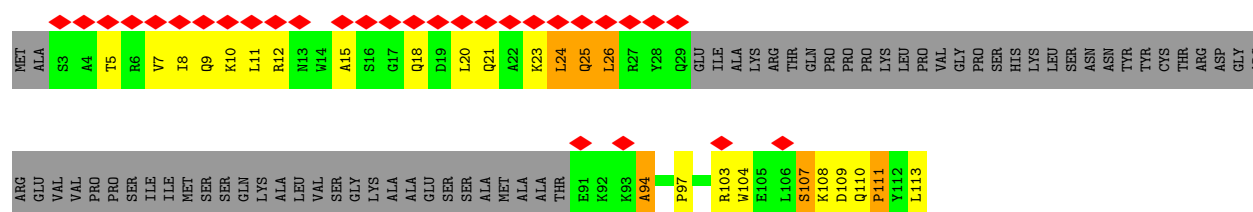
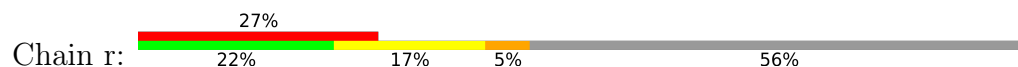
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



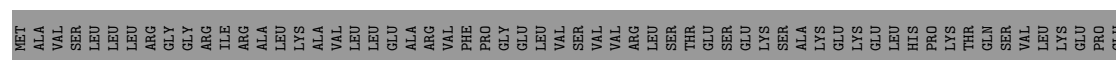
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



PRO	THR	ASP	THR	THR	THR	TYR	LYS	ASN	L35	Q36	H37	H38	D39	Y40	W41	T42	Y43	T44	F45	L46	D47	L48	W49	L50	D51	L52	S53	R54	F55	R56	L57	F58	Q59	P60	SER	SER	GLY	ARG	GLU	SER	PRO	ARG	HIS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	147426	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.196	Depositor
Minimum map value	-2.036	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.55	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.81	0/782	1.19	6/1066 (0.6%)
2	B	0.97	1/1278 (0.1%)	1.37	13/1730 (0.8%)
3	C	0.94	2/1687 (0.1%)	1.33	14/2297 (0.6%)
4	D	0.97	7/3169 (0.2%)	1.41	32/4286 (0.7%)
5	E	0.82	2/1675 (0.1%)	1.31	22/2282 (1.0%)
6	F	0.96	6/3363 (0.2%)	1.53	63/4543 (1.4%)
7	G	0.93	10/5374 (0.2%)	1.59	107/7281 (1.5%)
8	H	0.96	3/2600 (0.1%)	1.49	54/3550 (1.5%)
9	I	0.93	1/1427 (0.1%)	1.52	19/1927 (1.0%)
10	P	0.83	3/2804 (0.1%)	1.23	29/3802 (0.8%)
11	Q	0.87	1/980 (0.1%)	1.28	12/1324 (0.9%)
12	R	1.04	4/671 (0.6%)	1.38	13/903 (1.4%)
13	S	0.90	1/678 (0.1%)	1.47	11/915 (1.2%)
14	T	1.04	1/613 (0.2%)	1.56	12/826 (1.5%)
15	V	0.86	0/937	1.46	14/1270 (1.1%)
16	W	0.82	1/993 (0.1%)	1.00	3/1335 (0.2%)
17	X	0.78	0/1191	1.34	18/1605 (1.1%)
18	Z	0.82	1/1183 (0.1%)	1.22	12/1597 (0.8%)
19	a	0.88	0/561	1.38	8/755 (1.1%)
20	b	0.74	0/643	0.95	1/884 (0.1%)
21	q	0.98	2/1037 (0.2%)	1.41	17/1408 (1.2%)
22	r	0.94	2/421 (0.5%)	1.37	8/566 (1.4%)
23	s	0.43	0/233	0.75	1/317 (0.3%)
All	All	0.91	48/34300 (0.1%)	1.41	489/46469 (1.1%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	89	PRO	N-CD	-15.12	1.26	1.47
21	q	139	PRO	N-CD	-13.36	1.29	1.47
10	P	371	PRO	N-CD	12.95	1.65	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	532	PRO	N-CD	-12.57	1.30	1.47
14	T	141	PRO	N-CD	11.84	1.64	1.47
8	H	42	PRO	N-CD	10.85	1.62	1.47
6	F	234	GLY	CA-C	-10.28	1.41	1.52
6	F	227	PRO	N-CD	10.07	1.61	1.47
6	F	235	VAL	N-CA	-9.68	1.34	1.46
10	P	290	PRO	N-CD	9.62	1.61	1.47
7	G	275	PRO	N-CD	-9.48	1.34	1.47
8	H	75	PRO	N-CD	9.22	1.60	1.47
6	F	319	PRO	N-CD	9.07	1.60	1.47
9	I	107	PRO	N-CD	8.59	1.59	1.47
4	D	163	PRO	N-CD	-8.41	1.35	1.47
18	Z	73	PRO	N-CD	8.15	1.59	1.47
4	D	352	PRO	N-CD	-7.95	1.36	1.47
12	R	39	ASP	CA-C	7.91	1.64	1.53
11	Q	53	ILE	C-O	7.90	1.33	1.24
3	C	81	ASP	C-O	-7.88	1.14	1.24
13	S	63	PRO	N-CD	-7.88	1.36	1.47
5	E	218	ARG	CA-C	7.87	1.62	1.53
12	R	40	GLU	N-CA	7.68	1.56	1.46
22	r	111	PRO	N-CD	-7.45	1.37	1.47
7	G	449	PRO	N-CD	6.79	1.57	1.47
7	G	541	PRO	N-CD	-6.74	1.38	1.47
6	F	233	VAL	CA-C	-6.71	1.44	1.52
7	G	203	ASP	CA-C	6.71	1.62	1.52
4	D	106	VAL	C-N	-6.54	1.24	1.33
7	G	600	GLU	CA-C	6.48	1.61	1.52
4	D	266	ARG	C-O	-6.31	1.16	1.24
7	G	127	ASP	CA-C	6.24	1.62	1.52
6	F	384	PRO	N-CD	-6.18	1.39	1.47
2	B	110	PRO	C-O	-6.16	1.16	1.24
7	G	76	ARG	CA-C	6.08	1.61	1.53
7	G	361	VAL	CA-C	5.89	1.60	1.52
5	E	93	PRO	N-CD	-5.88	1.39	1.47
8	H	60	PRO	N-CD	5.83	1.55	1.47
22	r	25	GLN	CA-C	5.79	1.60	1.52
12	R	59	PHE	CA-C	-5.76	1.45	1.52
16	W	22	PRO	N-CD	5.66	1.55	1.47
4	D	107	ARG	C-N	5.50	1.40	1.33
4	D	392	PRO	C-O	-5.50	1.20	1.24
7	G	683	PRO	N-CD	-5.41	1.40	1.47
21	q	126	PRO	N-CD	5.33	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	235	THR	CA-C	5.32	1.59	1.53
4	D	266	ARG	CA-C	-5.14	1.45	1.52
3	C	61	GLY	C-N	-5.04	1.27	1.33

All (489) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	142	VAL	N-CA-CB	19.28	132.44	110.65
4	D	142	VAL	N-CA-C	-19.03	92.53	110.42
7	G	174	THR	N-CA-C	-16.87	89.00	114.64
6	F	125	CYS	N-CA-C	-15.62	93.48	113.17
6	F	332	CYS	N-CA-C	15.55	129.99	111.02
21	q	139	PRO	N-CA-CB	-13.57	95.59	103.19
7	G	251	ILE	N-CA-C	13.34	126.84	108.17
7	G	77	MET	N-CA-C	-13.05	97.32	113.38
7	G	500	ILE	N-CA-C	-12.50	98.78	110.53
19	a	3	PHE	CB-CA-C	-12.40	89.60	110.68
10	P	106	LEU	N-CA-C	12.19	128.70	109.07
6	F	171	VAL	N-CA-C	-11.86	99.38	110.53
7	G	204	MET	N-CA-C	-11.62	91.46	109.25
6	F	449	ARG	N-CA-C	-11.61	98.70	111.36
6	F	334	THR	N-CA-CB	11.51	127.31	109.82
11	Q	60	ASP	N-CA-C	-11.33	90.32	109.24
7	G	599	THR	N-CA-C	11.30	126.17	112.38
15	V	57	ASP	N-CA-C	-11.02	99.28	111.07
8	H	259	PHE	N-CA-C	-11.00	99.37	111.36
9	I	164	VAL	N-CA-C	-10.60	100.19	113.22
9	I	77	LEU	N-CA-C	-10.52	99.62	111.71
5	E	68	ASN	N-CA-C	-10.40	99.94	111.07
14	T	139	MET	N-CA-C	-10.39	97.48	113.89
2	B	195	PRO	N-CA-C	-10.34	98.08	110.70
7	G	280	ASP	N-CA-C	10.31	122.52	111.28
3	C	80	LEU	N-CA-C	-10.29	99.83	112.38
4	D	337	MET	N-CA-C	-10.21	100.14	111.07
4	D	140	ASP	CB-CA-C	-10.18	98.08	111.42
10	P	366	ILE	N-CA-C	10.15	120.97	110.62
7	G	414	PHE	N-CA-C	-10.14	101.40	113.88
9	I	161	ALA	N-CA-C	10.14	122.33	111.28
14	T	135	ALA	N-CA-C	-10.08	100.29	111.28
19	a	4	GLU	N-CA-C	10.05	124.80	112.54
7	G	325	ARG	N-CA-C	-9.87	100.21	110.97
9	I	166	ALA	N-CA-C	-9.84	100.82	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	178	GLU	N-CA-C	-9.84	99.31	111.11
6	F	103	ASN	N-CA-C	-9.81	101.00	113.16
6	F	141	GLY	N-CA-C	-9.78	101.16	112.50
7	G	654	VAL	N-CA-C	9.74	123.26	111.09
5	E	64	ALA	N-CA-C	-9.73	99.44	111.11
6	F	144	VAL	N-CA-C	-9.72	101.39	110.53
10	P	371	PRO	N-CA-CB	9.66	111.86	103.36
6	F	418	GLN	N-CA-C	-9.60	100.77	111.14
7	G	337	ALA	N-CA-C	-9.57	100.81	114.12
16	W	87	ILE	N-CA-C	-9.57	101.23	110.42
19	a	2	TRP	N-CA-C	-9.56	101.62	113.28
8	H	52	ALA	N-CA-C	-9.54	100.86	111.07
3	C	136	PHE	N-CA-C	-9.50	96.84	110.24
17	X	70	PHE	N-CA-C	-9.49	99.72	111.11
12	R	38	TYR	N-CA-C	-9.46	96.34	110.24
4	D	427	PRO	N-CA-C	-9.42	95.71	110.50
17	X	112	LEU	N-CA-C	-9.41	100.97	111.14
21	q	139	PRO	CA-N-CD	9.38	125.14	112.00
7	G	694	PHE	N-CA-C	9.32	121.44	111.28
14	T	133	ILE	N-CA-C	9.30	119.84	110.82
7	G	692	LYS	N-CA-C	-9.28	100.53	112.23
10	P	367	GLU	N-CA-C	9.27	122.57	111.82
10	P	369	THR	N-CA-CB	9.24	123.47	110.17
7	G	640	ASP	N-CA-C	-9.21	101.32	111.36
18	Z	69	ILE	N-CA-C	-9.20	100.70	110.36
7	G	389	THR	N-CA-C	-9.13	96.26	109.96
5	E	85	ALA	N-CA-C	-9.11	101.43	111.36
19	a	57	VAL	N-CA-C	-9.04	105.12	113.71
6	F	411	SER	N-CA-C	-8.86	101.59	111.07
7	G	133	GLN	N-CA-CB	8.80	121.54	110.45
7	G	212	LYS	N-CA-C	-8.79	94.58	108.90
7	G	365	ASN	N-CA-C	-8.69	102.23	112.92
9	I	154	TYR	N-CA-CB	-8.69	99.19	111.62
8	H	60	PRO	N-CA-CB	8.69	108.56	102.65
16	W	20	VAL	N-CA-C	8.65	120.74	108.36
10	P	96	LEU	N-CA-C	8.64	121.65	111.71
19	a	3	PHE	CA-CB-CG	8.54	122.34	113.80
13	S	18	GLU	N-CA-C	8.50	123.25	109.40
13	S	86	GLU	N-CA-C	-8.49	102.10	111.36
3	C	70	LYS	N-CA-C	8.49	121.60	111.33
10	P	373	LYS	N-CA-C	8.48	121.89	110.35
3	C	108	LYS	N-CA-C	8.42	120.08	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	99	HIS	N-CA-C	-8.37	102.23	111.36
8	H	141	SER	N-CA-C	-8.36	102.12	111.07
7	G	532	PRO	CA-N-CD	8.35	123.69	112.00
7	G	452	LEU	N-CA-C	-8.33	102.20	111.28
11	Q	54	THR	N-CA-C	8.32	123.28	109.46
7	G	558	GLN	N-CA-C	-8.29	102.20	111.07
8	H	196	ALA	N-CA-C	8.23	127.99	109.81
5	E	218	ARG	CB-CA-C	-8.20	99.81	112.12
8	H	311	THR	N-CA-C	-8.19	102.60	112.59
7	G	691	ILE	N-CA-C	8.17	123.66	111.89
6	F	298	GLU	N-CA-C	8.16	120.18	111.28
3	C	196	PRO	N-CA-C	8.15	124.86	113.53
6	F	411	SER	N-CA-CB	8.13	121.80	110.01
6	F	191	TYR	N-CA-C	8.12	121.68	110.24
1	A	64	LEU	N-CA-C	-8.11	102.39	111.07
7	G	484	ASP	N-CA-C	8.11	121.03	111.71
7	G	534	VAL	N-CA-C	-8.10	104.70	111.91
15	V	86	LYS	N-CA-C	-8.06	102.43	111.14
7	G	500	ILE	N-CA-CB	8.06	120.88	110.57
13	S	76	THR	N-CA-C	8.04	122.00	108.90
2	B	110	PRO	N-CA-C	8.03	124.49	113.65
5	E	219	SER	N-CA-CB	8.02	123.99	111.56
9	I	201	ILE	N-CA-C	-8.01	102.63	110.72
8	H	271	LEU	N-CA-C	-8.01	102.50	111.14
17	X	43	PHE	N-CA-C	-8.01	102.50	111.07
1	A	9	ILE	N-CA-C	-7.96	102.50	110.62
7	G	651	PRO	CB-CA-C	-7.95	98.44	111.56
21	q	67	GLU	CB-CA-C	-7.94	99.60	112.06
10	P	206	ILE	N-CA-C	7.93	120.93	108.87
17	X	46	CYS	N-CA-C	-7.93	102.72	111.36
15	V	6	LYS	N-CA-C	-7.88	100.12	110.53
8	H	311	THR	N-CA-CB	7.85	123.48	110.92
7	G	270	VAL	N-CA-CB	-7.84	100.67	110.31
9	I	160	GLU	N-CA-C	7.82	124.20	111.37
10	P	235	THR	CB-CA-C	-7.82	100.02	112.07
9	I	74	LEU	N-CA-C	-7.79	102.80	111.28
7	G	389	THR	N-CA-CB	7.77	121.43	109.85
17	X	58	LYS	N-CA-C	-7.76	102.76	111.07
4	D	141	TYR	CA-C-N	7.74	130.16	120.72
4	D	141	TYR	C-N-CA	7.74	130.16	120.72
21	q	44	TYR	N-CA-C	-7.70	98.89	110.28
8	H	253	GLU	N-CA-C	7.70	121.93	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	R	47	ARG	N-CA-C	7.69	120.63	111.33
6	F	334	THR	N-CA-C	-7.68	101.65	111.02
6	F	58	ARG	N-CA-C	-7.67	103.00	111.36
7	G	56	VAL	N-CA-C	-7.65	102.99	110.72
5	E	68	ASN	N-CA-CB	7.65	121.11	110.01
21	q	89	TRP	N-CA-C	-7.65	102.88	111.14
2	B	153	PRO	CB-CA-C	-7.62	98.98	111.56
4	D	361	ALA	N-CA-C	-7.59	103.12	112.38
7	G	569	GLN	N-CA-C	7.58	121.97	108.24
5	E	166	LYS	N-CA-C	-7.58	102.20	113.72
8	H	201	THR	N-CA-C	-7.58	102.62	111.03
6	F	171	VAL	N-CA-CB	7.58	120.27	110.57
14	T	141	PRO	N-CA-C	-7.57	103.00	113.53
12	R	74	HIS	N-CA-C	7.54	121.14	110.50
8	H	223	PHE	CB-CA-C	-7.51	99.09	110.88
9	I	119	CYS	N-CA-C	-7.51	103.18	111.36
2	B	183	ARG	N-CA-C	-7.50	104.37	113.97
7	G	277	MET	N-CA-C	7.49	120.60	109.59
7	G	467	LYS	N-CA-C	-7.48	102.27	111.33
18	Z	73	PRO	N-CA-C	-7.47	103.14	113.53
9	I	158	CYS	N-CA-C	-7.44	103.17	111.28
6	F	430	GLY	N-CA-C	7.43	121.64	112.73
7	G	510	TRP	N-CA-CB	7.41	120.90	109.85
4	D	350	LYS	CB-CA-C	-7.40	100.98	111.85
4	D	99	LEU	N-CA-C	7.39	120.98	109.07
12	R	39	ASP	N-CA-C	7.37	121.28	110.59
8	H	309	ILE	N-CA-C	7.36	117.44	110.30
7	G	303	THR	N-CA-C	7.35	122.96	113.18
15	V	57	ASP	N-CA-CB	7.33	120.64	110.01
13	S	94	VAL	N-CA-C	7.32	117.45	110.42
7	G	384	ASN	N-CA-C	-7.28	103.38	111.82
7	G	661	GLU	N-CA-C	7.27	118.89	110.97
14	T	105	MET	N-CA-C	7.27	119.28	111.36
3	C	195	HIS	CB-CA-C	7.27	117.36	110.17
7	G	374	THR	CB-CA-C	-7.23	99.85	111.28
8	H	139	THR	N-CA-CB	7.18	120.42	110.01
8	H	50	ALA	N-CA-C	7.17	118.74	111.07
15	V	68	LEU	N-CA-C	-7.15	103.48	111.28
8	H	254	LEU	N-CA-C	-7.14	103.53	111.82
7	G	497	VAL	N-CA-C	-7.14	103.34	110.62
6	F	73	PRO	N-CA-C	-7.13	103.85	113.40
7	G	461	SER	N-CA-C	7.11	119.94	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	81	LYS	N-CA-C	-7.11	103.61	111.36
7	G	465	VAL	N-CA-CB	7.10	118.39	110.51
7	G	217	GLU	N-CA-C	-7.09	101.69	110.41
15	V	95	LEU	N-CA-C	-7.07	103.58	111.28
7	G	148	SER	N-CA-C	7.06	120.91	109.40
6	F	78	GLY	N-CA-C	-7.06	104.26	112.73
11	Q	162	ALA	N-CA-C	7.05	118.96	111.28
7	G	150	ARG	N-CA-C	7.04	119.64	109.14
8	H	176	LEU	CA-C-N	-7.04	113.55	120.52
8	H	176	LEU	C-N-CA	-7.04	113.55	120.52
6	F	455	GLN	N-CA-C	7.03	118.59	111.07
6	F	169	LEU	N-CA-C	7.01	118.93	111.28
10	P	235	THR	CA-C-O	7.00	128.18	121.67
2	B	166	ASN	N-CA-C	-6.99	103.36	110.97
12	R	45	ARG	N-CA-C	-6.97	104.65	113.01
18	Z	34	SER	N-CA-C	-6.97	103.61	111.07
7	G	294	TYR	N-CA-C	-6.97	104.59	113.23
6	F	418	GLN	N-CA-CB	6.96	120.16	110.07
8	H	292	ASN	N-CA-C	6.95	118.93	111.36
6	F	428	GLY	N-CA-C	-6.94	103.88	112.77
6	F	103	ASN	N-CA-CB	6.93	121.05	110.44
7	G	582	VAL	N-CA-C	6.93	118.46	108.48
5	E	152	GLN	N-CA-C	-6.92	103.67	111.07
6	F	246	GLU	N-CA-C	-6.89	103.77	111.28
7	G	300	GLN	N-CA-CB	6.88	122.47	112.08
6	F	233	VAL	O-C-N	6.88	131.14	123.10
6	F	148	ALA	N-CA-C	-6.87	103.87	111.36
7	G	362	ASP	N-CA-C	6.86	125.42	110.80
14	T	145	VAL	N-CA-C	-6.86	103.79	110.72
8	H	300	LEU	N-CA-C	-6.86	104.17	112.54
18	Z	28	ARG	N-CA-C	6.85	119.69	108.52
6	F	329	LYS	N-CA-C	6.83	119.60	111.33
7	G	133	GLN	N-CA-C	-6.82	101.20	110.68
7	G	268	GLY	N-CA-C	6.81	124.77	115.30
12	R	56	ASN	N-CA-C	6.81	120.00	108.90
6	F	233	VAL	CA-C-O	-6.81	113.25	120.53
8	H	305	ILE	N-CA-C	-6.77	103.43	113.39
8	H	8	THR	N-CA-C	-6.77	101.14	110.35
6	F	244	ASN	N-CA-C	-6.76	100.97	110.50
7	G	434	SER	N-CA-C	-6.74	100.99	110.29
15	V	114	TRP	N-CA-CB	6.72	120.31	110.30
10	P	371	PRO	CA-N-CD	-6.71	102.61	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	208	ASP	N-CA-C	6.70	121.61	113.17
15	V	8	THR	N-CA-C	6.70	119.03	108.79
6	F	344	GLN	N-CA-C	-6.68	104.00	111.28
4	D	184	ILE	N-CA-C	-6.66	103.83	110.62
8	H	93	HIS	CB-CA-C	6.66	117.88	108.76
10	P	116	ILE	N-CA-C	-6.65	104.01	110.72
3	C	69	PRO	N-CA-C	-6.64	104.29	113.53
17	X	129	THR	N-CA-C	6.64	120.87	110.17
3	C	125	PHE	N-CA-CB	-6.64	100.60	110.17
7	G	640	ASP	N-CA-CB	6.63	119.97	110.16
14	T	141	PRO	N-CA-CB	6.63	110.62	103.33
7	G	601	GLY	N-CA-C	6.62	124.83	115.30
15	V	86	LYS	N-CA-CB	6.62	119.67	110.07
7	G	287	SER	N-CA-C	6.61	119.26	110.53
6	F	228	PRO	N-CA-C	-6.59	98.89	112.47
5	E	166	LYS	CB-CA-C	6.59	123.49	110.65
11	Q	141	ASN	N-CA-CB	6.58	120.79	110.46
7	G	435	PRO	N-CA-C	-6.58	100.17	110.50
8	H	267	SER	N-CA-C	-6.57	104.20	111.36
18	Z	65	LEU	N-CA-C	-6.56	104.21	111.36
8	H	182	ALA	N-CA-C	-6.55	104.06	111.07
2	B	97	LEU	N-CA-C	-6.55	101.44	110.35
6	F	336	LEU	N-CA-CB	-6.54	101.03	111.43
8	H	223	PHE	N-CA-C	-6.53	104.08	111.07
6	F	234	GLY	CA-C-N	-6.51	111.77	120.50
6	F	234	GLY	C-N-CA	-6.51	111.77	120.50
17	X	98	ARG	N-CA-C	6.51	120.48	112.54
7	G	275	PRO	CB-CA-C	-6.48	102.49	110.98
7	G	605	GLN	N-CA-C	6.48	119.08	108.52
9	I	66	LEU	N-CA-C	-6.48	104.30	111.36
14	T	141	PRO	CA-N-CD	-6.47	102.94	112.00
13	S	16	LEU	N-CA-C	-6.47	98.36	108.90
7	G	250	SER	N-CA-C	6.47	116.81	108.34
22	r	24	LEU	N-CA-C	6.46	119.61	110.50
4	D	388	GLY	N-CA-C	6.46	119.55	110.38
4	D	140	ASP	N-CA-C	-6.45	96.47	107.23
8	H	177	PRO	N-CA-C	-6.44	101.53	111.13
4	D	84	PHE	N-CA-C	-6.43	104.31	111.71
15	V	49	GLU	N-CA-C	-6.43	104.27	111.28
12	R	81	GLY	N-CA-C	-6.42	106.86	115.21
7	G	275	PRO	CA-N-CD	6.42	120.98	112.00
3	C	125	PHE	N-CA-C	6.41	119.54	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	255	TYR	N-CA-CB	6.41	119.30	110.01
6	F	178	GLU	N-CA-CB	6.41	119.48	109.94
7	G	95	PRO	N-CA-C	-6.40	101.14	110.80
6	F	370	LEU	N-CA-C	-6.39	104.40	111.36
11	Q	59	LEU	N-CA-C	-6.38	100.73	110.30
6	F	416	SER	N-CA-C	6.37	117.89	111.07
8	H	271	LEU	N-CA-CB	6.36	119.30	110.07
7	G	273	ILE	N-CA-C	-6.35	98.37	107.77
9	I	205	ILE	N-CA-C	-6.34	104.31	110.72
7	G	176	CYS	N-CA-C	6.34	119.68	110.42
15	V	71	LEU	N-CA-C	6.34	118.19	111.28
6	F	144	VAL	N-CA-CB	6.33	118.67	110.57
15	V	91	ALA	N-CA-C	-6.31	104.40	111.28
21	q	28	PHE	N-CA-C	6.29	117.80	111.07
6	F	415	ILE	N-CA-C	-6.27	104.39	110.72
17	X	99	HIS	N-CA-CB	6.27	119.44	110.16
7	G	383	SER	N-CA-C	-6.26	106.86	114.75
4	D	233	HIS	N-CA-C	6.24	119.01	111.40
5	E	50	THR	N-CA-CB	6.24	121.47	110.37
7	G	356	ASP	N-CA-CB	6.24	119.29	110.12
19	a	26	ILE	N-CA-C	-6.23	104.59	113.07
6	F	255	CYS	N-CA-C	-6.23	104.57	111.36
11	Q	141	ASN	N-CA-C	-6.22	105.69	113.28
1	A	101	GLY	N-CA-C	-6.22	105.28	112.50
4	D	141	TYR	N-CA-C	6.22	120.87	113.16
5	E	64	ALA	N-CA-CB	6.22	119.20	109.94
6	F	192	ASP	N-CA-C	6.21	119.07	109.07
2	B	113	ASP	N-CA-CB	6.21	119.46	109.28
22	r	26	LEU	N-CA-CB	-6.21	101.10	110.35
8	H	52	ALA	N-CA-CB	6.21	119.01	110.01
6	F	101	PHE	N-CA-C	6.20	118.83	111.33
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
21	q	69	ASN	N-CA-CB	6.19	121.32	111.66
6	F	409	ILE	N-CA-C	6.19	116.36	110.42
18	Z	69	ILE	N-CA-CB	6.18	117.37	110.51
8	H	269	THR	N-CA-C	6.18	118.01	111.28
7	G	420	LYS	N-CA-C	6.17	118.80	111.33
10	P	368	GLU	N-CA-CB	6.17	119.80	110.30
13	S	61	VAL	N-CA-C	-6.17	99.60	108.42
7	G	418	ILE	N-CA-C	-6.15	103.42	112.04
4	D	291	VAL	N-CA-C	-6.15	103.40	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Z	44	ILE	N-CA-C	-6.14	104.76	110.53
10	P	118	LYS	N-CA-C	6.13	118.94	111.82
6	F	212	LEU	N-CA-C	-6.13	104.59	111.28
8	H	202	GLU	N-CA-C	-6.13	105.78	113.20
7	G	325	ARG	N-CA-CB	6.12	118.85	109.91
8	H	276	SER	N-CA-C	6.12	118.92	111.82
13	S	87	VAL	N-CA-C	-6.08	104.42	110.62
7	G	508	ALA	N-CA-C	6.07	117.90	111.28
8	H	24	GLU	N-CA-C	-6.05	104.03	112.45
7	G	353	ALA	N-CA-C	-6.05	104.61	112.23
10	P	370	LYS	N-CA-C	6.05	119.29	108.47
8	H	103	LEU	N-CA-C	-6.04	104.77	111.36
8	H	185	TRP	N-CA-C	-6.04	104.05	112.45
7	G	638	THR	N-CA-C	-6.03	100.14	109.24
8	H	7	LEU	N-CA-C	-6.02	104.35	111.03
18	Z	65	LEU	N-CA-CB	6.02	119.07	110.16
7	G	532	PRO	N-CA-CB	-6.01	97.07	103.38
22	r	108	LYS	N-CA-C	6.01	117.91	111.36
2	B	196	PRO	N-CA-C	-5.97	101.84	111.03
4	D	352	PRO	N-CA-CB	-5.95	97.31	103.08
6	F	291	GLU	N-CA-C	5.93	118.20	110.43
17	X	38	LYS	N-CA-C	-5.93	104.73	111.07
7	G	387	LEU	CB-CA-C	-5.91	101.75	111.68
5	E	66	VAL	N-CA-C	5.89	116.55	110.36
6	F	127	ASP	N-CA-C	5.88	118.48	111.71
8	H	315	PRO	O-C-N	5.88	123.91	121.15
14	T	94	ASP	N-CA-CB	-5.87	105.14	111.66
7	G	639	LEU	N-CA-C	5.87	118.62	111.82
10	P	122	HIS	N-CA-C	5.86	120.12	112.92
7	G	480	ALA	N-CA-C	-5.85	104.98	111.36
9	I	116	CYS	N-CA-C	-5.85	105.64	112.89
17	X	97	PHE	N-CA-C	5.85	118.60	111.82
2	B	135	GLY	CA-C-O	-5.84	117.91	122.52
21	q	65	THR	N-CA-C	5.83	119.17	110.14
3	C	209	LEU	N-CA-CB	-5.82	100.71	110.83
4	D	258	VAL	N-CA-C	-5.82	103.99	110.62
7	G	672	ALA	N-CA-C	-5.81	104.94	111.28
15	V	19	THR	N-CA-CB	5.81	120.72	110.37
13	S	86	GLU	N-CA-CB	5.81	118.76	110.16
6	F	102	MET	CB-CA-C	-5.81	101.35	110.94
8	H	116	ILE	N-CA-C	-5.81	104.84	110.42
10	P	367	GLU	CB-CA-C	-5.80	99.53	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	q	7	LEU	N-CA-C	-5.80	104.86	111.07
11	Q	164	PHE	N-CA-CB	5.79	119.81	110.42
12	R	34	THR	N-CA-C	-5.79	106.83	112.97
19	a	3	PHE	N-CA-CB	5.79	118.75	110.06
4	D	414	ASP	N-CA-C	-5.78	101.40	110.36
17	X	36	CYS	CB-CA-C	-5.77	102.57	111.74
7	G	275	PRO	N-CA-CB	-5.75	97.98	103.33
8	H	252	PRO	N-CA-CB	-5.75	97.99	103.51
10	P	234	LYS	CB-CA-C	-5.73	103.44	111.80
6	F	299	LEU	N-CA-C	5.73	118.46	111.82
13	S	73	GLN	N-CA-C	-5.72	100.38	109.59
8	H	126	LYS	N-CA-C	5.72	117.52	111.28
10	P	272	LEU	N-CA-C	-5.72	101.81	110.28
7	G	289	LYS	N-CA-C	5.72	117.51	111.28
12	R	35	GLY	N-CA-C	5.71	121.81	113.48
6	F	393	ASN	N-CA-C	-5.69	104.98	111.07
1	A	105	GLU	N-CA-C	-5.69	105.08	111.28
5	E	119	THR	N-CA-C	-5.68	105.85	112.89
4	D	352	PRO	N-CA-C	5.68	117.63	110.70
10	P	119	ALA	N-CA-C	-5.67	105.02	111.14
6	F	457	HIS	N-CA-CB	-5.66	100.87	110.50
6	F	176	ALA	N-CA-C	5.66	118.18	111.33
7	G	59	GLN	N-CA-C	5.66	118.01	107.99
11	Q	124	MET	CA-C-N	-5.66	114.94	122.98
11	Q	124	MET	C-N-CA	-5.66	114.94	122.98
12	R	52	GLN	N-CA-C	5.64	117.98	110.53
7	G	599	THR	CA-C-N	-5.64	114.14	122.83
7	G	599	THR	C-N-CA	-5.64	114.14	122.83
21	q	140	PRO	N-CA-C	-5.63	102.29	110.80
18	Z	64	ASP	N-CA-C	5.61	119.85	112.89
6	F	304	ALA	CB-CA-C	-5.60	110.10	116.54
2	B	112	TYR	N-CA-C	5.60	122.73	110.80
9	I	191	LEU	N-CA-C	-5.59	105.27	111.36
17	X	40	ASN	N-CA-C	-5.58	104.88	110.97
5	E	222	PHE	CB-CA-C	-5.58	100.64	109.80
5	E	183	PRO	N-CA-C	-5.58	102.17	111.26
21	q	142	THR	N-CA-CB	5.57	119.86	109.68
2	B	201	LEU	N-CA-C	-5.55	105.13	111.07
7	G	530	TYR	N-CA-C	-5.55	102.06	110.28
13	S	63	PRO	CA-N-CD	5.55	119.77	112.00
6	F	118	ASP	N-CA-C	-5.54	102.08	110.28
21	q	68	MET	N-CA-C	5.54	119.30	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	r	94	ALA	N-CA-C	-5.54	101.66	109.96
6	F	294	VAL	CA-C-N	-5.53	114.07	119.76
6	F	294	VAL	C-N-CA	-5.53	114.07	119.76
12	R	89	PRO	N-CA-CB	-5.52	98.30	103.27
4	D	163	PRO	N-CA-CB	-5.51	97.73	103.08
4	D	200	PHE	CA-CB-CG	5.51	119.31	113.80
7	G	615	LEU	N-CA-C	-5.50	106.34	113.16
21	q	71	LYS	N-CA-C	5.50	119.98	113.16
7	G	127	ASP	CA-C-O	5.50	128.98	121.89
8	H	141	SER	N-CA-CB	5.50	117.98	110.01
4	D	132	ALA	N-CA-C	-5.49	106.58	113.72
19	a	25	TYR	N-CA-C	-5.49	107.83	114.75
7	G	363	SER	N-CA-C	-5.47	100.26	109.07
7	G	313	LEU	N-CA-C	5.47	118.47	109.72
2	B	98	ALA	CB-CA-C	-5.46	108.69	115.89
10	P	86	CYS	N-CA-C	-5.45	103.19	110.55
14	T	135	ALA	N-CA-CB	5.45	118.13	110.12
22	r	111	PRO	N-CA-C	-5.45	106.44	113.57
4	D	231	GLY	N-CA-C	-5.44	103.09	110.43
7	G	150	ARG	N-CA-CB	-5.43	102.83	111.62
7	G	404	GLY	N-CA-C	5.42	121.39	113.48
7	G	420	LYS	N-CA-CB	-5.42	101.94	110.06
7	G	682	ASP	CA-C-N	-5.41	114.19	119.76
7	G	682	ASP	C-N-CA	-5.41	114.19	119.76
10	P	374	THR	N-CA-C	5.41	117.55	108.73
17	X	27	ALA	N-CA-C	-5.41	105.03	111.69
18	Z	50	MET	N-CA-C	-5.39	105.41	111.28
18	Z	55	GLN	N-CA-C	-5.38	105.41	111.28
4	D	141	TYR	N-CA-CB	-5.38	102.21	110.44
14	T	92	LYS	N-CA-C	-5.37	106.32	112.92
5	E	219	SER	N-CA-C	-5.36	100.58	108.79
11	Q	163	ASN	CB-CA-C	-5.35	99.30	109.95
12	R	88	HIS	CB-CA-C	5.35	117.27	109.08
5	E	48	PRO	N-CA-C	5.35	120.79	113.84
4	D	201	PHE	N-CA-C	-5.35	105.53	111.36
7	G	510	TRP	N-CA-C	-5.35	101.94	109.96
8	H	252	PRO	CA-N-CD	5.33	119.47	112.00
8	H	284	GLN	N-CA-C	-5.33	105.55	111.36
11	Q	164	PHE	N-CA-C	-5.32	106.76	113.20
6	F	412	LEU	N-CA-C	-5.32	105.65	111.82
21	q	131	ARG	N-CA-C	5.31	117.68	110.35
5	E	74	GLN	N-CA-C	-5.31	107.46	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	94	PRO	N-CA-C	5.30	118.64	111.22
5	E	221	ARG	N-CA-C	5.29	117.91	110.23
7	G	362	ASP	CA-CB-CG	5.29	117.89	112.60
6	F	199	ARG	N-CA-C	5.29	117.36	109.59
9	I	54	THR	N-CA-C	-5.29	104.93	111.33
10	P	339	GLY	N-CA-C	5.29	122.62	115.00
4	D	391	VAL	CA-C-N	-5.28	115.86	119.66
4	D	391	VAL	C-N-CA	-5.28	115.86	119.66
7	G	356	ASP	N-CA-C	-5.27	105.53	111.28
7	G	449	PRO	N-CA-CB	5.26	109.07	103.39
9	I	160	GLU	N-CA-CB	-5.26	100.77	109.72
8	H	46	LEU	N-CA-C	-5.26	106.64	113.16
21	q	6	VAL	CB-CA-C	-5.26	105.05	112.14
8	H	199	ASP	CB-CA-C	-5.25	102.63	111.24
7	G	277	MET	N-CA-CB	-5.25	101.63	109.71
17	X	33	GLY	N-CA-C	-5.24	107.81	114.16
11	Q	72	ILE	N-CA-C	-5.24	108.40	113.53
5	E	48	PRO	CB-CA-C	-5.23	104.42	111.85
8	H	146	MET	N-CA-C	-5.23	105.47	111.07
8	H	310	PHE	N-CA-C	5.23	119.29	113.01
4	D	391	VAL	N-CA-C	5.23	113.88	109.02
6	F	300	ILE	N-CA-CB	5.23	119.29	110.56
21	q	21	ARG	N-CA-C	5.23	117.65	111.33
13	S	85	ASP	N-CA-C	5.22	117.88	111.82
22	r	111	PRO	CA-N-CD	5.22	119.31	112.00
22	r	25	GLN	N-CA-C	5.22	118.90	112.54
22	r	107	SER	N-CA-C	-5.21	102.14	109.96
15	V	84	ALA	N-CA-C	5.21	116.65	111.07
7	G	63	PHE	CA-C-O	-5.21	115.02	121.06
7	G	600	GLU	CB-CA-C	-5.21	102.99	111.06
7	G	435	PRO	CB-CA-C	-5.21	105.89	111.56
4	D	363	VAL	N-CA-C	5.20	116.28	111.81
7	G	556	THR	N-CA-C	-5.20	101.50	109.41
10	P	260	GLY	N-CA-C	-5.20	108.44	115.36
10	P	194	VAL	N-CA-CB	5.19	118.37	110.58
3	C	164	TRP	N-CA-C	5.19	117.01	111.36
8	H	101	GLY	N-CA-C	5.18	118.51	112.50
10	P	316	LYS	N-CA-C	-5.18	104.89	111.11
7	G	458	GLY	N-CA-C	-5.17	108.19	115.32
7	G	713	ALA	N-CA-C	-5.17	105.54	111.07
7	G	172	ILE	N-CA-C	-5.16	98.61	109.34
10	P	198	ALA	N-CA-C	-5.15	100.12	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	569	GLN	CB-CA-C	-5.15	104.23	112.05
1	A	2	ASN	CA-C-N	-5.14	113.00	120.29
1	A	2	ASN	C-N-CA	-5.14	113.00	120.29
8	H	196	ALA	CA-C-N	-5.14	113.46	119.32
8	H	196	ALA	C-N-CA	-5.14	113.46	119.32
20	b	82	LYS	N-CA-C	-5.14	103.75	110.53
3	C	156	VAL	N-CA-C	-5.12	104.10	111.17
6	F	337	MET	CB-CA-C	-5.12	103.07	111.68
7	G	387	LEU	N-CA-C	-5.12	98.35	107.98
8	H	277	TYR	N-CA-C	5.11	117.92	110.10
6	F	60	GLY	N-CA-C	-5.11	106.00	114.48
9	I	95	PRO	N-CA-C	5.10	121.20	113.81
17	X	140	ASN	CA-C-N	-5.10	114.53	119.78
17	X	140	ASN	C-N-CA	-5.10	114.53	119.78
21	q	5	GLU	N-CA-C	5.09	116.51	111.07
5	E	181	ASN	N-CA-C	-5.08	99.51	108.20
3	C	109	SER	N-CA-C	5.08	118.09	109.76
2	B	98	ALA	N-CA-C	5.07	117.54	109.02
7	G	280	ASP	N-CA-CB	-5.07	102.67	110.12
7	G	393	GLY	N-CA-C	-5.07	107.75	115.66
8	H	254	LEU	N-CA-CB	5.07	118.14	110.28
10	P	376	ASN	CB-CA-C	-5.07	102.24	110.85
23	s	38	HIS	N-CA-C	5.07	118.56	112.38
3	C	221	GLU	N-CA-C	-5.06	102.38	108.25
17	X	112	LEU	N-CA-CB	5.05	117.40	110.07
10	P	170	LEU	N-CA-C	5.05	117.05	110.43
12	R	43	TYR	N-CA-CB	-5.04	103.19	110.70
16	W	112	GLU	N-CA-C	5.04	116.86	111.36
5	E	222	PHE	N-CA-C	5.03	117.80	109.46
14	T	140	CYS	CB-CA-C	-5.03	104.12	109.85
4	D	224	ALA	N-CA-C	5.02	117.14	111.11
7	G	203	ASP	CA-C-O	5.01	127.14	121.32
18	Z	130	LYS	N-CA-C	-5.01	105.71	111.07
9	I	160	GLU	CB-CA-C	5.01	119.15	110.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	762	0	823	74	0
2	B	1247	0	1258	156	0
3	C	1641	0	1596	135	0
4	D	3095	0	3066	298	0
5	E	1635	0	1626	166	0
6	F	3288	0	3243	356	0
7	G	5287	0	5323	554	0
8	H	2525	0	2613	362	0
9	I	1398	0	1359	166	0
10	P	2730	0	2747	226	0
11	Q	957	0	949	70	0
12	R	660	0	639	73	0
13	S	667	0	683	71	0
14	T	604	0	596	93	0
15	V	915	0	954	80	0
16	W	970	0	991	80	0
17	X	1164	0	1154	96	0
18	Z	1152	0	1148	104	0
19	a	548	0	562	54	0
20	b	620	0	617	86	0
21	q	1004	0	962	90	0
22	r	413	0	429	45	0
23	s	226	0	214	14	0
24	A	46	0	69	11	0
24	I	46	0	69	10	0
24	b	46	0	69	11	0
25	B	8	0	0	5	0
25	F	8	0	0	10	0
25	G	16	0	0	5	0
25	I	16	0	0	16	0
26	B	18	0	18	12	0
27	B	35	0	44	3	0
27	I	47	0	71	7	0
28	E	4	0	0	4	0
28	G	4	0	0	4	0
29	F	31	0	19	3	0
30	H	35	0	43	16	0
31	P	48	0	26	4	0
32	R	1	0	0	0	0
33	W	32	0	0	7	0
34	a	57	0	58	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	34006	0	34038	2953	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 (2953) 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:445:LEU:CD2	7:G:460:HIS:CE1	2.17	1.28
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.27
10:P:93:HIS:CD2	10:P:94:LEU:HD12	1.75	1.22
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.20
8:H:251:LEU:HD12	8:H:251:LEU:O	1.41	1.20
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.40	1.19
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
6:F:382:CYS:SG	25:F:502:SF4:FE3	1.38	1.12
26:B:302:UQ1:HM33	4:D:185:MET:CE	1.78	1.12
9:I:123:CYS:SG	25:I:303:SF4:FE1	1.40	1.12
6:F:379:CYS:SG	25:F:502:SF4:FE4	1.43	1.09
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.08
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.08
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.08
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.08
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.27	1.08
17:X:4:ILE:HG22	17:X:5:VAL:H	0.96	1.08
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.07
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.07
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.31	1.06
9:I:152:CYS:SG	25:I:303:SF4:FE2	1.46	1.06
13:S:23:LEU:HD12	13:S:23:LEU:O	1.54	1.06
14:T:138:LEU:HD12	14:T:138:LEU:O	1.55	1.06
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.38	1.05
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.05
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.05
26:B:302:UQ1:HM33	4:D:185:MET:HE3	1.34	1.05
7:G:445:LEU:HD22	7:G:460:HIS:CE1	1.87	1.05
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.05
2:B:82:ILE:HG23	8:H:57:MET:SD	1.97	1.04
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.92	1.04
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.33	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:179:CYS:SG	28:E:301:FES:FE2	1.48	1.04
7:G:401:LEU:HD11	7:G:466:LEU:HD21	1.40	1.04
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.04
6:F:266:GLY:CA	6:F:271:SER:HA	1.86	1.03
8:H:142:TYR:CD1	8:H:289:LEU:HD12	1.94	1.03
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.22	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.75	1.02
16:W:32:LYS:HG2	33:W:201:EHZ:C19	1.90	1.02
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.96	1.01
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.86	1.00
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.00
21:q:66:THR:HG22	21:q:74:PHE:HB2	1.39	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
9:I:155:CYS:SG	25:I:303:SF4:FE4	1.52	1.00
6:F:266:GLY:HA3	6:F:271:SER:CA	1.90	1.00
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	0.99
5:E:179:CYS:HG	28:E:301:FES:FE2	0.70	0.99
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
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	0.98
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.98
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.98
2:B:82:ILE:HG12	8:H:57:MET:CE	1.93	0.98
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.78	0.98
8:H:30:TYR:CE1	19:a:1:MET:O	2.16	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
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
17:X:4:ILE:HG22	17:X:5:VAL:N	1.77	0.97
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.47	0.97
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.97
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.47	0.96
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.96
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.96
6:F:379:CYS:HG	25:F:502:SF4:FE4	0.73	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.96
7:G:92:CYS:SG	28:G:803:FES:S1	2.62	0.96
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.46	0.96
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.96
10:P:376:ASN:OD1	10:P:377:TYR:N	1.98	0.96
2:B:100:CYS:SG	25:B:301:SF4:FE4	1.59	0.95
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.95
13:S:16:LEU:HD11	13:S:51:LEU:HD11	1.46	0.95
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.95
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.95
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.95
12:R:38:TYR:HE2	21:q:127:TYR:HB2	1.30	0.95
5:E:240:PRO:HA	6:F:60:GLY:HA3	1.44	0.95
4:D:90:ALA:HB2	8:H:205:SER:HA	1.45	0.95
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.95
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.48	0.94
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.44	0.94
9:I:152:CYS:HG	25:I:303:SF4:FE2	0.69	0.94
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.32	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
8:H:224:PHE:CE2	30:H:400:UQ9:H13	2.02	0.94
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
6:F:382:CYS:HG	25:F:502:SF4:FE3	0.64	0.94
9:I:113:CYS:SG	25:I:304:SF4:FE3	1.59	0.94
10:P:333:PRO:HB2	10:P:337:ASP:HB2	1.47	0.94
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.93
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.93
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.93
7:G:445:LEU:HD23	7:G:460:HIS:CE1	2.00	0.93
10:P:93:HIS:CD2	10:P:94:LEU:CD1	2.52	0.93
10:P:262:THR:H	10:P:332:LEU:HD12	1.34	0.93
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.92
18:Z:86:ILE:HG23	18:Z:128:ARG:HE	1.33	0.92
22:r:9:GLN:HA	22:r:12:ARG:HD3	1.50	0.92
7:G:445:LEU:CD2	7:G:460:HIS:HE1	1.82	0.92
17:X:4:ILE:CG2	17:X:5:VAL:H	1.82	0.92
17:X:37:ASP:OD2	20:b:70:PRO:HD3	1.69	0.91
15:V:75:GLY:HA2	22:r:103:ARG:HD2	1.51	0.91
16:W:55:LEU:HB3	16:W:107:MET:HE1	1.52	0.91
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.86	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:425:CYS:HG	25:F:502:SF4:FE1	0.62	0.90
10:P:93:HIS:NE2	10:P:94:LEU:CD1	2.35	0.90
7:G:226:CYS:HG	25:G:802:SF4:FE1	0.75	0.90
9:I:80:GLU:HG3	19:a:1:MET:SD	2.11	0.90
6:F:110:PRO:HB3	6:F:152:ARG:CZ	2.03	0.89
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.89
6:F:266:GLY:HA3	6:F:271:SER:HA	0.94	0.89
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.53	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.89
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.88	0.88
7:G:32:ILE:HG23	7:G:98:LYS:HD2	1.54	0.88
7:G:176:CYS:HG	25:G:802:SF4:FE4	0.62	0.88
10:P:96:LEU:HD12	10:P:97:MET:N	1.88	0.88
4:D:99:LEU:CD2	4:D:109:CYS:SG	2.62	0.88
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.88
2:B:81:LEU:HG	8:H:53:MET:HE1	1.54	0.88
7:G:97:MET:HB2	7:G:100:TRP:CD1	2.09	0.88
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.56	0.88
26:B:302:UQ1:CM3	4:D:185:MET:HE3	2.04	0.87
6:F:327:ILE:HD11	6:F:331:VAL:HG11	1.56	0.87
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.87
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.09	0.87
10:P:192:ARG:HH22	10:P:198:ALA:HB3	1.36	0.87
13:S:16:LEU:HD22	13:S:19:ILE:HD11	1.53	0.87
20:b:60:ASP:OD1	20:b:61:GLY:N	2.07	0.87
14:T:79:ILE:HB	14:T:145:VAL:HG13	1.55	0.87
2:B:104:MET:HE3	26:B:302:UQ1:H112	1.58	0.86
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.86
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.86
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.86
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.56	0.86
13:S:16:LEU:HD12	13:S:16:LEU:O	1.76	0.86
7:G:78:CYS:SG	28:G:803:FES:FE2	1.68	0.86
3:C:80:LEU:O	3:C:81:ASP:HB2	1.73	0.86
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.86
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.86
16:W:55:LEU:HD22	16:W:107:MET:HE2	1.57	0.86
4:D:99:LEU:HD23	4:D:109:CYS:HA	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:44:ASN:HD21	6:F:51:TRP:HA	1.41	0.86
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.86
9:I:162:CYS:SG	25:I:304:SF4:FE4	1.68	0.86
17:X:53:PRO:HD2	18:Z:116:TRP:CD1	2.11	0.85
12:R:32:THR:HG22	12:R:36:GLN:H	1.40	0.85
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.59	0.85
4:D:137:ASP:OD1	4:D:148:GLU:CD	2.20	0.85
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.85
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.95	0.85
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.59	0.85
2:B:101:ALA:HB3	26:B:302:UQ1:HM23	1.59	0.84
7:G:78:CYS:HG	28:G:803:FES:FE2	0.55	0.84
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.84
10:P:206:ILE:H	31:P:401:NDP:H71N	1.24	0.84
15:V:56:LEU:HD12	15:V:57:ASP:N	1.92	0.84
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.84
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.84
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.07	0.84
10:P:192:ARG:NH2	10:P:198:ALA:HB3	1.92	0.84
4:D:266:ARG:HB2	9:I:65:GLU:OE2	1.77	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
6:F:300:ILE:HD13	6:F:307:VAL:H	1.41	0.84
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.58	0.84
8:H:224:PHE:CE2	30:H:400:UQ9:C13	2.59	0.84
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.84
12:R:38:TYR:CE2	21:q:127:TYR:HB2	2.13	0.84
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.83
8:H:187:ILE:HD12	24:I:301:3PE:H251	1.59	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
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.83
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.79	0.83
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.82
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.92	0.82
9:I:162:CYS:HG	25:I:304:SF4:FE4	0.53	0.82
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.82
6:F:117:ALA:HB1	6:F:131:MET:SD	2.19	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
3:C:217:ARG:NH1	16:W:112:GLU:HB2	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:183:MET:HE2	27:I:302:PC1:H2A1	1.61	0.82
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.60	0.82
2:B:89:SER:O	8:H:54:LYS:HD3	1.79	0.82
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.45	0.82
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.82
12:R:51:ARG:HH21	21:q:125:VAL:HG12	1.44	0.82
7:G:401:LEU:CD1	7:G:466:LEU:HD21	2.09	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
4:D:329:ARG:HD2	4:D:453:THR:HB	1.62	0.81
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
9:I:123:CYS:HG	25:I:303:SF4:FE1	0.53	0.81
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.81
21:q:71:LYS:O	21:q:72:ASN:OD1	1.99	0.81
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.96	0.81
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.81
16:W:55:LEU:CD2	16:W:107:MET:HE2	2.09	0.81
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.81
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.81
13:S:36:PHE:HZ	13:S:44:LEU:HD11	1.45	0.81
1:A:25:PRO:HG3	8:H:60:PRO:HD3	1.63	0.80
8:H:311:THR:HB	18:Z:51:MET:SD	2.21	0.80
20:b:20:VAL:HA	24:b:201:3PE:H282	1.64	0.80
2:B:89:SER:O	8:H:54:LYS:CD	2.29	0.80
6:F:109:ARG:NH1	6:F:237:GLY:O	2.13	0.80
6:F:234:GLY:HA3	6:F:238:CYS:O	1.82	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.80
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.80
8:H:181:MET:CE	8:H:304:HIS:ND1	2.45	0.80
8:H:251:LEU:O	8:H:251:LEU:CD1	2.27	0.80
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.63	0.80
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
9:I:113:CYS:HG	25:I:304:SF4:FE3	0.52	0.80
6:F:174:ARG:HA	23:s:52:LEU:HD21	1.64	0.80
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.63	0.80
7:G:73:GLY:HA2	28:G:803:FES:S1	2.21	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.79
14:T:87:LEU:HD21	14:T:104:PHE:HZ	1.47	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
14:T:93:ILE:HG21	14:T:110:LEU:HD22	1.63	0.79
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.46	0.79
8:H:142:TYR:OH	8:H:288:LEU:HD22	1.82	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
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
14:T:113:LEU:HD22	16:W:71:MET:HE2	1.63	0.79
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79
21:q:55:PHE:CD1	22:r:26:LEU:HD22	2.17	0.79
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.65	0.79
8:H:17:MET:SD	8:H:229:THR:OG1	2.41	0.79
13:S:20:ARG:HG3	13:S:54:LEU:HB2	1.64	0.79
4:D:280:ALA:CB	15:V:11:LEU:HG	2.13	0.78
15:V:48:THR:OG1	15:V:87:GLU:OE2	2.01	0.78
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.78
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.65	0.78
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.23	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.65	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.78
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.18	0.78
14:T:87:LEU:HD22	14:T:104:PHE:CE1	2.19	0.78
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.63	0.78
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.78
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
20:b:66:VAL:HG13	20:b:72:ASP:HB2	1.65	0.78
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.77
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.67	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
5:E:178:ALA:HA	6:F:125:CYS:SG	2.24	0.77
14:T:83:VAL:CG2	14:T:126:PHE:HZ	1.97	0.77
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
2:B:96:GLY:HA2	2:B:101:ALA:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.66	0.77
8:H:93:HIS:CE1	19:a:24:ALA:HA	2.19	0.77
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.65	0.77
21:q:9:ARG:HA	21:q:12:GLN:HG2	1.65	0.77
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.77
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.65	0.77
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.77
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.67	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77
3:C:217:ARG:HH12	16:W:112:GLU:HB2	1.50	0.77
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.77
4:D:99:LEU:HD22	4:D:109:CYS:SG	2.24	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.77
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.50	0.76
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.76
17:X:20:VAL:HG22	17:X:24:VAL:HG21	1.66	0.76
26:B:302:UQ1:HM33	4:D:185:MET:HE2	1.65	0.76
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.76
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.00	0.76
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.50	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
13:S:51:LEU:HD13	13:S:95:LEU:HD21	1.67	0.76
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.67	0.76
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.68	0.76
2:B:89:SER:O	8:H:54:LYS:HE2	1.85	0.76
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.13	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.76
14:T:93:ILE:HG23	14:T:110:LEU:HD13	1.66	0.76
4:D:271:ARG:HD2	8:H:279:ARG:O	1.86	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
6:F:109:ARG:CZ	6:F:237:GLY:O	2.34	0.76
10:P:143:ASP:HA	10:P:147:ASN:HB2	1.67	0.76
5:E:189:ASP:CG	6:F:163:TYR:HB3	2.11	0.76
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.68	0.76
27:B:303:PC1:H371	8:H:49:PHE:HB3	1.66	0.75
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.75
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.75
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.75
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.75
13:S:19:ILE:HG13	13:S:95:LEU:HD11	1.69	0.75
7:G:651:PRO:HG3	13:S:57:GLU:H	1.51	0.75
19:a:3:PHE:HE2	34:a:101:CDL:HA4	1.50	0.75
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.75
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.52	0.75
17:X:29:ALA:HB2	18:Z:71:LEU:HD11	1.67	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.75
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.75
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.75
8:H:91:MET:O	8:H:92:PRO:C	2.26	0.75
11:Q:167:ASN:O	11:Q:168:LYS:CD	2.35	0.75
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.75
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
16:W:28:LEU:HG	16:W:32:LYS:HE3	1.69	0.75
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.74
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.74
16:W:55:LEU:HB3	16:W:107:MET:HE2	1.66	0.74
20:b:23:PHE:HD2	24:b:201:3PE:H281	1.51	0.74
4:D:99:LEU:HD21	4:D:109:CYS:SG	2.26	0.74
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.69	0.74
10:P:336:GLU:HG3	10:P:342:PRO:HD3	1.67	0.74
14:T:117:GLU:HA	14:T:120:MET:HE3	1.67	0.74
1:A:4:TYR:CE2	24:A:401:3PE:H231	2.22	0.74
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.88	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
20:b:31:ILE:HA	20:b:34:MET:HE2	1.69	0.74
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.74
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.74
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.74
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.03	0.74
6:F:425:CYS:SG	25:F:502:SF4:FE1	1.78	0.74
7:G:674:LEU:HD11	13:S:46:LYS:HE2	1.69	0.74
8:H:180:PRO:HD3	18:Z:43:LEU:HD21	1.70	0.74
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.28	0.74
14:T:88:LYS:HG3	14:T:98:LEU:HD22	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:20:VAL:HG13	24:b:201:3PE:H2A1	1.69	0.74
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.70	0.74
14:T:103:HIS:CG	14:T:106:LYS:HD2	2.23	0.74
2:B:91:TRP:CZ3	30:H:400:UQ9:H1M	2.22	0.73
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.68	0.73
18:Z:93:GLU:O	18:Z:97:ILE:HG13	1.88	0.73
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.69	0.73
14:T:94:ASP:HB3	14:T:98:LEU:HB2	1.68	0.73
21:q:56:PHE:HD1	21:q:59:HIS:HE2	1.35	0.73
6:F:293:SER:HA	6:F:336:LEU:HD13	1.68	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.73
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.73
2:B:112:TYR:OH	9:I:91:GLY:CA	2.28	0.73
3:C:80:LEU:HG	4:D:396:THR:HG22	1.71	0.73
5:E:240:PRO:HG3	6:F:57:LEU:O	1.88	0.73
20:b:69:HIS:HD2	20:b:70:PRO:HD2	1.54	0.73
5:E:39:VAL:HG11	7:G:163:LYS:NZ	2.04	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.73
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.73
20:b:23:PHE:HE1	24:b:201:3PE:H371	1.53	0.73
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.87	0.73
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.54	0.73
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.70	0.73
16:W:32:LYS:HE2	33:W:201:EHZ:C19	2.18	0.73
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
11:Q:167:ASN:O	11:Q:168:LYS:HD2	1.88	0.72
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.72
18:Z:65:LEU:O	18:Z:69:ILE:HG12	1.89	0.72
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.72
21:q:56:PHE:HA	21:q:59:HIS:CD2	2.24	0.72
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.68	0.72
4:D:375:MET:HE1	7:G:126:LEU:HA	1.71	0.72
5:E:232:SER:HB3	6:F:288:VAL:HG23	1.69	0.72
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.72
10:P:169:HIS:H	10:P:184:LYS:HE3	1.54	0.72
4:D:90:ALA:HB2	8:H:205:SER:CA	2.18	0.72
1:A:21:ALA:O	1:A:25:PRO:HD3	1.88	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.20	0.72
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:327:ILE:HG23	6:F:332:CYS:SG	2.29	0.72
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.72
14:T:120:MET:HG2	16:W:44:ARG:HH11	1.54	0.72
9:I:200:GLU:OE2	21:q:93:MET:SD	2.48	0.72
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.71
4:D:266:ARG:CB	9:I:65:GLU:OE2	2.38	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
9:I:53:ALA:HB1	20:b:14:ALA:HB2	1.71	0.71
10:P:192:ARG:NH1	10:P:192:ARG:HA	2.05	0.71
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.71
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	0.71
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.71	0.71
5:E:240:PRO:CA	6:F:60:GLY:HA3	2.20	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.71
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.71
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.71
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
8:H:183:MET:HE2	27:I:302:PC1:H271	1.72	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.73	0.71
8:H:113:VAL:HG22	8:H:136:VAL:HG23	1.72	0.71
27:I:302:PC1:H2D1	27:I:302:PC1:H291	1.71	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
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.72	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.71
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.71
8:H:311:THR:O	18:Z:51:MET:HG3	1.91	0.71
10:P:170:LEU:O	10:P:171:ASN:OD1	2.09	0.71
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.56	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.70
18:Z:69:ILE:HG23	20:b:54:PRO:HD3	1.73	0.70
19:a:3:PHE:CE2	34:a:101:CDL:HA4	2.26	0.70
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.74	0.70
8:H:23:VAL:HG11	19:a:9:LEU:HD21	1.72	0.70
9:I:155:CYS:HG	25:I:303:SF4:FE4	1.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:67:GLN:HG2	12:R:109:LEU:CD2	2.21	0.70
2:B:116:ARG:O	8:H:39:ILE:HG22	1.91	0.70
4:D:137:ASP:OD1	4:D:148:GLU:CG	2.39	0.70
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.55	0.70
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.55	0.70
16:W:42:TRP:CZ2	16:W:93:LEU:HA	2.26	0.70
4:D:141:TYR:O	4:D:144:MET:SD	2.49	0.70
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.70
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.73	0.70
2:B:89:SER:O	8:H:54:LYS:CE	2.40	0.70
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.70
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.27	0.70
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.70
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.70
16:W:32:LYS:CG	33:W:201:EHZ:C19	2.69	0.70
2:B:82:ILE:HA	8:H:57:MET:HE1	1.74	0.70
2:B:136:THR:HG21	2:B:177:VAL:HG22	1.73	0.70
5:E:237:PRO:HG3	6:F:49:HIS:CD2	2.27	0.70
7:G:127:ASP:HA	12:R:106:TYR:OH	1.90	0.70
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.70
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.70
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.70
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.22	0.69
15:V:56:LEU:HD12	15:V:56:LEU:C	2.16	0.69
18:Z:86:ILE:HG23	18:Z:128:ARG:NE	2.06	0.69
2:B:95:PHE:HE2	2:B:131:MET:SD	2.15	0.69
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.73	0.69
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.21	0.69
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.69
14:T:100:VAL:HB	14:T:142:GLN:HB2	1.74	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	2.08	0.69
21:q:3:LEU:HD12	21:q:6:VAL:CG2	2.22	0.69
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
4:D:253:LEU:HB2	22:r:23:LYS:CD	2.23	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.74	0.69
9:I:92:PRO:HA	21:q:91:HIS:O	1.93	0.69
10:P:171:ASN:OD1	10:P:171:ASN:O	2.11	0.69
14:T:87:LEU:HD22	14:T:104:PHE:HE1	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.74	0.69
6:F:225:LEU:H	11:Q:160:TYR:HE2	1.38	0.69
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.74	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
7:G:126:LEU:HD11	12:R:89:PRO:CB	2.23	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.28	0.69
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.69
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.58	0.69
14:T:138:LEU:HD13	14:T:144:ILE:CG1	2.22	0.69
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.68
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.23	0.68
10:P:191:VAL:HA	10:P:194:VAL:HG22	1.73	0.68
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.75	0.68
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.68
17:X:50:GLU:HG3	17:X:56:CYS:SG	2.33	0.68
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
8:H:30:TYR:CZ	19:a:1:MET:O	2.45	0.68
8:H:33:LEU:HD23	22:r:25:GLN:HG2	1.76	0.68
8:H:85:LEU:HD21	8:H:108:THR:HB	1.74	0.68
8:H:224:PHE:CZ	30:H:400:UQ9:H13	2.28	0.68
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.75	0.68
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.68
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.68
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.68
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.08	0.68
22:r:20:LEU:C	22:r:20:LEU:HD12	2.18	0.68
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.74	0.68
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.68
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.76	0.68
20:b:23:PHE:HZ	24:b:201:3PE:H351	1.58	0.68
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.57	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
10:P:192:ARG:NH2	10:P:200:ILE:HD11	2.09	0.68
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.68
6:F:227:PRO:HG3	7:G:94:MET:SD	2.34	0.68
1:A:105:GLU:CG	1:A:111:LEU:HG	2.25	0.67
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.28	0.67
20:b:23:PHE:HE1	24:b:201:3PE:H3A2	1.59	0.67
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.67
7:G:126:LEU:CD1	12:R:89:PRO:HB3	2.24	0.67
2:B:94:THR:HB	2:B:104:MET:HE1	1.74	0.67
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.67
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.58	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.67
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
1:A:3:LEU:HD23	24:A:401:3PE:H251	1.75	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.67
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
9:I:188:GLU:OE2	12:R:56:ASN:HB2	1.94	0.67
6:F:300:ILE:HD13	6:F:307:VAL:HG23	1.77	0.67
9:I:188:GLU:CD	12:R:56:ASN:HB2	2.19	0.67
10:P:302:GLY:HA2	10:P:314:THR:HG23	1.77	0.67
15:V:116:ILE:HG23	15:V:116:ILE:O	1.92	0.67
21:q:138:VAL:CG2	21:q:139:PRO:HD2	2.25	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
10:P:197:GLU:HB3	10:P:259:VAL:CG2	2.24	0.67
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.05	0.67
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.67
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.09	0.67
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.76	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.77	0.67
13:S:16:LEU:HB3	13:S:69:TYR:HD1	1.58	0.67
17:X:18:VAL:HG21	18:Z:74:LEU:HD11	1.75	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.67
9:I:93:LEU:O	21:q:93:MET:HG2	1.94	0.67
10:P:94:LEU:HA	10:P:97:MET:HE3	1.77	0.67
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.66
9:I:54:THR:HG21	18:Z:33:TYR:CZ	2.29	0.66
10:P:192:ARG:HH22	10:P:198:ALA:CB	2.07	0.66
10:P:288:PHE:CZ	10:P:290:PRO:HB3	2.30	0.66
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.74	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
3:C:141:ARG:NH1	4:D:410:TYR:HE1	1.93	0.66
6:F:109:ARG:HE	6:F:239:PRO:HD3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.25	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.66
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.28	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
8:H:207:LEU:O	8:H:208:VAL:C	2.38	0.66
9:I:35:THR:CG2	22:r:107:SER:HA	2.26	0.66
14:T:87:LEU:CD2	14:T:104:PHE:CZ	2.78	0.66
14:T:130:ILE:HG23	14:T:131:PRO:HD2	1.77	0.66
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.77	0.66
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.66
9:I:80:GLU:OE2	22:r:26:LEU:CD1	2.44	0.66
12:R:42:ASP:HB3	12:R:44:ARG:HH11	1.61	0.66
16:W:121:PHE:HA	16:W:124:LYS:HE2	1.75	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
13:S:24:CYS:SG	13:S:61:VAL:O	2.53	0.66
14:T:83:VAL:HG22	14:T:126:PHE:CZ	2.31	0.66
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.66
3:C:79:CYS:C	3:C:81:ASP:N	2.48	0.66
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.74	0.66
10:P:169:HIS:H	10:P:184:LYS:CE	2.09	0.66
10:P:199:ILE:HD11	10:P:258:ALA:O	1.96	0.66
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.78	0.66
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.66
6:F:110:PRO:O	6:F:238:CYS:HB3	1.96	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
1:A:8:PHE:HE1	24:A:401:3PE:H2C1	1.60	0.65
3:C:98:PHE:CA	15:V:90:LEU:HD11	2.19	0.65
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.26	0.65
2:B:91:TRP:CH2	30:H:400:UQ9:H1M	2.31	0.65
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.65
8:H:130:PHE:HD2	8:H:207:LEU:HD21	1.61	0.65
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.65
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.77	0.65
8:H:283:ASP:OD1	8:H:284:GLN:N	2.29	0.65
10:P:59:PHE:HB2	10:P:130:ILE:HD11	1.79	0.65
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.77	0.65
6:F:236:PHE:HA	11:Q:166:TRP:CD1	2.30	0.65
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:16:LEU:HB3	13:S:69:TYR:CD1	2.32	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:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
13:S:58:CYS:HB2	13:S:61:VAL:HG12	1.78	0.65
2:B:93:MET:HE1	2:B:131:MET:HE2	1.78	0.65
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.65
10:P:236:VAL:CG1	10:P:270:ARG:HH21	2.10	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.65
9:I:79:ARG:HG2	22:r:12:ARG:HH21	1.62	0.65
14:T:118:ILE:HG23	14:T:122:MET:HE3	1.78	0.65
2:B:146:ARG:O	2:B:147:LYS:C	2.39	0.65
10:P:191:VAL:HG13	10:P:192:ARG:NH2	2.12	0.65
10:P:226:VAL:HG21	10:P:281:PHE:CZ	2.31	0.65
4:D:137:ASP:OD1	4:D:148:GLU:OE2	2.14	0.65
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.78	0.65
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.65
17:X:124:GLN:O	20:b:70:PRO:HB2	1.97	0.65
2:B:173:TYR:O	3:C:203:LEU:HD22	1.97	0.64
5:E:79:LEU:HB2	5:E:80:PRO:HD3	1.78	0.64
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.33	0.64
10:P:88:VAL:HG12	10:P:92:MET:HE2	1.80	0.64
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.64
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.64
8:H:33:LEU:CD2	22:r:25:GLN:HG2	2.26	0.64
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.79	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	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
11:Q:163:ASN:OD1	11:Q:164:PHE:N	2.31	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.78	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.64
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.64
14:T:138:LEU:O	14:T:138:LEU:CD1	2.40	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.79	0.64
12:R:32:THR:HG22	12:R:36:GLN:N	2.09	0.64
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.64
14:T:83:VAL:HG23	14:T:126:PHE:HZ	1.62	0.64
14:T:87:LEU:HD21	14:T:104:PHE:CZ	2.32	0.64
17:X:65:GLY:HA2	17:X:68:LEU:HD12	1.78	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.64
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.64
18:Z:86:ILE:HA	18:Z:128:ARG:HH21	1.62	0.64
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.33	0.64
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.64
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.64
17:X:37:ASP:OD1	17:X:38:LYS:N	2.31	0.64
2:B:92:PRO:HD2	2:B:120:VAL:HG12	1.80	0.63
2:B:136:THR:CG2	2:B:177:VAL:HG22	2.29	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.63
10:P:333:PRO:HB2	10:P:337:ASP:CB	2.25	0.63
2:B:94:THR:CB	2:B:104:MET:HE1	2.27	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	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
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.63
10:P:284:THR:HG23	10:P:356:HIS:HB2	1.79	0.63
18:Z:65:LEU:O	18:Z:68:ARG:HG2	1.98	0.63
2:B:70:ARG:HG3	2:B:73:TYR:H	1.63	0.63
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.63
10:P:180:SER:O	10:P:184:LYS:HG3	1.98	0.63
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.63
6:F:33:GLY:HA2	6:F:291:GLU:CB	2.16	0.63
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.63
13:S:16:LEU:HD12	13:S:16:LEU:C	2.22	0.63
13:S:16:LEU:HA	13:S:69:TYR:HA	1.79	0.63
18:Z:70:ALA:O	18:Z:73:PRO:HD2	1.99	0.63
4:D:142:VAL:HG13	4:D:207:ARG:NH1	2.14	0.63
10:P:93:HIS:NE2	10:P:94:LEU:HD11	2.14	0.63
14:T:93:ILE:CG2	14:T:110:LEU:HD13	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.79	0.63
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
22:r:109:ASP:O	22:r:110:GLN:HG2	1.99	0.63
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.63
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.63
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.63
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.99	0.63
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.63
13:S:15:GLY:HA3	13:S:17:ARG:HH22	1.63	0.63
21:q:6:VAL:HA	21:q:9:ARG:HG2	1.79	0.63
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.63
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.80	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.63
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.28	0.63
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.28	0.63
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.34	0.63
16:W:55:LEU:CB	16:W:107:MET:CE	2.75	0.63
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.62
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.80	0.62
1:A:52:SER:HB2	1:A:54:LYS:HG2	1.78	0.62
5:E:230:LEU:HD11	6:F:48:ARG:HE	1.64	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
8:H:195:ARG:O	8:H:199:ASP:HB2	1.99	0.62
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.61	0.62
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
4:D:260:GLU:HG3	18:Z:25:LEU:HD22	1.80	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
16:W:55:LEU:CB	16:W:107:MET:HE2	2.30	0.62
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.35	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
14:T:103:HIS:ND1	14:T:140:CYS:SG	2.73	0.62
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.34	0.62
18:Z:58:ARG:NH2	20:b:49:THR:HG21	2.13	0.62
2:B:194:CYS:O	25:B:301:SF4:S2	2.58	0.62
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.62
8:H:25:ARG:HD2	30:H:400:UQ9:H10A	1.80	0.62
10:P:240:VAL:HB	10:P:266:THR:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.79	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.29	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.62
22:r:20:LEU:HD12	22:r:21:GLN:N	2.14	0.62
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.26	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.82	0.62
7:G:399:VAL:CG2	7:G:462:PHE:HZ	2.12	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.65	0.62
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.62
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.48	0.62
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.62
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.80	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.82	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	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
13:S:23:LEU:O	13:S:23:LEU:CD1	2.41	0.62
18:Z:28:ARG:HG3	18:Z:28:ARG:O	1.99	0.62
20:b:11:ASN:O	20:b:15:LYS:N	2.31	0.62
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.81	0.61
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.81	0.61
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.61
7:G:651:PRO:CD	13:S:56:ARG:HB3	2.30	0.61
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.35	0.61
8:H:306:SER:HG	8:H:310:PHE:HE2	1.30	0.61
20:b:23:PHE:CE1	24:b:201:3PE:H371	2.35	0.61
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.65	0.61
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.63	0.61
7:G:176:CYS:SG	25:G:802:SF4:FE4	1.78	0.61
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.61
7:G:617:ARG:NH1	16:W:129:HIS:HA	2.14	0.61
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.61
17:X:69:ASN:O	17:X:73:GLN:HG3	2.00	0.61
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.36	0.61
3:C:80:LEU:H	3:C:80:LEU:HD22	1.64	0.61
5:E:71:GLU:HB2	23:s:59:GLN:HB3	1.82	0.61
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.83	0.61
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.30	0.61
12:R:98:GLU:CD	12:R:98:GLU:H	2.07	0.61
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.82	0.61
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
21:q:71:LYS:O	21:q:72:ASN:CG	2.43	0.61
4:D:202:TRP:CZ3	4:D:261:MET:HG3	2.36	0.61
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	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
21:q:3:LEU:HD12	21:q:6:VAL:HG21	1.81	0.61
2:B:93:MET:HB2	2:B:128:ALA:CB	2.30	0.61
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.61
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.82	0.61
7:G:82:ILE:CG2	7:G:100:TRP:HB3	2.30	0.61
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	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
10:P:191:VAL:HG13	10:P:192:ARG:HH21	1.66	0.61
14:T:138:LEU:HD12	14:T:138:LEU:C	2.24	0.61
20:b:23:PHE:CE1	24:b:201:3PE:H3A2	2.35	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.31	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
6:F:416:SER:O	6:F:419:ILE:HG22	2.01	0.61
9:I:53:ALA:CB	20:b:14:ALA:HB2	2.30	0.61
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.81	0.61
10:P:169:HIS:HD2	10:P:181:LEU:HD11	1.65	0.61
11:Q:167:ASN:O	11:Q:168:LYS:CG	2.48	0.61
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.61
14:T:79:ILE:CB	14:T:145:VAL:HG13	2.28	0.61
2:B:101:ALA:HB1	26:B:302:UQ1:O1	2.01	0.61
3:C:133:SER:OG	3:C:136:PHE:O	2.16	0.61
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.61
5:E:182:ALA:O	5:E:183:PRO:C	2.43	0.61
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	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:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.61
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.32	0.60
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.60
10:P:192:ARG:HA	10:P:192:ARG:CZ	2.30	0.60
21:q:34:ARG:NE	21:q:58:ARG:NH2	2.48	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.02	0.60
10:P:263:PHE:HD2	10:P:333:PRO:O	1.84	0.60
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.60
12:R:32:THR:HA	12:R:55:VAL:HG23	1.84	0.60
21:q:3:LEU:O	21:q:6:VAL:HG22	2.01	0.60
7:G:126:LEU:CD1	12:R:89:PRO:HB2	2.31	0.60
10:P:299:SER:HB3	10:P:316:LYS:HE3	1.83	0.60
14:T:103:HIS:HB2	14:T:106:LYS:HB2	1.83	0.60
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
13:S:19:ILE:HG13	13:S:95:LEU:CD1	2.31	0.60
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.60
18:Z:143:TYR:O	18:Z:144:THR:C	2.45	0.60
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.60
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.60
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.63	0.60
10:P:315:THR:O	10:P:316:LYS:C	2.45	0.60
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.60
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:239:THR:O	8:H:239:THR:HG22	2.01	0.60
9:I:80:GLU:OE2	22:r:26:LEU:HD11	2.01	0.60
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.37	0.60
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.67	0.60
2:B:97:LEU:CD2	2:B:141:MET:HG2	2.30	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
10:P:136:THR:CG2	10:P:139:PHE:HB2	2.31	0.60
13:S:16:LEU:CB	13:S:69:TYR:HD1	2.14	0.60
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.60
2:B:144:ALA:O	2:B:145:LEU:C	2.45	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
10:P:262:THR:N	10:P:332:LEU:HD12	2.12	0.60
14:T:83:VAL:HG22	14:T:126:PHE:HZ	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.37	0.60
7:G:304:GLU:OE2	10:P:41:ILE:HG12	2.01	0.60
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.60
17:X:37:ASP:HA	17:X:40:ASN:HB2	1.84	0.60
4:D:202:TRP:CH2	4:D:261:MET:HG3	2.37	0.59
6:F:297:LYS:HB2	6:F:333:GLU:CB	2.31	0.59
12:R:42:ASP:HB3	12:R:44:ARG:NH1	2.17	0.59
17:X:20:VAL:HG12	17:X:25:LEU:HD21	1.84	0.59
17:X:133:THR:HG23	20:b:58:ARG:HH12	1.65	0.59
3:C:70:LYS:O	15:V:103:LEU:HD12	2.02	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.59
4:D:95:LEU:HG	4:D:97:LEU:HG	1.84	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.37	0.59
20:b:8:PHE:HA	20:b:11:ASN:ND2	2.18	0.59
5:E:162:THR:CG2	5:E:166:LYS:HA	2.33	0.59
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
10:P:318:LYS:O	10:P:322:ILE:HG13	2.02	0.59
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.32	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.02	0.59
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.66	0.59
6:F:119:GLU:HB3	6:F:124:THR:CG2	2.32	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
1:A:68:GLU:CD	1:A:98:LEU:HG	2.28	0.59
2:B:91:TRP:CH2	30:H:400:UQ9:C1M	2.86	0.59
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
8:H:142:TYR:CG	8:H:289:LEU:HD12	2.37	0.59
10:P:96:LEU:HD12	10:P:96:LEU:C	2.28	0.59
18:Z:98:MET:HB2	18:Z:104:TRP:NE1	2.18	0.59
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.83	0.59
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	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
10:P:178:SER:O	10:P:182:ARG:HG2	2.02	0.59
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:51:ASP:O	21:q:59:HIS:HB2	2.02	0.59
23:s:57:LEU:HG	23:s:58:PRO:HD2	1.84	0.59
4:D:375:MET:HE1	7:G:126:LEU:CA	2.33	0.59
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.84	0.59
10:P:357:ARG:HD3	10:P:361:TRP:O	2.03	0.59
12:R:40:GLU:HA	12:R:45:ARG:CZ	2.32	0.59
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.85	0.59
16:W:93:LEU:HG	16:W:97:ILE:CD1	2.33	0.59
18:Z:105:LYS:O	18:Z:106:VAL:C	2.46	0.59
20:b:6:SER:O	20:b:9:LEU:HB3	2.03	0.59
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.59
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.36	0.59
8:H:310:PHE:O	20:b:38:TYR:HB2	2.02	0.59
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.59
14:T:123:GLU:OE1	16:W:44:ARG:NH1	2.36	0.59
17:X:78:CYS:SG	17:X:110:CYS:HB3	2.42	0.59
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.59
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.84	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
5:E:165:ASP:C	5:E:167:LEU:H	2.09	0.58
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.67	0.58
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.58
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.33	0.58
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.58
6:F:44:ASN:HB3	6:F:134:ASP:HB2	1.84	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.86	0.58
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.84	0.58
13:S:47:ALA:O	13:S:49:PRO:HD3	2.03	0.58
17:X:134:ASP:O	17:X:135:ARG:C	2.45	0.58
18:Z:122:GLY:O	18:Z:126:GLY:N	2.34	0.58
4:D:99:LEU:CD2	4:D:109:CYS:HA	2.32	0.58
6:F:382:CYS:SG	25:F:502:SF4:S1	3.02	0.58
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.58
7:G:445:LEU:HD21	7:G:462:PHE:HB2	1.85	0.58
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.86	0.58
10:P:122:HIS:CB	12:R:46:VAL:HG12	2.33	0.58
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.84	0.58
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
10:P:57:THR:HG23	10:P:123:SER:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:66:GLY:O	10:P:67:ARG:C	2.42	0.58
16:W:104:THR:O	16:W:108:ARG:HG3	2.02	0.58
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.68	0.58
4:D:99:LEU:HB3	4:D:101:LEU:CD1	2.34	0.58
4:D:388:GLY:HA3	4:D:417:SER:OG	2.03	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.16	0.58
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.85	0.58
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.58
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.58
34:a:101:CDL:HB4	21:q:3:LEU:HD13	1.86	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
8:H:201:THR:OG1	8:H:202:GLU:N	2.36	0.58
10:P:57:THR:HG23	10:P:123:SER:HB2	1.86	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.04	0.58
23:s:35:LEU:HB3	23:s:38:HIS:HB2	1.85	0.58
2:B:101:ALA:CB	26:B:302:UQ1:O1	2.52	0.58
4:D:128:THR:H	4:D:131:GLN:NE2	2.00	0.58
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.58
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.58
16:W:42:TRP:CH2	16:W:93:LEU:HA	2.39	0.58
17:X:90:ASP:OD2	19:a:62:VAL:HG11	2.04	0.58
2:B:115:ASP:HA	2:B:119:VAL:O	2.04	0.58
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.04	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
17:X:122:LEU:HD23	20:b:82:LYS:HG2	1.85	0.58
17:X:141:PRO:O	17:X:142:TYR:HB2	2.04	0.58
18:Z:62:ILE:HG12	20:b:49:THR:HA	1.85	0.58
18:Z:129:THR:HB	18:Z:132:GLU:HG3	1.86	0.58
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.58
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.58
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.86	0.58
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.58
10:P:245:VAL:O	10:P:249:ILE:HG13	2.04	0.58
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.86	0.58
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.57
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.86	0.57
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.57
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.57
2:B:164:CYS:SG	25:B:301:SF4:S4	3.02	0.57
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.39	0.57
3:C:186:ILE:HG13	3:C:187:LEU:N	2.18	0.57
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57
8:H:85:LEU:CD2	8:H:108:THR:HB	2.34	0.57
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.39	0.57
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.57
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.57
14:T:90:TYR:CE2	14:T:92:LYS:HB3	2.39	0.57
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.57
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
10:P:220:TYR:HA	10:P:223:PHE:HD2	1.67	0.57
14:T:90:TYR:CE2	14:T:92:LYS:CB	2.87	0.57
2:B:153:PRO:HB2	2:B:155:PRO:HD2	1.85	0.57
6:F:48:ARG:NH1	6:F:48:ARG:HA	2.19	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.57
2:B:99:CYS:C	2:B:101:ALA:N	2.59	0.57
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.57
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	2.02	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
7:G:372:PHE:H	7:G:532:PRO:HB2	1.69	0.57
8:H:307:LEU:HD11	18:Z:47:TYR:CG	2.39	0.57
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.85	0.57
10:P:192:ARG:CZ	10:P:198:ALA:HB3	2.34	0.57
12:R:37:VAL:O	12:R:38:TYR:C	2.44	0.57
20:b:69:HIS:CD2	20:b:70:PRO:HD2	2.36	0.57
2:B:110:PRO:HB3	8:H:33:LEU:O	2.03	0.57
2:B:170:TYR:OH	4:D:131:GLN:O	2.22	0.57
8:H:142:TYR:CE1	8:H:289:LEU:HD12	2.39	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.05	0.57
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.57
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.86	0.57
21:q:13:GLN:HB3	21:q:33:ILE:HG22	1.87	0.57
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.66	0.57
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.57
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.57
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.57
6:F:39:ASP:HA	6:F:261:TRP:HZ2	1.70	0.57
8:H:19:PHE:CE1	19:a:11:ILE:HD12	2.40	0.57
9:I:62:MET:SD	18:Z:35:MET:HG2	2.45	0.57
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.57
13:S:16:LEU:HD11	13:S:51:LEU:CD1	2.29	0.57
21:q:65:THR:HG22	21:q:66:THR:N	2.20	0.57
21:q:68:MET:SD	21:q:81:MET:HB3	2.44	0.57
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.57
5:E:222:PHE:H	5:E:225:GLU:CD	2.13	0.57
9:I:89:GLU:HG3	21:q:61:TRP:HB3	1.87	0.57
17:X:52:ASP:OD2	17:X:55:ARG:HG3	2.03	0.57
21:q:129:THR:O	21:q:129:THR:HG22	2.03	0.57
1:A:60:ILE:O	1:A:61:THR:C	2.46	0.57
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.05	0.57
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.57
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.57
10:P:320:GLU:O	10:P:324:ILE:HG12	2.05	0.57
16:W:42:TRP:CZ2	33:W:201:EHZ:O1	2.58	0.57
2:B:100:CYS:HG	25:B:301:SF4:FE4	1.22	0.56
4:D:148:GLU:OE2	4:D:225:ALA:HA	2.04	0.56
4:D:266:ARG:NH1	9:I:60:ILE:HA	2.20	0.56
4:D:348:LEU:O	18:Z:11:PRO:HB3	2.05	0.56
8:H:69:SER:C	8:H:71:PHE:H	2.12	0.56
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.88	0.56
10:P:188:GLU:O	10:P:192:ARG:HG2	2.05	0.56
17:X:5:VAL:HG13	17:X:7:LEU:HG	1.87	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
4:D:137:ASP:OD1	4:D:148:GLU:HG3	2.04	0.56
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.56
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.37	0.56
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.58	0.56
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.87	0.56
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.05	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.70	0.56
12:R:59:PHE:O	12:R:63:LEU:HG	2.06	0.56
12:R:62:ASP:O	12:R:66:GLN:HG3	2.06	0.56
18:Z:7:LYS:HB2	18:Z:7:LYS:NZ	2.20	0.56
18:Z:92:GLU:O	18:Z:96:ILE:HG13	2.05	0.56
1:A:105:GLU:HG2	1:A:111:LEU:HG	1.87	0.56
1:A:113:TRP:HH2	8:H:287:HIS:CD2	2.23	0.56
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.30	0.56
8:H:51:ASP:OD2	30:H:400:UQ9:H12	2.06	0.56
8:H:312:ALA:HB2	20:b:38:TYR:HB3	1.87	0.56
14:T:134:ASP:OD1	14:T:134:ASP:O	2.23	0.56
17:X:130:LYS:HE3	20:b:67:PRO:HB3	1.86	0.56
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.87	0.56
2:B:93:MET:HE1	2:B:95:PHE:CE2	2.40	0.56
2:B:194:CYS:HB2	9:I:153:ILE:O	2.05	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.56
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.87	0.56
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.36	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.40	0.56
8:H:19:PHE:HB3	19:a:12:MET:HG3	1.87	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.40	0.56
14:T:90:TYR:HE2	14:T:92:LYS:CB	2.19	0.56
17:X:137:LEU:HD23	17:X:138:PRO:O	2.05	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.21	0.56
11:Q:167:ASN:O	11:Q:168:LYS:HG2	2.05	0.56
14:T:83:VAL:CG2	14:T:126:PHE:CZ	2.83	0.56
14:T:130:ILE:HD11	14:T:148:ILE:HD11	1.86	0.56
34:a:101:CDL:H141	34:a:101:CDL:H321	1.86	0.56
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.40	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.56
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.56
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
4:D:338:ARG:NH1	18:Z:23:ARG:HA	2.21	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.56
7:G:401:LEU:HD11	7:G:462:PHE:HE2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.56
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.56
8:H:202:GLU:O	8:H:203:GLY:C	2.49	0.56
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.56
1:A:22:PHE:O	1:A:25:PRO:HD2	2.05	0.56
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.87	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56
11:Q:165:SER:HB3	11:Q:168:LYS:O	2.06	0.56
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.56
2:B:69:SER:O	2:B:70:ARG:C	2.48	0.56
2:B:97:LEU:HD21	2:B:141:MET:HG2	1.88	0.56
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.87	0.56
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.56
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.46	0.56
10:P:64:PHE:HE1	10:P:209:ARG:O	1.88	0.56
10:P:140:ASP:OD1	10:P:142:GLU:HB2	2.05	0.56
11:Q:110:PRO:HB3	12:R:43:TYR:OH	2.06	0.56
2:B:95:PHE:CE2	2:B:131:MET:SD	2.99	0.55
2:B:154:GLU:O	10:P:89:TYR:OH	2.21	0.55
4:D:266:ARG:HD3	24:I:301:3PE:O14	2.05	0.55
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.55
5:E:139:CYS:CB	5:E:144:SER:HB3	2.35	0.55
7:G:382:ARG:HD2	13:S:56:ARG:CD	2.36	0.55
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.55
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.88	0.55
18:Z:69:ILE:CG2	20:b:54:PRO:HD3	2.37	0.55
4:D:238:LEU:HA	18:Z:9:ASP:HB2	1.86	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55
1:A:102:LEU:CD1	1:A:111:LEU:HD11	2.37	0.55
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.72	0.55
4:D:266:ARG:NH2	9:I:59:ARG:O	2.39	0.55
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.07	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
8:H:175:LEU:HD21	27:I:302:PC1:H2C1	1.88	0.55
10:P:122:HIS:HB2	12:R:46:VAL:HG12	1.88	0.55
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.42	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.55
14:T:103:HIS:HD1	14:T:140:CYS:HG	1.49	0.55
17:X:124:GLN:C	17:X:125:LEU:HD12	2.32	0.55
2:B:174:SER:HA	3:C:203:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:279:THR:HA	15:V:12:VAL:HG13	1.87	0.55
7:G:35:PHE:O	7:G:101:ASN:HA	2.07	0.55
10:P:145:PHE:O	10:P:149:PRO:HG2	2.05	0.55
17:X:39:THR:HG23	17:X:40:ASN:N	2.20	0.55
4:D:84:PHE:HB2	4:D:97:LEU:HB2	1.87	0.55
4:D:89:PRO:HG2	8:H:204:GLU:HG3	1.88	0.55
5:E:233:LEU:HD11	6:F:289:GLU:OE2	2.07	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.55
8:H:249:ILE:HD13	17:X:99:HIS:CG	2.42	0.55
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.06	0.55
21:q:6:VAL:HG23	21:q:7:LEU:N	2.21	0.55
22:r:9:GLN:O	22:r:12:ARG:HB2	2.06	0.55
6:F:382:CYS:SG	25:F:502:SF4:S4	3.05	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
9:I:75:SER:O	22:r:12:ARG:HG2	2.07	0.55
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.49	0.55
16:W:23:ILE:HG13	16:W:80:ARG:HG2	1.87	0.55
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
6:F:170:GLN:HB3	23:s:48:LEU:HD22	1.89	0.55
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.71	0.55
10:P:376:ASN:OD1	10:P:376:ASN:C	2.50	0.55
16:W:25:SER:HB3	16:W:30:GLU:HB3	1.88	0.55
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.87	0.55
17:X:132:LYS:HB3	20:b:59:ASP:HB3	1.87	0.55
20:b:8:PHE:CG	20:b:9:LEU:N	2.74	0.55
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.88	0.55
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.55
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.46	0.55
6:F:48:ARG:HA	6:F:48:ARG:HH11	1.72	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
16:W:35:VAL:HG21	33:W:201:EHZ:N2	2.22	0.55
16:W:53:MET:HB2	16:W:55:LEU:HG	1.89	0.55
22:r:7:VAL:O	22:r:11:LEU:HG	2.06	0.55
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.32	0.55
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.55
8:H:69:SER:C	8:H:71:PHE:N	2.61	0.55
8:H:130:PHE:CD2	8:H:207:LEU:HD11	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:98:GLY:HA3	10:P:103:LEU:HG	1.87	0.55
10:P:236:VAL:HG13	10:P:270:ARG:HH21	1.71	0.55
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.55
18:Z:56:GLU:HA	18:Z:59:ARG:HH11	1.72	0.55
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.55
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.89	0.54
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.07	0.54
6:F:67:GLU:O	6:F:71:LYS:HG2	2.06	0.54
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.54
8:H:11:VAL:O	8:H:12:PRO:C	2.50	0.54
10:P:71:ASN:HA	10:P:97:MET:SD	2.47	0.54
14:T:87:LEU:HD22	14:T:104:PHE:CZ	2.41	0.54
14:T:128:PHE:CE2	14:T:130:ILE:HG13	2.42	0.54
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.54
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.54
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.37	0.54
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.37	0.54
6:F:119:GLU:HG3	6:F:127:ASP:OD2	2.07	0.54
6:F:300:ILE:HD11	6:F:311:TRP:HD1	1.72	0.54
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.54
9:I:123:CYS:SG	25:I:303:SF4:S3	3.06	0.54
19:a:31:ASN:HD21	19:a:36:LYS:HB2	1.71	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
7:G:617:ARG:HH12	16:W:128:GLY:C	2.16	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.54
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.54
19:a:58:ASN:HB2	19:a:61:TYR:CD2	2.43	0.54
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.23	0.54
6:F:299:LEU:CD1	6:F:300:ILE:HG23	2.37	0.54
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
7:G:445:LEU:HD23	7:G:460:HIS:HE1	1.55	0.54
8:H:133:LEU:O	8:H:136:VAL:HG12	2.08	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
10:P:300:TRP:O	10:P:304:LEU:HG	2.08	0.54
15:V:50:GLN:HE22	22:r:94:ALA:H	1.56	0.54
21:q:17:HIS:NE2	21:q:33:ILE:HG23	2.23	0.54
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:232:VAL:HG23	4:D:356:ILE:HD13	1.88	0.54
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.43	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
17:X:64:ASN:O	17:X:68:LEU:HG	2.07	0.54
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.54
2:B:126:ARG:HG3	8:H:213:VAL:O	2.08	0.54
4:D:145:MET:O	4:D:148:GLU:N	2.39	0.54
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.90	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:445:LEU:HD21	7:G:460:HIS:CE1	2.34	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.90	0.54
10:P:316:LYS:O	10:P:320:GLU:HG2	2.08	0.54
11:Q:160:TYR:CZ	11:Q:164:PHE:HZ	2.26	0.54
3:C:217:ARG:HH12	16:W:112:GLU:CB	2.19	0.54
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
5:E:162:THR:HG22	5:E:166:LYS:HA	1.89	0.54
5:E:199:ASP:O	5:E:203:ILE:HG13	2.08	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.54
8:H:43:TYR:CE2	21:q:27:PHE:HZ	2.26	0.54
10:P:207:PHE:CE1	10:P:214:LEU:HD22	2.43	0.54
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.33	0.54
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.14	0.54
5:E:180:VAL:CG1	5:E:224:CYS:SG	2.96	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.54
7:G:179:CYS:HG	25:G:802:SF4:FE3	1.23	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
10:P:172:ALA:H	10:P:202:ARG:NH2	2.06	0.54
14:T:97:LYS:HG3	14:T:97:LYS:O	2.08	0.54
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.90	0.54
17:X:133:THR:O	20:b:58:ARG:NH1	2.40	0.54
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.23	0.54
34:a:101:CDL:H511	22:r:8:ILE:HD11	1.88	0.54
20:b:8:PHE:O	20:b:9:LEU:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.54
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.89	0.54
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.91	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
9:I:80:GLU:CB	22:r:26:LEU:HD11	2.38	0.54
9:I:109:GLY:O	12:R:63:LEU:HD12	2.08	0.54
10:P:142:GLU:HA	10:P:146:VAL:HG12	1.90	0.54
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.54
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.54
1:A:110:GLY:O	1:A:111:LEU:HB2	2.08	0.54
4:D:259:GLU:HB3	18:Z:25:LEU:HD11	1.89	0.54
5:E:165:ASP:C	5:E:167:LEU:N	2.64	0.54
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.54
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.54
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.54
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.07	0.54
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.54
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
3:C:80:LEU:HG	4:D:396:THR:CG2	2.37	0.53
3:C:100:ARG:HH12	15:V:86:LYS:NZ	2.06	0.53
5:E:39:VAL:HG21	7:G:163:LYS:HZ2	1.73	0.53
5:E:139:CYS:C	5:E:144:SER:HB3	2.33	0.53
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.53
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.51	0.53
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.37	0.53
10:P:58:VAL:O	10:P:83:PRO:HD2	2.09	0.53
19:a:2:TRP:HH2	34:a:101:CDL:H522	1.73	0.53
4:D:253:LEU:HD11	22:r:18:GLN:HG3	1.90	0.53
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.53
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.53
14:T:118:ILE:HG23	14:T:122:MET:CE	2.37	0.53
16:W:88:LYS:O	16:W:92:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:VAL:HG11	7:G:163:LYS:HZ3	1.73	0.53
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.53
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.90	0.53
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.73	0.53
4:D:368:ARG:HA	4:D:371:MET:HG2	1.89	0.53
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.53
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.53
7:G:617:ARG:NH1	16:W:128:GLY:C	2.66	0.53
10:P:85:ARG:HE	31:P:401:NDP:C2A	2.21	0.53
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.53
13:S:30:SER:O	13:S:31:GLN:C	2.49	0.53
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.53
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.53
19:a:7:PRO:HD3	34:a:101:CDL:H181	1.90	0.53
20:b:59:ASP:HA	20:b:63:MET:HE2	1.89	0.53
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.53
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.89	0.53
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.53
6:F:80:MET:HE2	6:F:95:THR:HG21	1.89	0.53
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
9:I:67:ILE:HG13	27:I:302:PC1:H251	1.89	0.53
10:P:370:LYS:HG3	10:P:370:LYS:O	2.08	0.53
12:R:98:GLU:HA	12:R:113:GLN:CD	2.33	0.53
13:S:16:LEU:HD13	13:S:19:ILE:CD1	2.38	0.53
1:A:112:GLU:C	1:A:113:TRP:CG	2.86	0.53
2:B:122:ARG:HH21	4:D:89:PRO:HB3	1.74	0.53
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.53
5:E:77:ALA:C	5:E:80:PRO:HD2	2.33	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53
6:F:85:LEU:HD13	6:F:262:PHE:CE2	2.44	0.53
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.38	0.53
9:I:80:GLU:OE2	22:r:26:LEU:HD13	2.08	0.53
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.44	0.53
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.53
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.53
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.53
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.53
14:T:87:LEU:HD23	14:T:122:MET:HE1	1.91	0.53
21:q:73:THR:HA	21:q:76:ASP:OD1	2.09	0.53
2:B:126:ARG:NH1	8:H:61:MET:SD	2.76	0.53
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.22	0.53
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.90	0.53
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.53
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.91	0.53
8:H:292:ASN:O	20:b:18:VAL:HG11	2.09	0.53
10:P:353:LEU:HA	10:P:356:HIS:HD2	1.74	0.53
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.53
17:X:133:THR:HG23	20:b:58:ARG:NH1	2.23	0.53
18:Z:65:LEU:HB3	20:b:50:PRO:O	2.09	0.53
1:A:21:ALA:HB2	8:H:218:GLY:HA3	1.90	0.53
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.64	0.53
4:D:338:ARG:HH12	18:Z:23:ARG:HA	1.74	0.53
7:G:364:ASP:C	7:G:364:ASP:OD1	2.52	0.53
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.53
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.53
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.53
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.53
21:q:9:ARG:HA	21:q:12:GLN:CG	2.37	0.53
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.53
7:G:126:LEU:HD13	12:R:89:PRO:HB3	1.90	0.53
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.53
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.91	0.53
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.91	0.53
10:P:265:PHE:HD1	10:P:334:GLY:HA3	1.74	0.53
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.53
12:R:69:VAL:HG12	12:R:112:LYS:N	2.24	0.53
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.53
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.91	0.53
3:C:135:ARG:O	3:C:136:PHE:C	2.47	0.52
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.52
8:H:249:ILE:HG21	17:X:99:HIS:CE1	2.45	0.52
9:I:80:GLU:HB3	22:r:26:LEU:HD11	1.90	0.52
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.52
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.52
21:q:55:PHE:CG	22:r:26:LEU:HD22	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:O	1:A:12:LEU:HG	2.09	0.52
2:B:136:THR:HG21	4:D:118:ARG:HG2	1.90	0.52
3:C:80:LEU:O	3:C:81:ASP:CB	2.52	0.52
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.27	0.52
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.69	0.52
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.73	0.52
5:E:39:VAL:HG21	7:G:163:LYS:NZ	2.25	0.52
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.75	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
10:P:305:PHE:CG	10:P:314:THR:HG22	2.45	0.52
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.52
19:a:42:GLN:O	19:a:43:TYR:C	2.50	0.52
2:B:92:PRO:HD3	2:B:119:VAL:HG13	1.91	0.52
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.52
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.45	0.52
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.75	0.52
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.23	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52
9:I:54:THR:HG22	20:b:13:TRP:HE1	1.74	0.52
10:P:283:MET:HE2	10:P:366:ILE:HG22	1.92	0.52
16:W:93:LEU:HG	16:W:97:ILE:HD12	1.92	0.52
20:b:66:VAL:HG11	20:b:70:PRO:HA	1.92	0.52
21:q:29:ARG:HD3	21:q:74:PHE:CE1	2.44	0.52
3:C:104:ASN:O	22:r:97:PRO:HD3	2.10	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.52
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.52
14:T:130:ILE:CG2	14:T:131:PRO:HD2	2.40	0.52
17:X:80:GLU:HB3	17:X:81:PRO:HD3	1.91	0.52
1:A:3:LEU:HA	8:H:96:ILE:CD1	2.40	0.52
4:D:381:HIS:HE1	9:I:161:ALA:O	1.93	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.52
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.52
10:P:336:GLU:CG	10:P:342:PRO:HD3	2.38	0.52
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.42	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52
21:q:125:VAL:HG23	21:q:125:VAL:O	2.08	0.52
1:A:113:TRP:CH2	8:H:287:HIS:CD2	2.98	0.52
5:E:177:GLY:O	28:E:301:FES:S1	2.68	0.52
6:F:238:CYS:O	6:F:239:PRO:C	2.51	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.10	0.52
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.74	0.52
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.52
8:H:23:VAL:HG11	19:a:9:LEU:CD2	2.39	0.52
21:q:56:PHE:HD1	21:q:59:HIS:NE2	2.06	0.52
1:A:113:TRP:CH2	8:H:287:HIS:HD2	2.27	0.52
4:D:101:LEU:HG	4:D:106:VAL:HA	1.91	0.52
6:F:126:LYS:HG3	6:F:275:LEU:CB	2.39	0.52
10:P:236:VAL:HG11	10:P:270:ARG:HH21	1.75	0.52
17:X:77:HIS:HD2	17:X:115:LEU:HD21	1.75	0.52
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.52
21:q:138:VAL:HG23	21:q:139:PRO:HD2	1.92	0.52
2:B:127:GLN:H	2:B:127:GLN:CD	2.18	0.52
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.52
7:G:617:ARG:HH12	16:W:129:HIS:N	2.07	0.52
14:T:79:ILE:CG2	14:T:145:VAL:HG13	2.40	0.52
19:a:1:MET:HG3	34:a:101:CDL:HB21	1.92	0.52
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.52
1:A:102:LEU:HD11	1:A:111:LEU:HD11	1.91	0.52
3:C:73:GLN:NE2	15:V:112:TRP:HE1	2.07	0.52
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	2.98	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.52
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.52
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.52
20:b:48:ALA:O	20:b:49:THR:C	2.53	0.52
1:A:19:LEU:O	1:A:20:VAL:C	2.50	0.52
2:B:81:LEU:HD22	27:B:303:PC1:H262	1.92	0.52
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.43	0.52
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.91	0.52
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.45	0.52
6:F:296:LEU:HD22	6:F:337:MET:CE	2.39	0.52
7:G:126:LEU:HD11	12:R:89:PRO:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
9:I:155:CYS:SG	25:I:303:SF4:S2	3.08	0.52
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.52
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.75	0.52
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.51
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.51
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.51
7:G:399:VAL:HG21	7:G:462:PHE:CZ	2.44	0.51
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.51
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.99	0.51
10:P:192:ARG:NH1	10:P:198:ALA:HB3	2.25	0.51
18:Z:61:LEU:O	18:Z:64:ASP:OD1	2.29	0.51
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	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
21:q:29:ARG:HD3	21:q:74:PHE:CD1	2.44	0.51
21:q:65:THR:CG2	21:q:66:THR:N	2.72	0.51
1:A:105:GLU:HG3	1:A:111:LEU:HG	1.91	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.11	0.51
6:F:259:GLY:O	6:F:263:ALA:N	2.40	0.51
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.92	0.51
7:G:275:PRO:HB2	11:Q:86:ASN:ND2	2.25	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:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
13:S:16:LEU:O	13:S:16:LEU:CD1	2.51	0.51
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.92	0.51
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.91	0.51
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.92	0.51
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.25	0.51
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.51
8:H:142:TYR:CA	8:H:289:LEU:CD1	2.74	0.51
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.51
4:D:259:GLU:C	4:D:261:MET:H	2.18	0.51
5:E:188:ASN:O	5:E:189:ASP:HB3	2.10	0.51
6:F:40:ARG:HB3	6:F:289:GLU:CD	2.35	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
10:P:157:LYS:O	10:P:158:GLU:C	2.53	0.51
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.93	0.51
1:A:106:TRP:CD1	1:A:111:LEU:HD12	2.45	0.51
4:D:299:GLN:HB3	22:r:104:TRP:CE3	2.45	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
6:F:296:LEU:CD1	6:F:337:MET:HE3	2.34	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	2.09	0.51
17:X:25:LEU:O	17:X:29:ALA:N	2.44	0.51
34:a:101:CDL:HA62	21:q:10:GLY:HA3	1.93	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.75	0.51
8:H:222:LEU:O	8:H:223:PHE:C	2.51	0.51
9:I:71:GLY:O	22:r:15:ALA:HB1	2.11	0.51
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.51
14:T:140:CYS:HB2	14:T:143:GLU:CG	2.40	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.92	0.51
2:B:81:LEU:CG	8:H:53:MET:HE1	2.34	0.51
3:C:241:PHE:H	7:G:146:PHE:HE1	1.58	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	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:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.51
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.51
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.51
16:W:65:LYS:HE3	16:W:69:MET:HE2	1.92	0.51
34:a:101:CDL:H311	21:q:7:LEU:HD23	1.91	0.51
6:F:109:ARG:NE	6:F:239:PRO:HD3	2.25	0.51
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.24	0.51
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.40	0.51
6:F:217:GLU:CD	11:Q:166:TRP:HE1	2.18	0.51
10:P:374:THR:HG23	10:P:374:THR:O	2.11	0.51
20:b:11:ASN:OD1	20:b:12:ALA:N	2.44	0.51
1:A:11:ILE:CD1	24:A:401:3PE:H2D1	2.41	0.51
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.46	0.51
4:D:304:LYS:HE2	9:I:35:THR:N	2.25	0.51
6:F:225:LEU:HB3	6:F:227:PRO:CD	2.37	0.51
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
10:P:305:PHE:HB2	10:P:314:THR:HG22	1.92	0.51
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.51
14:T:87:LEU:HD23	14:T:122:MET:CE	2.41	0.51
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.50
2:B:125:PRO:HB3	2:B:148:VAL:HG13	1.93	0.50
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.08	0.50
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:639:LEU:HD23	7:G:639:LEU:C	2.36	0.50
8:H:307:LEU:HD11	18:Z:47:TYR:CD1	2.46	0.50
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.50
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.91	0.50
17:X:137:LEU:HG	17:X:138:PRO:HD2	1.92	0.50
4:D:345:GLU:HB2	18:Z:19:ILE:HD12	1.93	0.50
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	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:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.46	0.50
10:P:65:LEU:HD23	10:P:129:LEU:HD22	1.93	0.50
10:P:108:TRP:CZ2	31:P:401:NDP:H2A	2.46	0.50
10:P:209:ARG:N	10:P:352:VAL:HG22	2.26	0.50
10:P:234:LYS:HG2	10:P:234:LYS:O	2.10	0.50
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.11	0.50
14:T:105:MET:HB2	14:T:139:MET:SD	2.51	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
17:X:130:LYS:CE	20:b:67:PRO:HB3	2.42	0.50
3:C:190:TYR:HB3	16:W:101:LYS:HG2	1.94	0.50
7:G:651:PRO:HD2	13:S:56:ARG:HD2	1.94	0.50
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.50
4:D:359:ASP:O	7:G:150:ARG:NH2	2.44	0.50
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.50
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.50
10:P:212:ARG:O	10:P:213:PHE:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.50
11:Q:167:ASN:C	11:Q:168:LYS:HG2	2.36	0.50
12:R:55:VAL:HG22	12:R:56:ASN:H	1.77	0.50
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.46	0.50
14:T:130:ILE:HG23	14:T:131:PRO:CD	2.40	0.50
15:V:44:TYR:O	15:V:48:THR:HG22	2.11	0.50
2:B:99:CYS:C	2:B:101:ALA:H	2.19	0.50
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
17:X:38:LYS:O	17:X:42:GLU:HG3	2.11	0.50
4:D:97:LEU:HD23	4:D:111:PRO:HA	1.94	0.50
6:F:49:HIS:O	6:F:50:ASP:C	2.54	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
8:H:230:ASN:O	8:H:231:ILE:C	2.53	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
10:P:205:ASP:OD1	10:P:205:ASP:O	2.30	0.50
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.94	0.50
2:B:171:TYR:HE1	4:D:120:THR:HG22	1.76	0.50
4:D:89:PRO:HG2	8:H:204:GLU:CG	2.42	0.50
5:E:70:PRO:HB3	23:s:60:PRO:HG3	1.92	0.50
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.50
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.50
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.94	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
9:I:63:TRP:CZ2	24:I:301:3PE:H321	2.46	0.50
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.50
2:B:84:TRP:HA	2:B:87:ARG:HG2	1.93	0.50
2:B:99:CYS:O	2:B:101:ALA:N	2.44	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.50
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.50
10:P:150:ARG:O	10:P:151:ALA:C	2.55	0.50
10:P:207:PHE:HE1	10:P:214:LEU:HD22	1.76	0.50
14:T:140:CYS:O	14:T:144:ILE:HG13	2.12	0.50
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.50
3:C:79:CYS:C	3:C:81:ASP:H	2.18	0.50
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.50
4:D:145:MET:O	4:D:146:CYS:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:70:VAL:HG12	10:P:97:MET:SD	2.52	0.50
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.50
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.50
18:Z:129:THR:HG22	18:Z:131:GLU:H	1.77	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.49
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.49
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.49
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.49
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.49
7:G:272:ARG:HH11	7:G:274:LEU:HD23	1.77	0.49
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.49
8:H:17:MET:CE	8:H:225:MET:HB3	2.41	0.49
10:P:192:ARG:CZ	10:P:200:ILE:HD11	2.42	0.49
14:T:138:LEU:HD13	14:T:144:ILE:CD1	2.42	0.49
18:Z:66:GLU:HA	18:Z:69:ILE:HG12	1.93	0.49
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.42	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.95	0.49
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.49
5:E:245:GLN:HB3	6:F:256:ARG:O	2.11	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.48	0.49
6:F:185:ASN:HA	6:F:189:SER:O	2.11	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
6:F:427:LEU:HB2	29:F:501:FMN:C7M	2.43	0.49
8:H:30:TYR:HE1	19:a:1:MET:O	1.87	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.95	0.49
8:H:155:LEU:O	8:H:315:PRO:HG3	2.12	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
10:P:135:GLU:CG	10:P:140:ASP:HA	2.41	0.49
13:S:24:CYS:N	13:S:58:CYS:SG	2.85	0.49
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.49
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.49
18:Z:140:PHE:O	18:Z:141:THR:C	2.55	0.49
19:a:4:GLU:O	19:a:7:PRO:HD2	2.11	0.49
34:a:101:CDL:OB3	22:r:5:THR:N	2.34	0.49
6:F:296:LEU:HD23	6:F:332:CYS:HB3	1.95	0.49
13:S:42:VAL:O	13:S:46:LYS:HG3	2.12	0.49
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.49
17:X:33:GLY:CA	18:Z:70:ALA:HB1	2.43	0.49
17:X:49:GLU:HB3	17:X:138:PRO:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:289:SER:N	4:D:293:LEU:HG	2.27	0.49
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.49
4:D:460:GLU:O	4:D:463:ARG:HG2	2.12	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.12	0.49
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
10:P:172:ALA:H	10:P:202:ARG:HH21	1.59	0.49
10:P:238:GLN:HB2	10:P:270:ARG:HG2	1.94	0.49
10:P:367:GLU:HG2	10:P:368:GLU:N	2.26	0.49
12:R:67:GLN:HG2	12:R:109:LEU:HD21	1.95	0.49
24:A:401:3PE:O14	24:A:401:3PE:N	2.38	0.49
2:B:171:TYR:CE1	4:D:120:THR:HG22	2.46	0.49
3:C:73:GLN:HE21	15:V:112:TRP:HE1	1.60	0.49
3:C:224:GLU:OE2	10:P:45:LYS:HB3	2.13	0.49
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.31	0.49
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.49
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.93	0.49
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.41	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.27	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
8:H:12:PRO:O	19:a:15:CYS:HB3	2.13	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.49
16:W:32:LYS:CD	33:W:201:EHZ:C19	2.90	0.49
17:X:73:GLN:OE1	17:X:117:TRP:HZ2	1.96	0.49
1:A:54:LYS:O	1:A:58:VAL:HG23	2.12	0.49
4:D:259:GLU:C	4:D:261:MET:N	2.68	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:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.49
14:T:88:LYS:NZ	14:T:96:GLU:H	2.11	0.49
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.49
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.26	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
8:H:93:HIS:CE1	19:a:24:ALA:CA	2.94	0.49
10:P:64:PHE:CZ	10:P:211:ASP:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:235:THR:O	10:P:236:VAL:C	2.56	0.49
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.49
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.13	0.49
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.49
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.49
5:E:134:CYS:SG	5:E:139:CYS:SG	3.06	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
10:P:315:THR:H	10:P:318:LYS:HB3	1.76	0.49
15:V:56:LEU:HA	15:V:59:VAL:HB	1.94	0.49
17:X:4:ILE:CG2	17:X:5:VAL:N	2.50	0.49
17:X:115:LEU:HD13	17:X:117:TRP:CZ3	2.48	0.49
1:A:18:ILE:O	1:A:21:ALA:HB3	2.13	0.49
4:D:279:THR:HA	15:V:12:VAL:CG1	2.43	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.49
6:F:379:CYS:SG	25:F:502:SF4:S1	3.11	0.49
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.42	0.49
8:H:303:TRP:CZ3	20:b:28:LEU:HG	2.48	0.49
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.49
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.49
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.49
9:I:49:ASP:O	9:I:50:MET:C	2.55	0.49
9:I:114:ILE:HD13	12:R:106:TYR:CD1	2.48	0.49
13:S:36:PHE:CZ	13:S:44:LEU:HD11	2.36	0.49
18:Z:69:ILE:HG23	20:b:54:PRO:CD	2.41	0.49
2:B:127:GLN:NE2	8:H:215:TYR:O	2.46	0.48
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.48
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.48
12:R:32:THR:CG2	12:R:36:GLN:H	2.18	0.48
17:X:112:LEU:HD13	17:X:118:VAL:HG22	1.95	0.48
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.48
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.95	0.48
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.48
8:H:66:THR:HA	8:H:124:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:I:302:PC1:H133	18:Z:30:LEU:O	2.13	0.48
10:P:59:PHE:CB	10:P:130:ILE:HD11	2.42	0.48
10:P:228:LEU:HD11	10:P:288:PHE:HZ	1.78	0.48
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.48
14:T:90:TYR:HE2	14:T:92:LYS:HB3	1.78	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
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.48
5:E:143:ASP:O	5:E:144:SER:C	2.55	0.48
6:F:126:LYS:HG3	6:F:275:LEU:HB3	1.94	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.47	0.48
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.48
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.48
1:A:109:LYS:HD2	1:A:112:GLU:OE2	2.14	0.48
3:C:234:LEU:O	4:D:387:GLU:HG3	2.13	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.48
6:F:226:LYS:O	6:F:227:PRO:C	2.56	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.48
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.48
19:a:37:ARG:CB	19:a:48:MET:HE2	2.43	0.48
1:A:113:TRP:CH2	8:H:287:HIS:HB2	2.49	0.48
8:H:42:PRO:HG3	21:q:28:PHE:HE1	1.79	0.48
8:H:224:PHE:CZ	30:H:400:UQ9:C13	2.94	0.48
10:P:197:GLU:HB3	10:P:259:VAL:HG23	1.93	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.95	0.48
20:b:23:PHE:CD2	24:b:201:3PE:H281	2.40	0.48
1:A:72:LEU:HB3	8:H:151:LEU:HD21	1.96	0.48
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.49	0.48
3:C:79:CYS:O	3:C:80:LEU:C	2.55	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48
7:G:33:GLU:OE2	7:G:40:SER:HA	2.14	0.48
7:G:34:VAL:HG11	7:G:96:VAL:HG22	1.94	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
9:I:55:ASP:OD1	18:Z:32:GLY:N	2.43	0.48
10:P:79:GLN:NE2	10:P:102:GLN:O	2.47	0.48
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.43	0.48
15:V:35:LEU:HD13	15:V:48:THR:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:85:GLN:O	18:Z:89:GLU:HG3	2.14	0.48
1:A:11:ILE:HD11	24:A:401:3PE:H2D1	1.95	0.48
2:B:174:SER:HB2	4:D:123:LEU:HD21	1.96	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
10:P:191:VAL:CG1	10:P:192:ARG:HH21	2.26	0.48
14:T:104:PHE:CZ	14:T:118:ILE:HG21	2.48	0.48
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.95	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.49	0.48
5:E:45:GLU:H	5:E:45:GLU:CD	2.21	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
6:F:296:LEU:HD13	6:F:337:MET:CE	2.34	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
8:H:20:LEU:HA	19:a:12:MET:SD	2.53	0.48
8:H:272:TRP:HH2	27:I:302:PC1:H381	1.79	0.48
9:I:49:ASP:O	9:I:53:ALA:N	2.41	0.48
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.14	0.48
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.48
14:T:119:ILE:HG13	14:T:135:ALA:HB1	1.95	0.48
16:W:103:ARG:O	16:W:104:THR:C	2.56	0.48
17:X:17:GLU:HB3	17:X:19:LYS:HG3	1.96	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48
3:C:100:ARG:HH12	15:V:86:LYS:HZ1	1.62	0.48
3:C:151:PRO:HG2	16:W:23:ILE:HG23	1.96	0.48
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.49	0.48
4:D:202:TRP:CH2	9:I:72:MET:HG2	2.48	0.48
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
9:I:171:PRO:HB3	21:q:93:MET:CE	2.38	0.48
10:P:294:PRO:HB3	10:P:296:PHE:HD1	1.79	0.48
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.48
20:b:68:SER:O	20:b:69:HIS:C	2.56	0.48
1:A:102:LEU:HG	1:A:106:TRP:HE1	1.79	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.79	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
9:I:54:THR:HG21	18:Z:33:TYR:CE2	2.49	0.48
12:R:79:CYS:O	12:R:88:HIS:CE1	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:50:ASN:O	13:S:51:LEU:C	2.57	0.48
20:b:69:HIS:HD2	20:b:70:PRO:CD	2.26	0.48
2:B:115:ASP:O	2:B:116:ARG:C	2.55	0.47
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.47
6:F:297:LYS:HB2	6:F:333:GLU:HB3	1.95	0.47
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.47
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	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
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.47
2:B:117:PHE:HA	8:H:39:ILE:HG21	1.95	0.47
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.47
5:E:142:ARG:O	5:E:143:ASP:HB2	2.13	0.47
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.47
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.47
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.48	0.47
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.73	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
10:P:335:LEU:O	10:P:336:GLU:HB2	2.15	0.47
10:P:360:ARG:HD3	10:P:360:ARG:O	2.15	0.47
17:X:53:PRO:HD2	18:Z:116:TRP:HD1	1.75	0.47
17:X:80:GLU:O	17:X:81:PRO:C	2.56	0.47
17:X:123:GLY:HA2	18:Z:66:GLU:OE2	2.14	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.47
22:r:113:LEU:HD12	22:r:113:LEU:HA	1.77	0.47
2:B:224:ARG:HG3	10:P:85:ARG:HH22	1.79	0.47
3:C:209:LEU:HD21	16:W:108:ARG:NH1	2.29	0.47
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.49	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.47
10:P:304:LEU:O	10:P:307:LEU:HB3	2.14	0.47
16:W:120:ASP:OD1	16:W:121:PHE:N	2.46	0.47
25:B:301:SF4:S4	4:D:138:ARG:HD3	2.54	0.47
4:D:142:VAL:HG13	4:D:207:ARG:HH12	1.78	0.47
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.47
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.14	0.47
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.15	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	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.47
3:C:70:LYS:HB2	15:V:99:PRO:O	2.14	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:82:ILE:HG21	7:G:100:TRP:HB3	1.96	0.47
10:P:311:GLU:O	10:P:312:PRO:C	2.57	0.47
16:W:46:VAL:O	16:W:50:VAL:HG23	2.14	0.47
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.50	0.47
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
5:E:145:ASP:O	5:E:146:SER:C	2.56	0.47
6:F:217:GLU:CD	6:F:224:ARG:HH22	2.23	0.47
6:F:425:CYS:SG	25:F:502:SF4:S4	3.13	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
13:S:58:CYS:HB2	13:S:61:VAL:CG1	2.43	0.47
17:X:122:LEU:HD21	20:b:81:LEU:HD23	1.95	0.47
17:X:139:GLU:O	17:X:140:ASN:C	2.57	0.47
21:q:55:PHE:CD1	22:r:26:LEU:CD2	2.95	0.47
1:A:108:GLN:C	1:A:110:GLY:N	2.72	0.47
2:B:99:CYS:O	2:B:102:VAL:N	2.45	0.47
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.45	0.47
4:D:279:THR:HG23	15:V:13:GLY:CA	2.23	0.47
4:D:280:ALA:CB	15:V:11:LEU:CG	2.90	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47
6:F: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	2.48	0.47
6:F:299:LEU:HD11	6:F:300:ILE:HG23	1.95	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:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:93:HIS:HE1	19:a:24:ALA:HA	1.74	0.47
8:H:224:PHE:CZ	30:H:400:UQ9:H11	2.49	0.47
8:H:310:PHE:HB3	20:b:33:PRO:HA	1.96	0.47
9:I:188:GLU:OE1	12:R:56:ASN:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:55:VAL:HG12	10:P:123:SER:HA	1.96	0.47
10:P:76:MET:HE1	10:P:254:LYS:CE	2.45	0.47
10:P:170:LEU:HG	10:P:171:ASN:N	2.28	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
15:V:116:ILE:O	15:V:116:ILE:CG2	2.61	0.47
16:W:32:LYS:O	16:W:36:ARG:HG3	2.15	0.47
17:X:39:THR:CG2	17:X:40:ASN:N	2.77	0.47
18:Z:144:THR:HA	19:a:45:TRP:HZ3	1.79	0.47
19:a:22:SER:O	19:a:23:THR:C	2.57	0.47
20:b:69:HIS:CD2	20:b:71:GLN:H	2.33	0.47
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.50	0.47
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.47	0.47
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.29	0.47
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.47
6:F:281:HIS:HB3	6:F:358:ASP:CG	2.40	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.97	0.47
18:Z:87:LEU:HD21	18:Z:119:PRO:HG3	1.97	0.47
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.96	0.47
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.47
4:D:299:GLN:OE1	22:r:104:TRP:HB2	2.14	0.47
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.97	0.47
5:E:221:ARG:HB2	5:E:225:GLU:HG2	1.97	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
9:I:63:TRP:HZ2	24:I:301:3PE:H321	1.80	0.47
10:P:287:THR:HG23	10:P:289:ILE:HD11	1.97	0.47
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.48	0.47
15:V:56:LEU:HD12	15:V:57:ASP:CA	2.44	0.47
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.39	0.47
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.47
23:s:55:PHE:O	23:s:56:ARG:C	2.57	0.47
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.47
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.50	0.47
6:F:44:ASN:ND2	6:F:133:HIS:O	2.48	0.47
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
7:G:496:MET:O	7:G:500:ILE:HG13	2.14	0.47
8:H:180:PRO:CD	18:Z:43:LEU:HD21	2.43	0.47
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.03	0.47
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:7:LEU:CD1	18:Z:87:LEU:HB3	2.45	0.47
21:q:14:VAL:HA	21:q:23:LEU:HD13	1.97	0.47
2:B:140:LYS:O	2:B:143:PRO:HD2	2.14	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.97	0.46
9:I:79:ARG:HG2	22:r:12:ARG:NH2	2.29	0.46
10:P:207:PHE:CD2	10:P:241:TYR:HD1	2.33	0.46
12:R:33:HIS:HE1	12:R:56:ASN:HD22	1.63	0.46
16:W:42:TRP:CZ2	16:W:93:LEU:CA	2.95	0.46
17:X:20:VAL:CG2	17:X:24:VAL:HG21	2.40	0.46
21:q:8:LYS:HG2	21:q:12:GLN:HE21	1.79	0.46
22:r:109:ASP:O	22:r:110:GLN:OE1	2.32	0.46
4:D:264:ASN:O	9:I:65:GLU:OE1	2.32	0.46
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.97	0.46
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.46
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
8:H:1:MET:HE3	19:a:29:PHE:CE1	2.50	0.46
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.96	0.46
10:P:209:ARG:O	10:P:210:GLU:HB2	2.15	0.46
13:S:19:ILE:HD12	13:S:94:VAL:CG1	2.44	0.46
17:X:115:LEU:HD13	17:X:117:TRP:CZ2	2.51	0.46
19:a:49:GLU:CD	19:a:52:ARG:HH11	2.22	0.46
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.97	0.46
2:B:116:ARG:HA	8:H:37:PRO:HA	1.97	0.46
4:D:142:VAL:HG21	4:D:185:MET:HG2	1.98	0.46
6:F:39:ASP:CA	6:F:261:TRP:HZ2	2.28	0.46
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.46
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.96	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
15:V:22:GLU:O	15:V:26:ILE:HG12	2.16	0.46
17:X:35:GLN:HG3	17:X:70:PHE:HE1	1.80	0.46
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.44	0.46
1:A:87:MET:HE3	1:A:87:MET:HB3	1.84	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.39	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
10:P:276:LEU:O	10:P:280:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:50:VAL:HA	16:W:55:LEU:HD12	1.97	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.59	0.46
2:B:93:MET:HB2	2:B:128:ALA:HB2	1.97	0.46
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.46
3:C:141:ARG:NH1	4:D:410:TYR:CE1	2.80	0.46
6:F:51:TRP:HZ2	23:s:36:GLN:HG3	1.80	0.46
9:I:64:THR:HG21	18:Z:35:MET:HE1	1.97	0.46
12:R:38:TYR:CD1	12:R:44:ARG:HB2	2.51	0.46
14:T:87:LEU:CD2	14:T:104:PHE:HZ	2.12	0.46
14:T:114:ASP:OD1	16:W:67:ARG:NH1	2.48	0.46
18:Z:72:MET:N	18:Z:73:PRO:CD	2.78	0.46
23:s:52:LEU:HB3	23:s:56:ARG:HH11	1.81	0.46
2:B:94:THR:HB	2:B:104:MET:CE	2.45	0.46
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.46
5:E:143:ASP:O	5:E:146:SER:N	2.49	0.46
6:F:109:ARG:NH2	6:F:232:ASP:O	2.45	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
9:I:53:ALA:O	9:I:54:THR:C	2.56	0.46
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.97	0.46
10:P:235:THR:HG22	10:P:323:HIS:O	2.15	0.46
14:T:117:GLU:HG2	16:W:43:TYR:CZ	2.51	0.46
15:V:72:LEU:C	15:V:72:LEU:CD1	2.89	0.46
16:W:32:LYS:CE	33:W:201:EHZ:C19	2.90	0.46
21:q:48:TYR:OH	21:q:83:PRO:HD2	2.15	0.46
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.46
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.51	0.46
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.46
10:P:131:GLY:HA3	31:P:401:NDP:O3D	2.15	0.46
12:R:32:THR:HA	12:R:55:VAL:CG2	2.45	0.46
17:X:33:GLY:HA3	18:Z:70:ALA:HB1	1.98	0.46
2:B:96:GLY:HA3	26:B:302:UQ1:O1	2.15	0.46
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.81	0.46
4:D:198:THR:HA	8:H:32:GLN:HG2	1.98	0.46
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.46
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:82:ILE:HG23	7:G:100:TRP:HB3	1.96	0.46
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.46
8:H:186:PHE:HB2	24:I:301:3PE:H2G1	1.98	0.46
10:P:157:LYS:O	10:P:160:GLY:N	2.49	0.46
10:P:245:VAL:HA	10:P:265:PHE:CD2	2.49	0.46
12:R:39:ASP:CG	12:R:40:GLU:N	2.74	0.46
14:T:87:LEU:CD2	14:T:122:MET:HE1	2.46	0.46
15:V:56:LEU:HD13	15:V:60:LYS:HE2	1.98	0.46
17:X:5:VAL:CG1	17:X:7:LEU:HG	2.46	0.46
18:Z:86:ILE:CG2	18:Z:128:ARG:HE	2.16	0.46
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.28	0.46
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.24	0.46
6:F:35:LEU:HG	6:F:39:ASP:HB2	1.97	0.46
6:F:51:TRP:CB	6:F:133:HIS:O	2.64	0.46
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.46
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.46
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.46
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.46
8:H:140:ILE:HG13	8:H:141:SER:N	2.30	0.46
9:I:80:GLU:N	19:a:1:MET:HE1	2.31	0.46
17:X:54:ARG:HD3	18:Z:116:TRP:CE3	2.51	0.46
18:Z:62:ILE:CG1	20:b:49:THR:HG22	2.44	0.46
19:a:58:ASN:HB2	19:a:61:TYR:CE2	2.50	0.46
20:b:45:ILE:N	20:b:80:TRP:HH2	2.14	0.46
21:q:71:LYS:HB2	21:q:73:THR:HG23	1.97	0.46
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.46
4:D:368:ARG:NH2	9:I:165:ASP:HB2	2.31	0.46
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.46
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.46
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.46
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.46
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.46
9:I:123:CYS:SG	25:I:303:SF4:S4	3.13	0.46
24:I:301:3PE:H362	24:I:301:3PE:H331	1.75	0.46
10:P:261:LYS:HB2	10:P:263:PHE:CE1	2.51	0.46
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.46
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.45
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.45
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.45
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.30	0.45
9:I:90:LYS:HG2	21:q:90:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:28:LEU:O	20:b:32:MET:HG2	2.15	0.45
20:b:38:TYR:O	20:b:39:THR:C	2.59	0.45
2:B:136:THR:HG21	2:B:177:VAL:CG2	2.44	0.45
7:G:176:CYS:SG	25:G:802:SF4:S1	3.14	0.45
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.45
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.45
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.45
9:I:60:ILE:HG23	24:I:301:3PE:O14	2.16	0.45
10:P:66:GLY:O	10:P:69:VAL:N	2.48	0.45
10:P:285:HIS:CE1	10:P:364:SER:HB3	2.51	0.45
14:T:119:ILE:CD1	14:T:138:LEU:HD11	2.43	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
2:B:99:CYS:O	2:B:100:CYS:C	2.57	0.45
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.32	0.45
4:D:92:HIS:O	4:D:458:PHE:CE2	2.70	0.45
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.45
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.99	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.45
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.31	0.45
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.45
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.45
10:P:315:THR:HB	10:P:318:LYS:HB2	1.98	0.45
15:V:56:LEU:HD11	15:V:57:ASP:OD1	2.17	0.45
16:W:83:ASP:O	16:W:87:ILE:HG12	2.17	0.45
3:C:85:ILE:CD1	3:C:140:ILE:HD11	2.47	0.45
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.98	0.45
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.45
5:E:184:MET:HG3	5:E:192:TYR:O	2.16	0.45
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
10:P:218:ALA:HB2	10:P:280:ILE:CG2	2.47	0.45
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.45
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.45
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.45
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.44	0.45
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.45
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:355:LYS:NZ	7:G:528:LEU:O	2.47	0.45
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.45
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.45
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.80	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
9:I:92:PRO:HB3	21:q:92:CYS:HB2	1.98	0.45
9:I:188:GLU:OE1	12:R:56:ASN:HB2	2.16	0.45
10:P:170:LEU:HD12	10:P:171:ASN:H	1.81	0.45
10:P:220:TYR:HA	10:P:223:PHE:CD2	2.50	0.45
14:T:87:LEU:CD2	14:T:104:PHE:CE1	2.94	0.45
14:T:117:GLU:HA	14:T:120:MET:CE	2.41	0.45
18:Z:69:ILE:CG2	20:b:54:PRO:CD	2.94	0.45
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.45
24:A:401:3PE:H352	24:A:401:3PE:H262	1.98	0.45
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.16	0.45
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.51	0.45
2:B:126:ARG:C	2:B:128:ALA:H	2.24	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.45
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
7:G:97:MET:HB2	7:G:100:TRP:NE1	2.30	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:382:ARG:HD2	13:S:56:ARG:HD3	1.99	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
10:P:259:VAL:H	10:P:261:LYS:HG2	1.82	0.45
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.32	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
3:C:243:ALA:C	7:G:105:ASN:ND2	2.75	0.45
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.74	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.52	0.45
7:G:163:LYS:HE2	12:R:97:LYS:NZ	2.31	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:CD1	2.47	0.45
7:G:401:LEU:HD11	7:G:462:PHE:CE2	2.51	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.45
13:S:42:VAL:HB	13:S:46:LYS:HE3	1.98	0.45
14:T:83:VAL:HG21	14:T:145:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:53:PRO:HG2	18:Z:116:TRP:NE1	2.32	0.45
21:q:21:ARG:O	21:q:25:ARG:HG3	2.17	0.45
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.32	0.45
4:D:91:ALA:O	4:D:92:HIS:C	2.58	0.45
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.45
9:I:93:LEU:O	21:q:93:MET:CG	2.65	0.45
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.45
14:T:90:TYR:O	14:T:91:ASP:HB2	2.17	0.45
14:T:130:ILE:CG2	14:T:131:PRO:CD	2.95	0.45
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.45
16:W:71:MET:C	16:W:73:ASN:N	2.70	0.45
17:X:7:LEU:HD13	18:Z:87:LEU:HB3	1.98	0.45
18:Z:66:GLU:HA	18:Z:69:ILE:CG1	2.46	0.45
2:B:99:CYS:HB3	4:D:141:TYR:CD2	2.52	0.45
4:D:84:PHE:CE2	4:D:91:ALA:HB2	2.51	0.45
5:E:163:THR:HG23	5:E:168:PHE:O	2.17	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	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
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.45
10:P:209:ARG:CA	10:P:352:VAL:HG22	2.47	0.45
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.45
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.98	0.45
14:T:133:ILE:HG23	14:T:134:ASP:N	2.32	0.45
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.45
3:C:73:GLN:NE2	15:V:107:PRO:HB3	2.31	0.45
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.98	0.45
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.45
5:E:81:VAL:O	5:E:82:LEU:C	2.60	0.45
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
8:H:25:ARG:NH1	30:H:400:UQ9:H10A	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:192:ARG:HH12	10:P:198:ALA:HB3	1.80	0.45
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.45
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.45
1:A:109:LYS:HA	1:A:112:GLU:CD	2.42	0.44
2:B:124:SER:HB3	2:B:125:PRO:HD2	2.00	0.44
3:C:98:PHE:HB2	15:V:94:MET:CE	2.47	0.44
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.44
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.44
5:E:52:PHE:O	5:E:99:LYS:HG3	2.17	0.44
5:E:90:GLY:HA3	5:E:126:VAL:HG12	1.99	0.44
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.52	0.44
5:E:221:ARG:NH2	5:E:227:ALA:HB2	2.31	0.44
6:F:382:CYS:HA	7:G:74:ASN:O	2.17	0.44
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.44
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.98	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
8:H:16:ALA:HB2	19:a:15:CYS:HB2	1.99	0.44
8:H:295:PRO:HB3	24:b:201:3PE:H382	1.98	0.44
9:I:50:MET:O	9:I:51:LYS:C	2.60	0.44
10:P:55:VAL:HA	10:P:79:GLN:O	2.18	0.44
10:P:245:VAL:HA	10:P:265:PHE:HD2	1.82	0.44
12:R:39:ASP:H	12:R:42:ASP:CG	2.21	0.44
13:S:20:ARG:HG3	13:S:54:LEU:CB	2.43	0.44
14:T:82:ARG:NH2	14:T:126:PHE:HD1	2.15	0.44
16:W:45:GLU:O	16:W:46:VAL:C	2.58	0.44
16:W:71:MET:O	16:W:72:LYS:C	2.59	0.44
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.52	0.44
18:Z:68:ARG:O	18:Z:69:ILE:C	2.60	0.44
18:Z:98:MET:HB2	18:Z:104:TRP:CE2	2.52	0.44
2:B:80:ASP:O	2:B:81:LEU:C	2.59	0.44
3:C:55:LYS:HE2	3:C:55:LYS:HB3	1.84	0.44
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.83	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
6:F:299:LEU:CD1	6:F:300:ILE:N	2.67	0.44
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.44
9:I:42:LYS:HD3	9:I:42:LYS:HA	1.84	0.44
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.44
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.44
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:46:CYS:SG	17:X:135:ARG:NH1	2.90	0.44
23:s:52:LEU:O	23:s:56:ARG:HG2	2.17	0.44
2:B:71:ALA:O	2:B:75:VAL:N	2.47	0.44
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.81	0.44
4:D:78:THR:O	4:D:79:ASN:C	2.59	0.44
4:D:100:GLU:C	4:D:101:LEU:HD12	2.41	0.44
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.44
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.97	0.44
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.44
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.44
6:F:427:LEU:HB2	29:F:501:FMN:HM73	2.00	0.44
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.44
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44
14:T:79:ILE:O	14:T:83:VAL:HG23	2.17	0.44
14:T:133:ILE:O	14:T:136:GLU:N	2.46	0.44
22:r:109:ASP:O	22:r:110:GLN:CG	2.64	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44
6:F:119:GLU:HB3	6:F:124:THR:HG22	2.00	0.44
6:F:126:LYS:O	6:F:129:GLU:HG2	2.18	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.44
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.48	0.44
10:P:156:SER:HB2	10:P:161:VAL:CG2	2.47	0.44
10:P:305:PHE:CB	10:P:314:THR:HG22	2.47	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
12:R:32:THR:HG21	21:q:129:THR:HG23	1.98	0.44
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.44
2:B:90:LEU:O	2:B:119:VAL:HA	2.17	0.44
2:B:105:MET:CE	26:B:302:UQ1:C6	2.96	0.44
3:C:107:PHE:CE1	3:C:133:SER:HB3	2.53	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.18	0.44
4:D:258:VAL:O	4:D:261:MET:HB2	2.17	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.57	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:4:ILE:HD12	8:H:4:ILE:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:78:PHE:HB2	22:r:12:ARG:CG	2.48	0.44
9:I:90:LYS:HG3	21:q:90:LEU:CD2	2.48	0.44
24:I:301:3PE:C27	24:I:301:3PE:H231	2.47	0.44
10:P:122:HIS:HB3	12:R:46:VAL:HG12	1.98	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44
16:W:86:VAL:O	16:W:90:LYS:HG3	2.18	0.44
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.44
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.44
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
7:G:607:LYS:HG2	11:Q:78:ARG:HH11	1.82	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.47	0.44
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.44
16:W:95:GLU:HB3	16:W:101:LYS:HG3	2.00	0.44
1:A:18:ILE:HG12	8:H:222:LEU:CD2	2.48	0.44
2:B:93:MET:CE	2:B:95:PHE:CE2	3.00	0.44
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.99	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.44
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.44
10:P:168:SER:O	10:P:202:ARG:HA	2.17	0.44
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
12:R:47:ARG:HG3	12:R:48:PHE:N	2.32	0.44
17:X:40:ASN:O	17:X:41:LYS:C	2.58	0.44
19:a:37:ARG:HB2	19:a:48:MET:HE2	1.99	0.44
21:q:3:LEU:O	21:q:6:VAL:CG2	2.66	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.44
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.44
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.80	0.44
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.44
10:P:130:ILE:N	10:P:130:ILE:HD12	2.33	0.44
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:23:LEU:HB3	13:S:33:VAL:HG12	2.00	0.44
16:W:20:VAL:HG21	16:W:80:ARG:CZ	2.48	0.44
18:Z:129:THR:HG22	18:Z:131:GLU:N	2.33	0.44
2:B:146:ARG:NH2	3:C:211:TYR:CZ	2.85	0.44
3:C:70:LYS:O	15:V:103:LEU:HA	2.18	0.44
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.44
4:D:271:ARG:CD	8:H:279:ARG:O	2.62	0.44
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.46	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
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.44
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.44
8:H:63:PRO:HD2	8:H:66:THR:HG21	2.00	0.44
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.52	0.44
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.77	0.44
9:I:66:LEU:CD1	24:I:301:3PE:H271	2.48	0.44
14:T:113:LEU:O	14:T:116:VAL:HB	2.17	0.44
16:W:87:ILE:O	16:W:91:MET:HG3	2.18	0.44
24:A:401:3PE:H322	24:A:401:3PE:H32	1.85	0.43
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.43
4:D:338:ARG:NH1	18:Z:23:ARG:CA	2.80	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:362:ASP:HB2	13:S:71:PHE:CD1	2.52	0.43
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.96	0.43
9:I:78:PHE:HB2	22:r:12:ARG:HG2	2.00	0.43
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.43
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.43
22:r:110:GLN:HA	22:r:111:PRO:HD2	1.85	0.43
2:B:96:GLY:CA	2:B:101:ALA:HB2	2.40	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.43
5:E:183:PRO:HB2	5:E:195:LEU:N	2.33	0.43
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.43
6:F:126:LYS:HE2	6:F:274:LYS:HZ3	1.83	0.43
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.43
7:G:466:LEU:O	7:G:467:LYS:C	2.61	0.43
8:H:200:LEU:HD21	8:H:282:TYR:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.43
10:P:197:GLU:HB3	10:P:259:VAL:HG22	1.99	0.43
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.43
2:B:70:ARG:HG3	2:B:70:ARG:O	2.18	0.43
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
5:E:192:TYR:OH	5:E:213:PRO:HD2	2.19	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:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.43
8:H:200:LEU:CD2	8:H:282:TYR:HD1	2.31	0.43
8:H:200:LEU:C	8:H:200:LEU:HD12	2.43	0.43
13:S:30:SER:O	13:S:33:VAL:N	2.51	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.43
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.53	0.43
20:b:23:PHE:CZ	24:b:201:3PE:H351	2.46	0.43
1:A:112:GLU:O	1:A:113:TRP:C	2.58	0.43
2:B:104:MET:HE3	26:B:302:UQ1:C11	2.40	0.43
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
5:E:124:LYS:HB3	5:E:125:PRO:HD2	2.00	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.60	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
9:I:197:TRP:CZ3	21:q:84:PRO:HA	2.53	0.43
10:P:76:MET:HE1	10:P:254:LYS:HE2	2.01	0.43
10:P:310:PHE:O	10:P:311:GLU:C	2.60	0.43
14:T:92:LYS:O	14:T:92:LYS:HG2	2.16	0.43
15:V:56:LEU:CD1	15:V:57:ASP:OD1	2.67	0.43
20:b:82:LYS:HB3	20:b:82:LYS:HE2	1.81	0.43
1:A:63:LEU:O	1:A:64:LEU:C	2.61	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
3:C:221:GLU:OE1	16:W:114:GLU:HB2	2.18	0.43
4:D:99:LEU:HB3	4:D:101:LEU:HD11	2.00	0.43
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.43
7:G:82:ILE:HG22	7:G:100:TRP:HE3	1.83	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:292:ASN:HD21	24:I:301:3PE:H121	1.84	0.43
10:P:64:PHE:CE1	10:P:209:ARG:O	2.69	0.43
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.43
13:S:24:CYS:SG	13:S:61:VAL:HG12	2.58	0.43
16:W:71:MET:O	16:W:74:ALA:N	2.39	0.43
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.19	0.43
4:D:232:VAL:CG2	4:D:356:ILE:HB	2.48	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
5:E:63:GLU:O	5:E:64:ALA:C	2.61	0.43
5:E:162:THR:HG21	5:E:166:LYS:HA	2.01	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43
6:F:166:ALA:HB1	23:s:45:PHE:HD2	1.84	0.43
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.18	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
8:H:43:TYR:CE2	21:q:27:PHE:CZ	3.06	0.43
8:H:138:GLN:HG3	8:H:139:THR:N	2.34	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.43
8:H:306:SER:OG	20:b:33:PRO:HG3	2.19	0.43
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.82	0.43
10:P:170:LEU:O	10:P:171:ASN:CG	2.61	0.43
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.43
20:b:15:LYS:O	20:b:15:LYS:HG3	2.18	0.43
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.43
1:A:23:TRP:O	1:A:26:GLN:HG3	2.19	0.43
2:B:105:MET:HE2	26:B:302:UQ1:C8	2.48	0.43
5:E:81:VAL:HB	5:E:104:LEU:HD11	2.00	0.43
7:G:279:GLU:HG3	11:Q:154:LYS:HG3	2.00	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
7:G:466:LEU:HD13	7:G:500:ILE:HD13	2.00	0.43
8:H:257:THR:O	8:H:260:MET:HB3	2.19	0.43
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.18	0.43
11:Q:104:ARG:HA	11:Q:104:ARG:HD3	1.88	0.43
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	2.00	0.43
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.43
14:T:109:GLY:O	14:T:110:LEU:C	2.61	0.43
15:V:56:LEU:C	15:V:56:LEU:CD1	2.85	0.43
17:X:29:ALA:CB	18:Z:71:LEU:HD11	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:28:ARG:O	18:Z:28:ARG:CG	2.64	0.43
18:Z:86:ILE:HA	18:Z:128:ARG:NH2	2.33	0.43
21:q:4:VAL:HG23	21:q:5:GLU:N	2.33	0.43
21:q:79:GLY:O	21:q:82:VAL:HG22	2.19	0.43
1:A:73:LEU:O	1:A:76:PRO:HD2	2.18	0.43
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.43
5:E:140:MET:HE1	6:F:366:ALA:HA	2.01	0.43
6:F:38:GLU:HG3	6:F:39:ASP:N	2.34	0.43
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.43
8:H:123:SER:HB3	8:H:214:GLU:HG3	2.00	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.43
16:W:120:ASP:HB3	16:W:123:SER:OG	2.18	0.43
21:q:22:GLY:O	21:q:26:VAL:HG23	2.18	0.43
2:B:117:PHE:HA	8:H:39:ILE:CG2	2.49	0.43
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.43
5:E:62:ILE:HD12	5:E:81:VAL:HG13	2.00	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.43
6:F:409:ILE:HG12	6:F:446:LEU:HD23	1.96	0.43
6:F:410:ASP:OD1	6:F:410:ASP:C	2.62	0.43
6:F:419:ILE:HG23	6:F:432:ALA:HB2	2.01	0.43
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.43
7:G:617:ARG:NH1	16:W:129:HIS:N	2.67	0.43
8:H:17:MET:HE1	8:H:225:MET:HE3	2.00	0.43
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.43
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.43
14:T:87:LEU:HD11	14:T:141:PRO:HB3	2.01	0.43
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.43
19:a:12:MET:HE2	19:a:12:MET:HB3	1.90	0.43
21:q:14:VAL:HG13	21:q:23:LEU:CD2	2.43	0.43
2:B:82:ILE:CG1	8:H:57:MET:CE	2.82	0.43
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.43
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.43
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.34	0.43
7:G:117:MET:SD	7:G:143:SER:HB2	2.59	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
8:H:179:TRP:CD1	18:Z:43:LEU:HD21	2.54	0.43
9:I:152:CYS:SG	25:I:303:SF4:S3	3.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:237:LYS:HE3	10:P:322:ILE:O	2.19	0.43
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.00	0.43
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.83	0.43
10:P:306:GLY:HA2	10:P:312:PRO:HB3	2.01	0.43
16:W:38:LEU:HG	16:W:70:PHE:HZ	1.84	0.43
16:W:99:VAL:O	16:W:99:VAL:HG12	2.19	0.43
16:W:102:GLN:O	16:W:103:ARG:C	2.60	0.43
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.43
19:a:55:SER:O	19:a:56:GLY:C	2.61	0.43
1:A:73:LEU:O	8:H:160:TYR:OH	2.25	0.42
4:D:83:ASN:C	4:D:85:GLY:N	2.74	0.42
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.42
4:D:198:THR:HG23	8:H:275:ALA:O	2.18	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
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.42
8:H:33:LEU:HD21	22:r:25:GLN:HG2	2.01	0.42
9:I:162:CYS:SG	25:I:304:SF4:S2	3.17	0.42
10:P:259:VAL:N	10:P:261:LYS:HG2	2.33	0.42
14:T:93:ILE:HD11	14:T:118:ILE:HD11	2.00	0.42
17:X:10:LEU:H	17:X:10:LEU:HD12	1.84	0.42
22:r:12:ARG:HB3	22:r:20:LEU:CD2	2.49	0.42
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
2:B:111:ARG:CZ	4:D:208:GLU:HG2	2.49	0.42
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.42
5:E:137:THR:HG22	6:F:370:LEU:HD21	2.02	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
6:F:126:LYS:HG3	6:F:275:LEU:HB2	2.01	0.42
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.42
6:F:416:SER:O	6:F:419:ILE:CG2	2.65	0.42
7:G:496:MET:HG2	7:G:500:ILE:HD11	2.01	0.42
8:H:93:HIS:CD2	19:a:27:HIS:ND1	2.87	0.42
9:I:35:THR:HG22	22:r:107:SER:HA	1.97	0.42
10:P:169:HIS:CD2	10:P:181:LEU:HD11	2.52	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.54	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.62	0.42
1:A:73:LEU:N	1:A:74:PRO:HD2	2.35	0.42
3:C:101:ASP:OD1	15:V:86:LYS:HE3	2.19	0.42
3:C:124:ARG:HD2	11:Q:140:LYS:HZ1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:133:SER:OG	3:C:133:SER:O	2.32	0.42
4:D:162:GLN:HB2	4:D:163:PRO:HD2	2.01	0.42
6:F:291:GLU:OE2	6:F:292:MET:N	2.53	0.42
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.42
7:G:664:TYR:OH	13:S:23:LEU:HD11	2.20	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.53	0.42
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
10:P:376:ASN:O	10:P:377:TYR:C	2.61	0.42
12:R:45:ARG:HA	12:R:48:PHE:HE1	1.83	0.42
12:R:48:PHE:CD2	21:q:125:VAL:HG21	2.54	0.42
13:S:16:LEU:HD13	13:S:19:ILE:HD11	2.02	0.42
13:S:30:SER:HB3	13:S:63:PRO:HG3	2.00	0.42
17:X:75:LYS:O	17:X:79:ALA:HB2	2.19	0.42
18:Z:74:LEU:O	18:Z:78:GLU:HG3	2.20	0.42
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42
5:E:94:ILE:HD13	7:G:209:TYR:CE2	2.53	0.42
5:E:179:CYS:C	5:E:181:ASN:N	2.78	0.42
6:F:47:GLY:N	6:F:133:HIS:ND1	2.68	0.42
6:F:50:ASP:O	6:F:55:GLY:HA3	2.19	0.42
6:F:296:LEU:HD22	6:F:337:MET:HE1	2.01	0.42
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.42
7:G:36:VAL:O	7:G:39:GLN:HG2	2.19	0.42
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
30:H:400:UQ9:H15B	30:H:400:UQ9:H17	1.80	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
18:Z:108:GLU:O	18:Z:109:SER:C	2.61	0.42
1:A:25:PRO:HG3	8:H:60:PRO:CD	2.42	0.42
2:B:91:TRP:CE3	30:H:400:UQ9:H1M	2.54	0.42
3:C:64:VAL:HG11	3:C:85:ILE:HD13	2.02	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
9:I:78:PHE:HD1	19:a:2:TRP:CD1	2.37	0.42
10:P:207:PHE:O	10:P:241:TYR:HA	2.19	0.42
10:P:220:TYR:CG	10:P:226:VAL:HG13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:300:TRP:NE1	10:P:304:LEU:HD21	2.35	0.42
16:W:120:ASP:OD1	16:W:120:ASP:C	2.61	0.42
17:X:26:LYS:HD3	17:X:95:GLN:OE1	2.19	0.42
19:a:17:VAL:O	19:a:18:ILE:C	2.62	0.42
1:A:52:SER:O	1:A:53:MET:C	2.61	0.42
2:B:94:THR:OG1	2:B:104:MET:HE1	2.20	0.42
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
7:G:404:GLY:HA2	7:G:684:LEU:HD11	2.00	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.42
8:H:196:ALA:C	8:H:198:PHE:N	2.77	0.42
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.42
9:I:68:ARG:HH22	18:Z:26:PRO:HD2	1.83	0.42
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.42
10:P:354:ARG:HG3	10:P:362:LEU:CD2	2.48	0.42
12:R:44:ARG:C	12:R:46:VAL:N	2.73	0.42
23:s:35:LEU:HA	23:s:37:HIS:CE1	2.55	0.42
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.49	0.42
2:B:126:ARG:O	2:B:128:ALA:N	2.50	0.42
4:D:259:GLU:O	4:D:261:MET:N	2.53	0.42
6:F:47:GLY:C	6:F:49:HIS:H	2.27	0.42
6:F:261:TRP:CE2	6:F:265:PHE:CZ	3.08	0.42
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.20	0.42
8:H:8:THR:O	8:H:9:LEU:CB	2.68	0.42
8:H:68:MET:HG3	8:H:68:MET:O	2.19	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
8:H:179:TRP:HE1	18:Z:43:LEU:HG	1.85	0.42
10:P:242:VAL:HG13	10:P:243:ALA:N	2.35	0.42
11:Q:55:VAL:HG21	16:W:78:ASP:OD1	2.19	0.42
13:S:19:ILE:O	13:S:53:ILE:HD12	2.20	0.42
17:X:41:LYS:O	17:X:42:GLU:C	2.59	0.42
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.42
23:s:53:SER:HA	23:s:56:ARG:HG2	2.02	0.42
24:A:401:3PE:H362	8:H:104:PHE:CE2	2.55	0.42
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.83	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.20	0.42
3:C:133:SER:OG	3:C:138:SER:N	2.53	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:227:PRO:HB3	7:G:95:PRO:HD3	2.01	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.42
17:X:132:LYS:HB3	17:X:132:LYS:HE2	1.84	0.42
18:Z:120:LEU:HD12	18:Z:121:ILE:H	1.85	0.42
20:b:11:ASN:O	20:b:15:LYS:HG2	2.20	0.42
21:q:5:GLU:HG3	21:q:9:ARG:HE	1.84	0.42
1:A:93:ILE:HD13	1:A:93:ILE:HA	1.90	0.42
2:B:94:THR:CB	2:B:104:MET:CE	2.97	0.42
4:D:144:MET:HG2	4:D:223:HIS:H	1.85	0.42
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.42
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.42
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.42
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.42
12:R:31:ILE:HG22	12:R:55:VAL:HG21	2.02	0.42
14:T:80:LYS:O	14:T:84:LEU:HG	2.20	0.42
17:X:52:ASP:O	17:X:53:PRO:C	2.61	0.42
20:b:15:LYS:O	20:b:16:GLU:HB2	2.20	0.42
20:b:59:ASP:HA	20:b:63:MET:CE	2.50	0.42
22:r:18:GLN:OE1	22:r:18:GLN:N	2.53	0.42
3:C:48:PRO:HD3	4:D:162:GLN:OE1	2.20	0.42
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.42
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.42
4:D:339:GLN:HE21	9:I:37:LYS:HZ2	1.67	0.42
5:E:62:ILE:HG21	5:E:103:VAL:HG11	2.01	0.42
5:E:136:THR:HB	28:E:301:FES:S2	2.60	0.42
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.42
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.42
8:H:172:MET:HE3	8:H:176:LEU:CB	2.47	0.42
16:W:28:LEU:O	16:W:32:LYS:HG3	2.20	0.42
16:W:53:MET:SD	16:W:106:VAL:HG21	2.60	0.42
18:Z:102:PRO:O	18:Z:103:ASN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:25:ARG:O	21:q:26:VAL:C	2.62	0.42
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.55	0.42
22:r:10:LYS:O	22:r:11:LEU:C	2.62	0.42
1:A:24:LEU:HD13	1:A:24:LEU:O	2.20	0.41
1:A:81:THR:O	20:b:46:ASN:ND2	2.53	0.41
3:C:243:ALA:C	7:G:105:ASN:HD21	2.28	0.41
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.41
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.41
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	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
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.41
8:H:311:THR:O	18:Z:51:MET:CG	2.66	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41
10:P:331:ASP:CG	10:P:332:LEU:H	2.28	0.41
14:T:90:TYR:CD2	14:T:92:LYS:HB3	2.54	0.41
16:W:76:VAL:HG13	16:W:82:VAL:HG22	2.02	0.41
16:W:78:ASP:HA	16:W:79:PRO:HD3	1.94	0.41
34:a:101:CDL:HA22	21:q:6:VAL:HG12	2.01	0.41
1:A:112:GLU:O	1:A:113:TRP:CD1	2.73	0.41
2:B:146:ARG:NH2	3:C:211:TYR:CE2	2.89	0.41
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.46	0.41
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.41
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.41
27:B:303:PC1:H372	8:H:53:MET:SD	2.60	0.41
3:C:72:VAL:HG23	3:C:72:VAL:O	2.20	0.41
3:C:82:GLU:OE1	3:C:141:ARG:NH2	2.53	0.41
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.41
4:D:266:ARG:CA	9:I:65:GLU:OE2	2.68	0.41
5:E:134:CYS:SG	5:E:175:CYS:HA	2.60	0.41
7:G:32:ILE:CG2	7:G:98:LYS:HA	2.50	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.02	0.41
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.89	0.41
8:H:19:PHE:CB	19:a:12:MET:HG3	2.49	0.41
9:I:152:CYS:SG	25:I:303:SF4:S1	3.17	0.41
10:P:228:LEU:HD11	10:P:288:PHE:CZ	2.54	0.41
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.21	0.41
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.41
14:T:115:GLN:O	14:T:116:VAL:C	2.63	0.41
17:X:70:PHE:CE1	17:X:117:TRP:CZ3	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:64:TYR:CD1	21:q:77:VAL:HG11	2.54	0.41
2:B:91:TRP:CZ2	30:H:400:UQ9:C1M	3.03	0.41
3:C:170:TRP:HE1	16:W:91:MET:HE1	1.86	0.41
4:D:140:ASP:O	4:D:147:ASN:ND2	2.53	0.41
4:D:198:THR:N	4:D:199:PRO:CD	2.84	0.41
4:D:201:PHE:HB2	8:H:32:GLN:HB3	2.02	0.41
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
7:G:272:ARG:HH11	7:G:274:LEU:CD2	2.33	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.54	0.41
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.56	0.41
8:H:174:LEU:HD23	8:H:174:LEU:HA	1.81	0.41
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.41
14:T:123:GLU:HG2	14:T:130:ILE:HD12	2.02	0.41
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.41
20:b:61:GLY:O	20:b:63:MET:HG3	2.20	0.41
24:A:401:3PE:H2E1	24:A:401:3PE:H2H2	1.83	0.41
2:B:95:PHE:HE2	2:B:131:MET:CE	2.33	0.41
4:D:261:MET:HE3	4:D:261:MET:HB3	1.90	0.41
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.41
4:D:448:VAL:HG11	8:H:205:SER:HB2	2.02	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	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:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.41
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
9:I:50:MET:O	9:I:54:THR:N	2.37	0.41
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.41
9:I:89:GLU:CG	21:q:61:TRP:HB3	2.50	0.41
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.41
10:P:243:ALA:O	10:P:244:ASP:C	2.63	0.41
14:T:87:LEU:CD2	14:T:122:MET:CE	2.98	0.41
14:T:100:VAL:O	14:T:141:PRO:HD2	2.20	0.41
14:T:118:ILE:HD13	14:T:118:ILE:HA	1.83	0.41
19:a:49:GLU:OE2	19:a:49:GLU:HA	2.20	0.41
20:b:25:VAL:O	20:b:26:TRP:C	2.64	0.41
20:b:31:ILE:O	20:b:32:MET:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.36	0.41
3:C:241:PHE:O	3:C:242:PRO:C	2.62	0.41
4:D:339:GLN:NE2	9:I:37:LYS:HZ2	2.17	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.41
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.41
5:E:192:TYR:CD2	5:E:203:ILE:HD13	2.56	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.41
6:F:217:GLU:OE2	6:F:224:ARG:NH2	2.53	0.41
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.51	0.41
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.41
6:F:299:LEU:HD12	6:F:300:ILE:HG23	2.01	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:160:VAL:CG1	7:G:161:GLU:N	2.83	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
8:H:206:GLU:O	8:H:207:LEU:HB2	2.20	0.41
10:P:230:SER:O	10:P:231:LEU:C	2.63	0.41
10:P:316:LYS:C	10:P:316:LYS:HD3	2.46	0.41
11:Q:85:ASN:C	11:Q:87:MET:N	2.76	0.41
12:R:64:ILE:HD12	12:R:64:ILE:HA	1.95	0.41
13:S:20:ARG:HD2	13:S:22:HIS:NE2	2.35	0.41
19:a:49:GLU:O	19:a:50:ARG:C	2.62	0.41
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.84	0.41
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.41
4:D:265:ASN:C	4:D:267:ILE:H	2.29	0.41
4:D:339:GLN:HE21	9:I:37:LYS:NZ	2.18	0.41
4:D:376:GLU:HG2	7:G:121:LEU:CD1	2.51	0.41
5:E:48:PRO:HD3	5:E:94:ILE:CG2	2.51	0.41
6:F:119:GLU:CD	29:F:501:FMN:HN3	2.28	0.41
6:F:300:ILE:CD1	6:F:307:VAL:HG23	2.49	0.41
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
8:H:90:PRO:O	8:H:91:MET:C	2.60	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
10:P:265:PHE:N	10:P:265:PHE:CD1	2.87	0.41
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.35	0.41
16:W:86:VAL:O	16:W:87:ILE:C	2.62	0.41
34:a:101:CDL:HA62	21:q:10:GLY:CA	2.51	0.41
21:q:50:GLU:HA	21:q:59:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:LEU:HD11	2:B:142:ALA:HA	2.03	0.41
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
5:E:138:PRO:CG	6:F:122:PRO:HB3	2.47	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
13:S:16:LEU:CB	13:S:69:TYR:CD1	2.97	0.41
17:X:26:LYS:HE2	17:X:26:LYS:HB3	1.85	0.41
17:X:70:PHE:O	17:X:74:ILE:HG13	2.21	0.41
18:Z:90:ASN:O	18:Z:94:GLU:HB2	2.21	0.41
19:a:48:MET:HE3	19:a:48:MET:HB2	1.77	0.41
1:A:8:PHE:CE1	24:A:401:3PE:H2C1	2.48	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.02	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
4:D:202:TRP:HZ2	9:I:73:THR:HG22	1.86	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
6:F:42:PHE:HE1	6:F:249:ALA:HB1	1.86	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:296:LEU:HD22	6:F:337:MET:HE3	2.02	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.02	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.41
8:H:75:PRO:HB2	8:H:222:LEU:HB2	2.03	0.41
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.41
8:H:172:MET:HE1	18:Z:46:GLY:HA3	2.01	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
12:R:60:ALA:O	12:R:61:ILE:C	2.63	0.41
14:T:87:LEU:HD11	14:T:141:PRO:HG3	2.03	0.41
20:b:16:GLU:N	20:b:17:PRO:HD3	2.35	0.41
21:q:64:TYR:CE2	21:q:81:MET:HB2	2.56	0.41
21:q:85:GLU:HG2	21:q:98:PRO:HB3	2.01	0.41
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.41
2:B:111:ARG:NE	4:D:208:GLU:HG2	2.35	0.41
2:B:145:LEU:O	2:B:146:ARG:C	2.64	0.41
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.41
3:C:47:ARG:HG3	4:D:160:ASN:HA	2.03	0.41
3:C:70:LYS:HD3	3:C:71:TYR:CZ	2.56	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:197:MET:HG3	8:H:32:GLN:NE2	2.36	0.41
4:D:310:VAL:C	4:D:312:ASP:H	2.29	0.41
5:E:142:ARG:HB3	5:E:182:ALA:HB3	2.03	0.41
5:E:145:ASP:OD1	5:E:145:ASP:N	2.54	0.41
5:E:225:GLU:O	5:E:226:PRO:C	2.60	0.41
5:E:238:LYS:HB3	5:E:242:PHE:CG	2.56	0.41
6:F:88:ARG:HA	6:F:88:ARG:HD3	1.85	0.41
6:F:109:ARG:HH21	6:F:239:PRO:CD	2.33	0.41
6:F:280:GLY:O	6:F:356:VAL:HB	2.20	0.41
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.41
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.86	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.41
7:G:163:LYS:HD3	7:G:163:LYS:HA	1.84	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.41
8:H:25:ARG:HD2	30:H:400:UQ9:C10	2.48	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.56	0.41
8:H:224:PHE:CD2	30:H:400:UQ9:H13	2.50	0.41
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.41
8:H:264:LEU:HD23	8:H:264:LEU:HA	1.81	0.41
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
10:P:135:GLU:HG3	10:P:140:ASP:HA	2.03	0.41
10:P:362:LEU:HA	10:P:362:LEU:HD23	1.88	0.41
12:R:55:VAL:HG22	12:R:56:ASN:N	2.35	0.41
15:V:96:LYS:HE2	15:V:96:LYS:HB2	1.95	0.41
15:V:98:LYS:HG2	15:V:100:TRP:CZ2	2.55	0.41
17:X:37:ASP:OD1	17:X:37:ASP:C	2.62	0.41
18:Z:19:ILE:HG22	18:Z:20:ASP:N	2.36	0.41
18:Z:62:ILE:HG13	20:b:49:THR:HG22	2.02	0.41
19:a:2:TRP:CH2	34:a:101:CDL:H522	2.55	0.41
20:b:49:THR:HA	20:b:50:PRO:HD3	1.89	0.41
1:A:102:LEU:O	1:A:106:TRP:HD1	2.04	0.41
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.56	0.41
4:D:79:ASN:HB2	4:D:100:GLU:HB3	2.03	0.41
4:D:240:LEU:O	4:D:241:LEU:C	2.62	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.21	0.41
6:F:70:LEU:O	6:F:71:LYS:C	2.63	0.41
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.55	0.41
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:82:ALA:HA	8:H:85:LEU:HD12	2.02	0.41
8:H:300:LEU:HD23	20:b:25:VAL:HG11	2.02	0.41
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.55	0.41
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.85	0.41
14:T:107:ASP:OD1	14:T:108:LEU:N	2.54	0.41
14:T:120:MET:O	14:T:121:ALA:C	2.63	0.41
2:B:163:SER:HB2	9:I:150:THR:O	2.20	0.40
3:C:101:ASP:O	15:V:90:LEU:HD13	2.21	0.40
3:C:141:ARG:HE	3:C:141:ARG:HB2	1.41	0.40
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.85	0.40
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.57	0.40
6:F:226:LYS:HD3	6:F:226:LYS:HA	1.84	0.40
7:G:32:ILE:HG22	7:G:33:GLU:N	2.36	0.40
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.40
7:G:312:GLY:O	21:q:143:PRO:HA	2.21	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:306:SER:CB	8:H:310:PHE:HE2	2.34	0.40
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.40
10:P:146:VAL:HG13	10:P:147:ASN:OD1	2.21	0.40
10:P:293:LEU:HD12	10:P:294:PRO:HD2	2.01	0.40
11:Q:55:VAL:HG21	16:W:80:ARG:HH11	1.85	0.40
13:S:22:HIS:CD2	13:S:66:TRP:HD1	2.38	0.40
18:Z:10:MET:HE2	18:Z:10:MET:HB3	1.72	0.40
34:a:101:CDL:OB7	21:q:3:LEU:HD13	2.21	0.40
21:q:39:VAL:CG1	21:q:97:PRO:HB3	2.52	0.40
21:q:68:MET:HE1	21:q:81:MET:O	2.21	0.40
1:A:16:THR:O	1:A:20:VAL:HG23	2.22	0.40
2:B:138:THR:HG21	4:D:116:LEU:HA	2.02	0.40
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.54	0.40
5:E:109:MET:HE2	7:G:196:GLY:CA	2.51	0.40
5:E:190:ASN:HD22	5:E:192:TYR:HE1	1.69	0.40
6:F:257:ARG:HG2	6:F:261:TRP:CE3	2.55	0.40
7:G:277:MET:HE1	11:Q:153:PRO:HD3	2.03	0.40
8:H:89:LEU:HD12	8:H:89:LEU:HA	1.87	0.40
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.40
10:P:96:LEU:HD12	10:P:97:MET:CA	2.51	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
10:P:191:VAL:HG13	10:P:192:ARG:CZ	2.51	0.40
14:T:99:SER:HB2	14:T:102:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:23:ALA:HB2	17:X:95:GLN:HE22	1.82	0.40
22:r:24:LEU:HD23	22:r:24:LEU:HA	1.85	0.40
6:F:196:PHE:HD1	23:s:56:ARG:HH21	1.70	0.40
6:F:306:GLY:O	6:F:307:VAL:C	2.64	0.40
6:F:335:VAL:HG12	6:F:336:LEU:N	2.36	0.40
6:F:338:ASP:OD1	6:F:341:ALA:HB2	2.20	0.40
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.40
7:G:217:GLU:C	7:G:219:SER:N	2.79	0.40
7:G:302:LEU:N	7:G:571:HIS:O	2.45	0.40
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.40
8:H:63:PRO:O	8:H:66:THR:HG22	2.21	0.40
14:T:140:CYS:HB2	14:T:143:GLU:HB2	2.02	0.40
18:Z:58:ARG:CZ	20:b:49:THR:HG21	2.51	0.40
19:a:9:LEU:O	19:a:10:ALA:C	2.64	0.40
22:r:20:LEU:C	22:r:20:LEU:CD1	2.89	0.40
1:A:20:VAL:O	1:A:21:ALA:C	2.63	0.40
1:A:102:LEU:HG	1:A:106:TRP:NE1	2.36	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
3:C:224:GLU:OE1	10:P:50:SER:OG	2.40	0.40
4:D:181:LEU:HD21	4:D:210:MET:CB	2.51	0.40
4:D:213:PHE:O	4:D:214:TYR:C	2.64	0.40
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.37	0.40
6:F:102:MET:HE2	6:F:149:MET:HB2	2.03	0.40
7:G:49:VAL:HG13	7:G:102:ILE:HG12	2.03	0.40
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.42	0.40
8:H:87:VAL:HB	8:H:88:PRO:HD3	2.04	0.40
8:H:114:TYR:O	8:H:117:LEU:N	2.55	0.40
8:H:251:LEU:HD11	8:H:254:LEU:HB2	2.03	0.40
9:I:90:LYS:CG	21:q:90:LEU:CD2	3.00	0.40
10:P:315:THR:HB	10:P:318:LYS:H	1.85	0.40
11:Q:57:GLU:O	11:Q:58:LYS:C	2.65	0.40
17:X:53:PRO:HG2	18:Z:116:TRP:HE1	1.87	0.40
21:q:7:LEU:O	21:q:11:VAL:HG23	2.21	0.40
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.40
4:D:128:THR:HG22	4:D:131:GLN:CG	2.52	0.40
4:D:144:MET:HE2	4:D:144:MET:HB2	1.91	0.40
6:F:114:VAL:CG1	6:F:212:LEU:HD23	2.52	0.40
6:F:119:GLU:OE1	6:F:119:GLU:HA	2.21	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.09	0.40
7:G:314:LEU:HD23	7:G:583:ILE:HG13	2.02	0.40
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:204:GLU:O	8:H:208:VAL:HA	2.21	0.40
9:I:50:MET:HB3	18:Z:33:TYR:OH	2.21	0.40
10:P:56:ALA:HA	10:P:125:VAL:O	2.20	0.40
10:P:96:LEU:C	10:P:96:LEU:CD1	2.94	0.40
10:P:302:GLY:HA2	10:P:314:THR:CG2	2.50	0.40
11:Q:166:TRP:O	11:Q:167:ASN:C	2.64	0.40
13:S:23:LEU:HB3	13:S:33:VAL:CG1	2.51	0.40
18:Z:140:PHE:C	18:Z:142:TRP:N	2.77	0.40
20:b:43:SER:O	20:b:47:LYS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	89/115 (77%)	82 (92%)	7 (8%)	0	100	100
2	B	154/224 (69%)	142 (92%)	10 (6%)	2 (1%)	9	40
3	C	196/263 (74%)	186 (95%)	8 (4%)	2 (1%)	12	45
4	D	384/463 (83%)	357 (93%)	27 (7%)	0	100	100
5	E	208/248 (84%)	191 (92%)	17 (8%)	0	100	100
6	F	424/464 (91%)	406 (96%)	18 (4%)	0	100	100
7	G	685/727 (94%)	631 (92%)	54 (8%)	0	100	100
8	H	310/318 (98%)	291 (94%)	18 (6%)	1 (0%)	36	68
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	P	338/377 (90%)	312 (92%)	26 (8%)	0	100	100
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	75 (93%)	6 (7%)	0	100	100
13	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
15	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
16	W	112/131 (86%)	110 (98%)	1 (1%)	1 (1%)	14	47
17	X	140/172 (81%)	130 (93%)	10 (7%)	0	100	100
18	Z	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
19	a	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
20	b	77/84 (92%)	71 (92%)	6 (8%)	0	100	100
21	q	116/145 (80%)	113 (97%)	3 (3%)	0	100	100
22	r	46/113 (41%)	44 (96%)	2 (4%)	0	100	100
23	s	24/104 (23%)	24 (100%)	0	0	100	100
All	All	4136/5036 (82%)	3897 (94%)	233 (6%)	6 (0%)	49	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	127	GLN
3	C	135	ARG
8	H	92	PRO
3	C	81	ASP
16	W	99	VAL
2	B	195	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/104 (82%)	85 (100%)	0	100	100
2	B	132/185 (71%)	132 (100%)	0	100	100
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	333/395 (84%)	333 (100%)	0	100	100
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	89
8	H	278/280 (99%)	278 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	P	297/325 (91%)	295 (99%)	2 (1%)	76	83
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%)	68 (99%)	1 (1%)	59	77
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	129 (100%)	0	100	100
18	Z	120/123 (98%)	119 (99%)	1 (1%)	73	82
19	a	57/60 (95%)	57 (100%)	0	100	100
20	b	70/73 (96%)	70 (100%)	0	100	100
21	q	108/131 (82%)	108 (100%)	0	100	100
22	r	44/96 (46%)	44 (100%)	0	100	100
23	s	26/95 (27%)	26 (100%)	0	100	100
All	All	3635/4292 (85%)	3626 (100%)	9 (0%)	85	89

All (9) residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	54	HIS
3	C	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	132	GLN
5	E	152	GLN
5	E	245	GLN
6	F	44	ASN
6	F	49	HIS
6	F	168	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	277	ASN
6	F	346	GLN
7	G	59	GLN
7	G	74	ASN
7	G	105	ASN
7	G	140	GLN
7	G	164	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

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Mol	Chain	Res	Type
7	G	569	GLN
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	163	GLN
8	H	169	GLN
8	H	258	ASN
8	H	287	HIS
10	P	71	ASN
10	P	154	GLN
10	P	166	HIS
10	P	216	HIS
10	P	251	ASN
10	P	269	ASN
10	P	275	HIS
10	P	323	HIS
10	P	341	GLN
10	P	356	HIS
11	Q	51	GLN
11	Q	88	GLN
12	R	33	HIS
15	V	41	HIS
15	V	50	GLN
16	W	54	GLN
17	X	30	HIS
17	X	77	HIS
18	Z	135	ASN
19	a	31	ASN
20	b	69	HIS
20	b	83	ASN
21	q	12	GLN
21	q	31	ASN
21	q	52	ASN
21	q	54	GLN
21	q	87	HIS
21	q	91	HIS
22	r	9	GLN

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Mol	Chain	Res	Type
22	r	21	GLN
22	r	110	GLN
23	s	59	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.13	2 (5%)
25	SF4	G	802	7	0,12,12	-	-	-	-	-
33	EHZ	W	201	-	27,31,37	1.90	7 (25%)	37,41,47	1.86	11 (29%)
34	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.28	6 (9%)
28	FES	G	803	7	0,4,4	-	-	-	-	-
25	SF4	F	502	6	0,12,12	-	-	-	-	-
24	3PE	b	201	-	45,45,50	1.11	5 (11%)	48,50,55	1.23	3 (6%)
29	FMN	F	501	-	33,33,33	1.38	4 (12%)	48,50,50	1.21	6 (12%)
27	PC1	I	302	-	46,46,53	0.99	2 (4%)	52,54,61	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	SF4	I	303	9	0,12,12	-	-	-		
24	3PE	A	401	-	45,45,50	1.12	5 (11%)	48,50,55	1.19	3 (6%)
31	NDP	P	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.66	11 (16%)
30	UQ9	H	400	-	35,35,58	0.83	2 (5%)	42,45,73	0.52	0
25	SF4	I	304	9	0,12,12	-	-	-		
25	SF4	G	801	7	0,12,12	-	-	-		
28	FES	E	301	5	0,4,4	-	-	-		
26	UQ1	B	302	-	18,18,18	1.94	2 (11%)	22,25,25	1.35	3 (13%)
25	SF4	B	301	2	0,12,12	-	-	-		
24	3PE	I	301	-	45,45,50	0.98	2 (4%)	48,50,55	1.08	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PC1	B	303	-	-	8/38/38/57	-
25	SF4	G	802	7	-	-	0/6/5/5
33	EHZ	W	201	-	-	21/39/39/45	-
34	CDL	a	101	-	-	18/67/67/110	-
28	FES	G	803	7	-	-	0/1/1/1
25	SF4	F	502	6	-	-	0/6/5/5
24	3PE	b	201	-	-	19/49/49/54	-
29	FMN	F	501	-	-	3/18/18/18	0/3/3/3
27	PC1	I	302	-	-	10/50/50/57	-
25	SF4	I	303	9	-	-	0/6/5/5
24	3PE	A	401	-	-	18/49/49/54	-
31	NDP	P	401	-	-	3/34/77/77	0/5/5/5
30	UQ9	H	400	-	-	14/30/54/81	0/1/1/1
25	SF4	I	304	9	-	-	0/6/5/5
25	SF4	G	801	7	-	-	0/6/5/5
28	FES	E	301	5	-	-	0/1/1/1
26	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
25	SF4	B	301	2	-	-	0/6/5/5
24	3PE	I	301	-	-	12/49/49/54	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	302	UQ1	C6-C5	7.36	1.48	1.35
33	W	201	EHZ	C15-N2	5.38	1.45	1.33
33	W	201	EHZ	C12-N1	5.16	1.45	1.33
29	F	501	FMN	C9A-C5A	4.82	1.49	1.41
24	I	301	3PE	O31-C31	4.25	1.45	1.33
31	P	401	NDP	C5A-C4A	4.23	1.46	1.39
24	I	301	3PE	O21-C21	4.20	1.46	1.34
34	a	101	CDL	OA8-CA7	4.19	1.45	1.33
27	B	303	PC1	O31-C31	4.18	1.45	1.33
34	a	101	CDL	OB8-CB7	4.17	1.45	1.33
27	I	302	PC1	O31-C31	4.16	1.45	1.33
27	B	303	PC1	O21-C21	4.10	1.45	1.34
34	a	101	CDL	OA6-CA5	4.07	1.45	1.34
34	a	101	CDL	OB6-CB5	4.05	1.45	1.34
27	I	302	PC1	O21-C21	4.03	1.45	1.34
31	P	401	NDP	C6N-C5N	3.35	1.39	1.33
24	A	401	3PE	O21-C21	3.18	1.43	1.34
24	b	201	3PE	O21-C21	3.13	1.43	1.34
29	F	501	FMN	C8-C7	3.08	1.48	1.40
26	B	302	UQ1	C3-C2	3.03	1.48	1.36
24	b	201	3PE	O31-C31	3.01	1.42	1.33
24	A	401	3PE	O31-C31	3.01	1.42	1.33
30	H	400	UQ9	C3-C2	-2.78	1.40	1.48
29	F	501	FMN	C4-N3	-2.67	1.33	1.38
33	W	201	EHZ	P1-O7	2.57	1.64	1.54
30	H	400	UQ9	C4-C5	-2.52	1.41	1.48
33	W	201	EHZ	O4-C15	-2.52	1.18	1.23
31	P	401	NDP	C5A-C6A	2.48	1.48	1.41
33	W	201	EHZ	C9-S1	2.43	1.82	1.76
33	W	201	EHZ	O3-C12	-2.39	1.18	1.23
31	P	401	NDP	C5A-N7A	-2.38	1.34	1.39
31	P	401	NDP	C8A-N7A	2.38	1.36	1.31
29	F	501	FMN	C5A-N5	-2.29	1.35	1.39
24	b	201	3PE	O21-C2	-2.27	1.40	1.46
33	W	201	EHZ	P1-OP3	-2.24	1.46	1.54
24	A	401	3PE	O31-C3	-2.20	1.40	1.45
24	A	401	3PE	O21-C2	-2.19	1.41	1.46
24	b	201	3PE	O31-C3	-2.15	1.40	1.45
24	A	401	3PE	P-O12	-2.12	1.45	1.55
24	b	201	3PE	P-O12	-2.09	1.45	1.55

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	W	201	EHZ	C8-C9-S1	6.35	121.48	113.63
31	P	401	NDP	C5A-C4A-N3A	-6.07	118.83	126.75
31	P	401	NDP	N3A-C4A-N9A	4.76	134.92	127.08
24	I	301	3PE	O21-C21-C22	4.36	120.90	111.50
34	a	101	CDL	OA6-CA5-C11	4.26	120.69	111.50
24	A	401	3PE	O21-C21-C22	4.25	120.65	111.50
27	B	303	PC1	O21-C21-C22	4.08	120.30	111.50
24	b	201	3PE	O21-C21-C22	4.05	120.22	111.50
27	I	302	PC1	O21-C21-C22	3.97	120.05	111.50
34	a	101	CDL	OB6-CB5-C51	3.90	119.90	111.50
31	P	401	NDP	C2A-N3A-C4A	3.88	120.91	111.75
31	P	401	NDP	PN-O3-PA	-3.65	120.29	132.83
31	P	401	NDP	N3A-C2A-N1A	-3.20	123.59	128.60
31	P	401	NDP	C4A-C5A-N7A	-3.19	106.73	110.62
33	W	201	EHZ	C13-C12-N1	3.08	121.60	116.42
33	W	201	EHZ	C14-C13-C12	-3.04	107.30	112.36
27	B	303	PC1	O31-C31-C32	2.91	121.04	111.91
33	W	201	EHZ	OP3-P1-O9	-2.89	99.35	110.68
33	W	201	EHZ	C7-C8-C9	-2.85	107.37	113.89
34	a	101	CDL	OA8-CA7-C31	2.80	120.68	111.91
26	B	302	UQ1	CM5-C5-C6	-2.77	119.88	124.40
34	a	101	CDL	CA4-OA6-CA5	-2.77	110.97	117.79
31	P	401	NDP	C4A-N9A-C8A	2.73	108.68	105.73
31	P	401	NDP	C5A-N7A-C8A	2.72	107.38	103.51
27	I	302	PC1	C2-O21-C21	-2.69	111.17	117.79
26	B	302	UQ1	C11-C9-C10	2.68	120.52	114.60
34	a	101	CDL	OB8-CB7-C71	2.58	120.00	111.91
29	F	501	FMN	C4A-C10-N1	-2.57	118.76	124.73
24	A	401	3PE	O31-C31-C32	2.52	119.81	111.91
24	b	201	3PE	O31-C31-C32	2.50	119.76	111.91
24	I	301	3PE	C2-O21-C21	-2.43	111.80	117.79
29	F	501	FMN	O4-C4-C4A	-2.40	120.23	126.60
27	I	302	PC1	O31-C31-C32	2.39	119.41	111.91
29	F	501	FMN	C4-C4A-N5	2.39	121.63	118.23
33	W	201	EHZ	C5-C6-C7	-2.38	107.99	114.85
34	a	101	CDL	CB4-OB6-CB5	-2.36	111.99	117.79
26	B	302	UQ1	C7-C8-C9	-2.34	119.92	127.26
33	W	201	EHZ	C10-S1-C9	2.27	108.93	101.87
24	I	301	3PE	O31-C31-C32	2.22	118.89	111.91
29	F	501	FMN	O2-C2-N1	-2.22	118.15	121.83
29	F	501	FMN	C4A-C10-N10	2.21	119.70	116.48
31	P	401	NDP	C3D-C2D-C1D	2.20	105.60	101.43
31	P	401	NDP	C6A-C5A-N7A	2.19	136.11	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	W	201	EHZ	C11-N1-C12	-2.18	118.79	122.84
24	b	201	3PE	O12-P-O14	-2.17	101.49	112.24
33	W	201	EHZ	O2-C9-S1	-2.17	119.80	122.61
31	P	401	NDP	N9A-C8A-N7A	-2.16	110.96	113.91
29	F	501	FMN	C10-N1-C2	2.13	121.16	116.90
33	W	201	EHZ	O6-P1-O9	2.12	112.42	106.47
33	W	201	EHZ	O3-C12-N1	-2.10	119.04	123.01
24	A	401	3PE	O12-P-O14	-2.06	102.07	112.24

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	401	3PE	C11-O13-P-O12
24	A	401	3PE	C11-O13-P-O14
24	A	401	3PE	C12-C11-O13-P
24	A	401	3PE	O32-C31-O31-C3
24	A	401	3PE	C32-C31-O31-C3
24	I	301	3PE	C1-O11-P-O12
24	I	301	3PE	C22-C21-O21-C2
24	b	201	3PE	C1-O11-P-O12
24	b	201	3PE	C1-O11-P-O14
24	b	201	3PE	O22-C21-O21-C2
27	I	302	PC1	C11-O13-P-O14
29	F	501	FMN	C5'-O5'-P-O2P
29	F	501	FMN	C5'-O5'-P-O3P
30	H	400	UQ9	C19-C21-C22-C23
30	H	400	UQ9	C20-C19-C21-C22
30	H	400	UQ9	C18-C19-C21-C22
30	H	400	UQ9	C17-C18-C19-C21
30	H	400	UQ9	C17-C18-C19-C20
30	H	400	UQ9	C15-C14-C16-C17
30	H	400	UQ9	C12-C13-C14-C16
30	H	400	UQ9	C12-C13-C14-C15
31	P	401	NDP	C2B-O2B-P2B-O2X
33	W	201	EHZ	O1-C7-C8-C9
33	W	201	EHZ	C6-C7-C8-C9
33	W	201	EHZ	C7-C8-C9-S1
33	W	201	EHZ	S1-C10-C11-N1
33	W	201	EHZ	C11-C10-S1-C9
33	W	201	EHZ	C16-C17-C20-O6
33	W	201	EHZ	C20-O6-P1-O7

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Mol	Chain	Res	Type	Atoms
33	W	201	EHZ	C20-O6-P1-O9
33	W	201	EHZ	C20-O6-P1-OP3
34	a	101	CDL	CA3-OA5-PA1-OA2
34	a	101	CDL	CA3-OA5-PA1-OA3
34	a	101	CDL	CA3-OA5-PA1-OA4
27	I	302	PC1	O32-C31-O31-C3
24	I	301	3PE	O22-C21-O21-C2
27	I	302	PC1	C32-C31-O31-C3
24	b	201	3PE	C22-C21-O21-C2
30	H	400	UQ9	C24-C26-C27-C28
24	I	301	3PE	C32-C31-O31-C3
30	H	400	UQ9	C22-C23-C24-C25
30	H	400	UQ9	C22-C23-C24-C26
24	A	401	3PE	C22-C21-O21-C2
24	I	301	3PE	O32-C31-O31-C3
30	H	400	UQ9	C13-C14-C16-C17
30	H	400	UQ9	C9-C11-C12-C13
24	b	201	3PE	C2B-C2C-C2D-C2E
24	A	401	3PE	O22-C21-O21-C2
24	b	201	3PE	C32-C31-O31-C3
24	b	201	3PE	C39-C3A-C3B-C3C
34	a	101	CDL	C12-C13-C14-C15
24	b	201	3PE	O32-C31-O31-C3
30	H	400	UQ9	C14-C16-C17-C18
24	A	401	3PE	C11-O13-P-O11
24	I	301	3PE	C1-O11-P-O13
24	b	201	3PE	C1-O11-P-O13
27	B	303	PC1	C22-C21-O21-C2
24	b	201	3PE	C27-C28-C29-C2A
27	B	303	PC1	O22-C21-O21-C2
24	I	301	3PE	C11-O13-P-O11
24	A	401	3PE	C37-C38-C39-C3A
34	a	101	CDL	C11-CA5-OA6-CA4
24	b	201	3PE	C1-C2-C3-O31
34	a	101	CDL	C71-CB7-OB8-CB6
24	A	401	3PE	C3-C2-O21-C21
29	F	501	FMN	C5'-O5'-P-O1P
34	a	101	CDL	C31-CA7-OA8-CA6
24	b	201	3PE	O11-C1-C2-C3
33	W	201	EHZ	N2-C15-C16-C17
24	I	301	3PE	C23-C24-C25-C26
34	a	101	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
24	b	201	3PE	C24-C25-C26-C27
27	I	302	PC1	C11-O13-P-O11
33	W	201	EHZ	C3-C4-C5-C6
34	a	101	CDL	OA9-CA7-OA8-CA6
24	I	301	3PE	C21-C22-C23-C24
33	W	201	EHZ	C5-C6-C7-O1
27	B	303	PC1	C32-C31-O31-C3
34	a	101	CDL	OA7-CA5-OA6-CA4
33	W	201	EHZ	O2-C9-S1-C10
24	A	401	3PE	C2A-C2B-C2C-C2D
24	A	401	3PE	C2-C1-O11-P
34	a	101	CDL	CB3-CB4-CB6-OB8
24	b	201	3PE	O11-C1-C2-O21
34	a	101	CDL	OB6-CB4-CB6-OB8
27	B	303	PC1	O32-C31-O31-C3
24	b	201	3PE	C11-O13-P-O11
27	I	302	PC1	C1-O11-P-O13
34	a	101	CDL	CA4-CA3-OA5-PA1
24	I	301	3PE	C11-O13-P-O12
24	I	301	3PE	C11-O13-P-O14
24	b	201	3PE	C11-O13-P-O12
31	P	401	NDP	O4D-C1D-N1N-C6N
27	B	303	PC1	C11-C12-N-C15
27	I	302	PC1	C11-C12-N-C15
24	b	201	3PE	O21-C2-C3-O31
33	W	201	EHZ	O4-C15-C16-O5
33	W	201	EHZ	C19-C17-C20-O6
24	b	201	3PE	C3-C2-O21-C21
27	I	302	PC1	C11-C12-N-C13
34	a	101	CDL	CB2-OB2-PB2-OB5
33	W	201	EHZ	C2-C3-C4-C5
31	P	401	NDP	PN-O3-PA-O2A
24	A	401	3PE	C2B-C2C-C2D-C2E
27	B	303	PC1	C11-C12-N-C14
24	A	401	3PE	C28-C29-C2A-C2B
27	B	303	PC1	C11-C12-N-C13
27	I	302	PC1	C11-C12-N-C14
34	a	101	CDL	C1-CA2-OA2-PA1
24	A	401	3PE	O11-C1-C2-O21
24	A	401	3PE	C25-C26-C27-C28
27	I	302	PC1	C2C-C2D-C2E-C2F
24	A	401	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
33	W	201	EHZ	N2-C15-C16-O5
24	b	201	3PE	C25-C26-C27-C28
33	W	201	EHZ	C18-C17-C20-O6
27	I	302	PC1	C2E-C2F-C2G-C2H
24	A	401	3PE	C33-C34-C35-C36
33	W	201	EHZ	C15-C16-C17-C18
33	W	201	EHZ	O5-C16-C17-C18
34	a	101	CDL	C32-C31-CA7-OA8
34	a	101	CDL	C1-CB2-OB2-PB2
34	a	101	CDL	C32-C31-CA7-OA9
24	I	301	3PE	C1-C2-O21-C21
33	W	201	EHZ	O4-C15-C16-C17
27	B	303	PC1	O21-C21-C22-C23

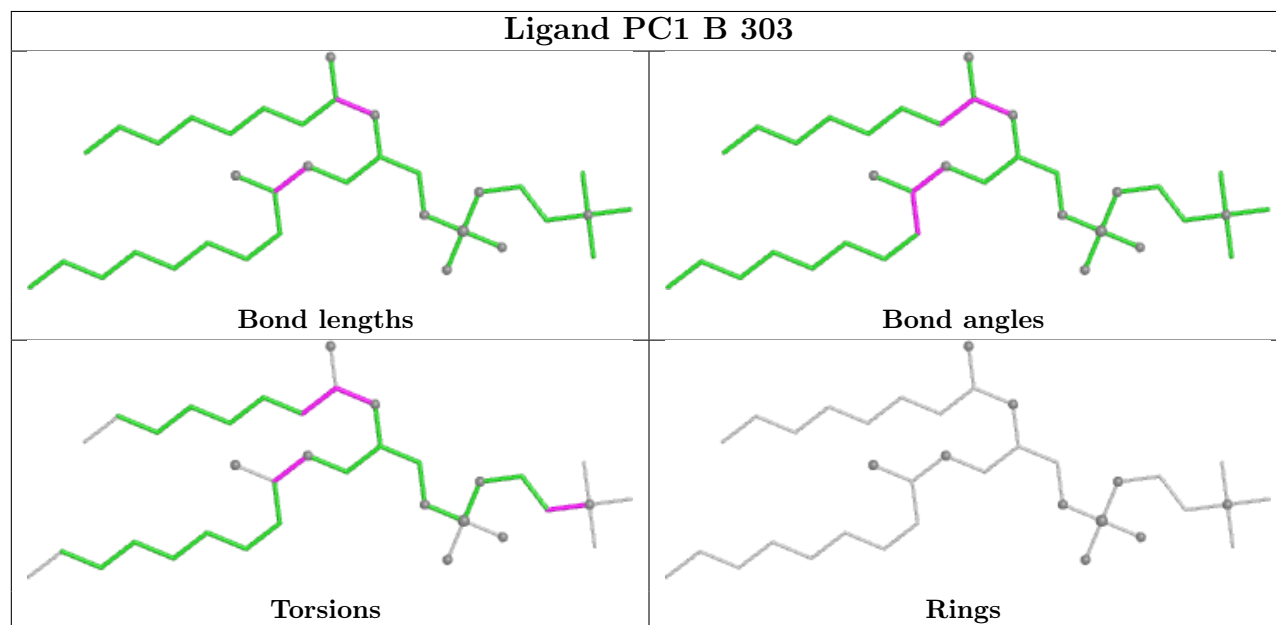
There are no ring outliers.

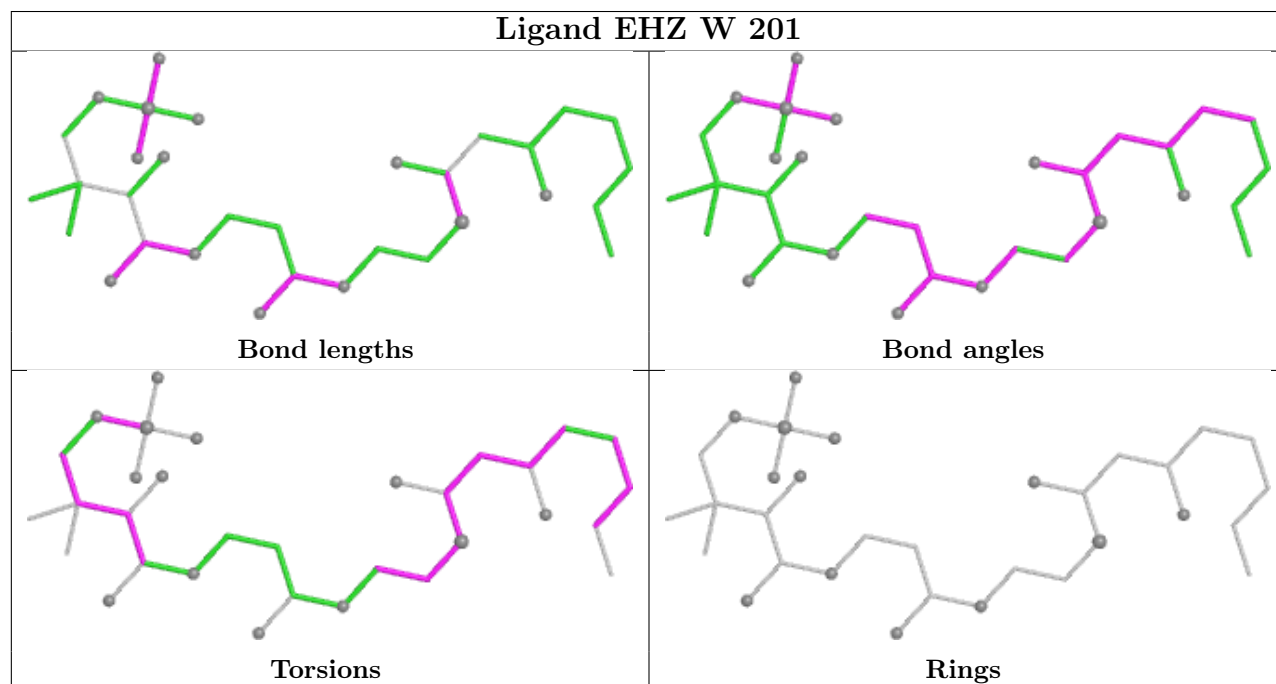
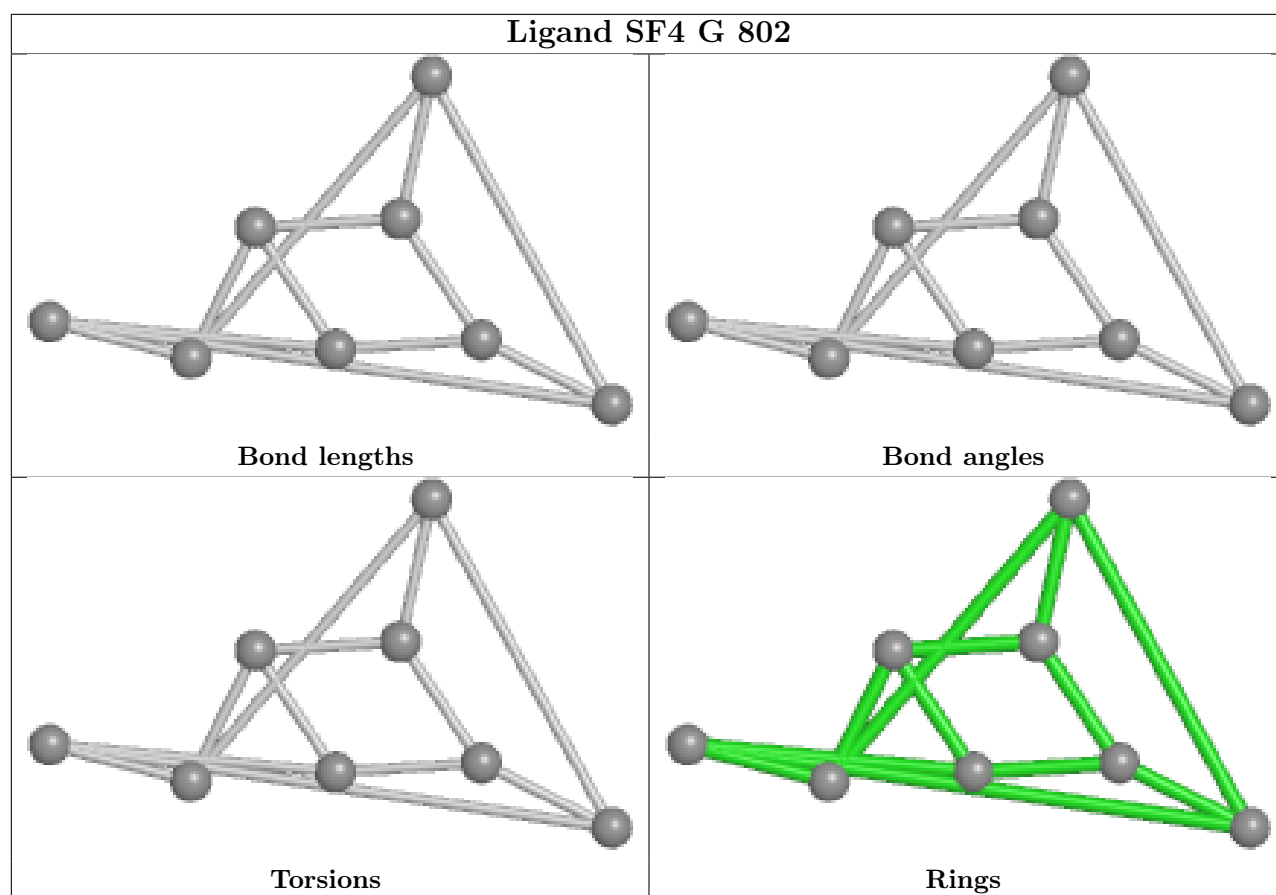
18 monomers are involved in 143 short contacts:

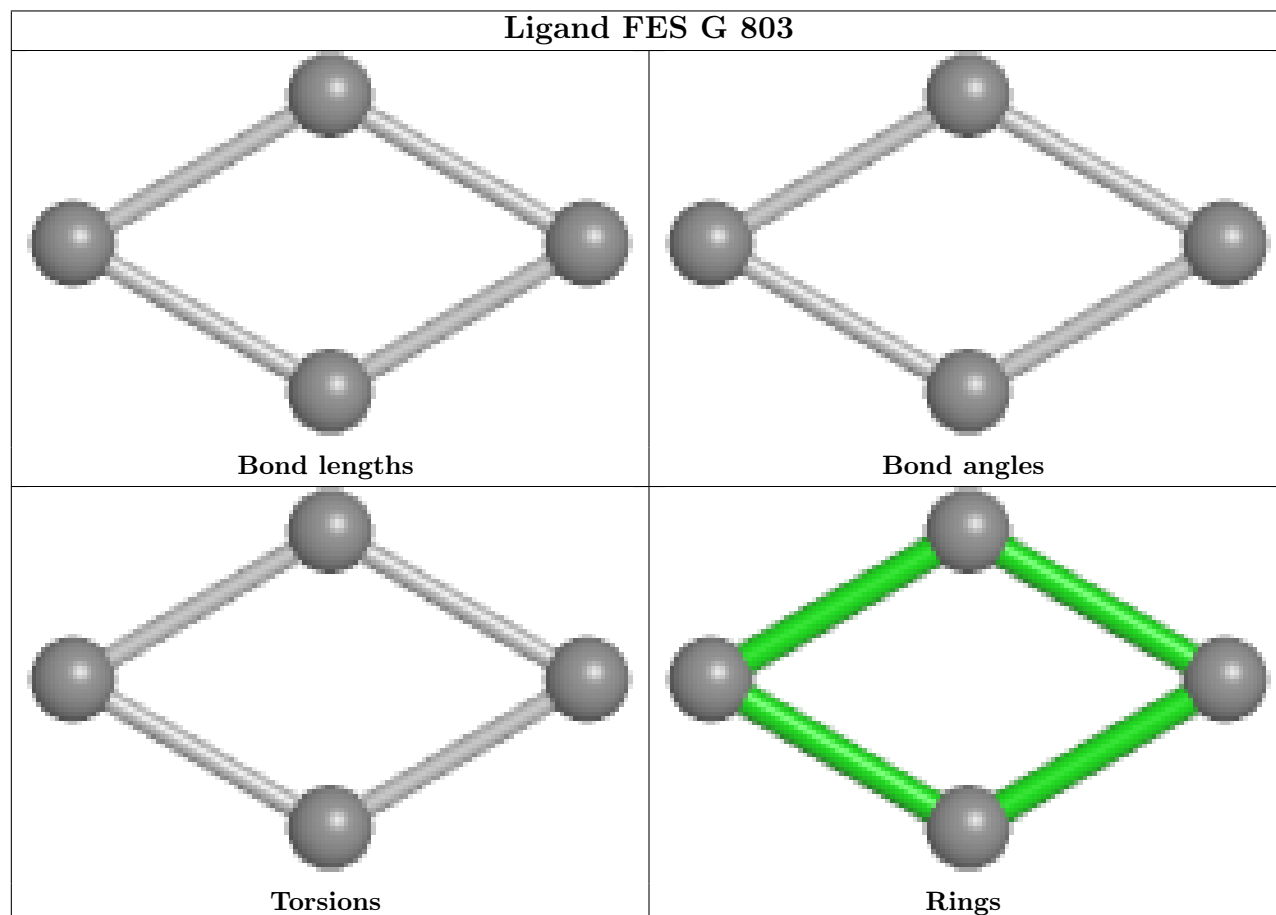
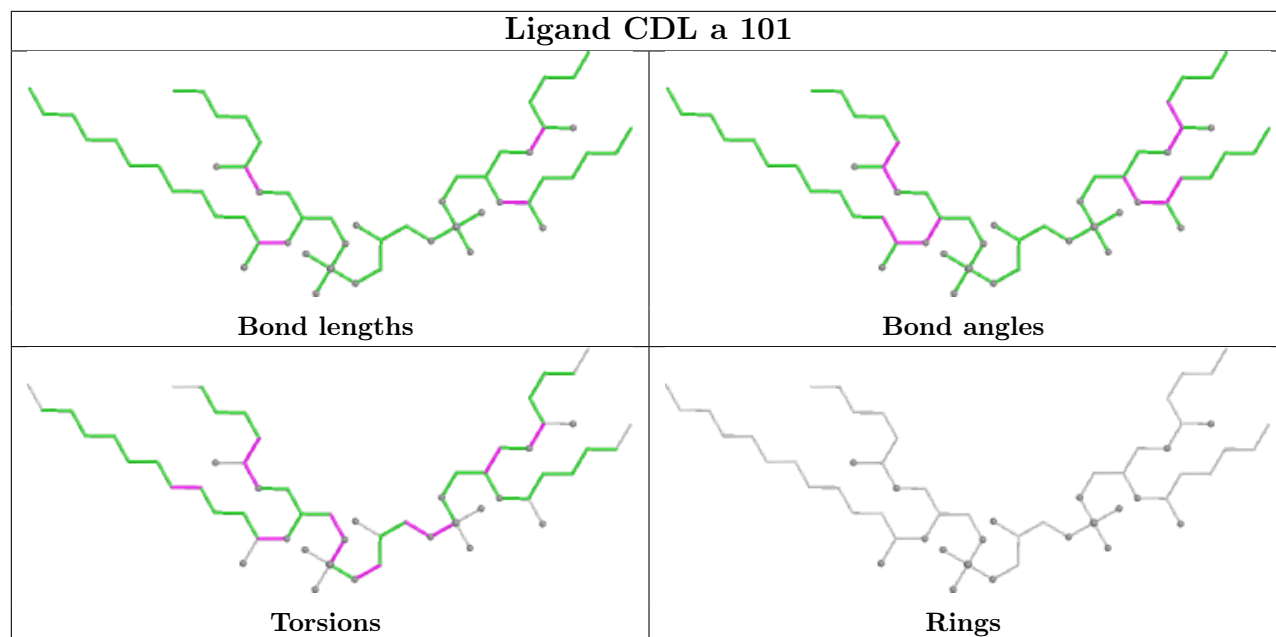
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	303	PC1	3	0
25	G	802	SF4	5	0
33	W	201	EHZ	7	0
34	a	101	CDL	15	0
28	G	803	FES	4	0
25	F	502	SF4	10	0
24	b	201	3PE	11	0
29	F	501	FMN	3	0
27	I	302	PC1	7	0
25	I	303	SF4	11	0
24	A	401	3PE	11	0
31	P	401	NDP	4	0
30	H	400	UQ9	16	0
25	I	304	SF4	5	0
28	E	301	FES	4	0
26	B	302	UQ1	12	0
25	B	301	SF4	5	0
24	I	301	3PE	10	0

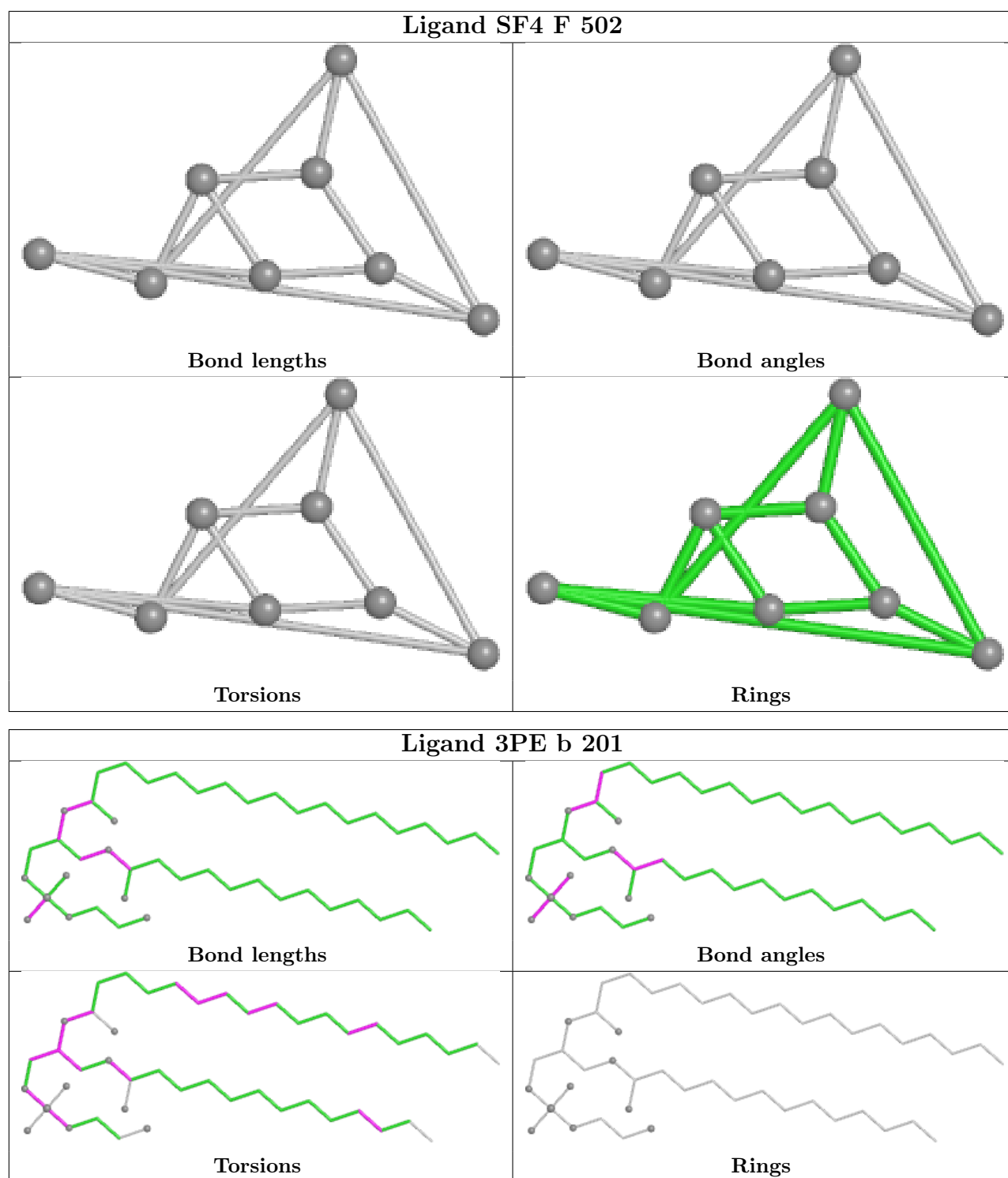
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

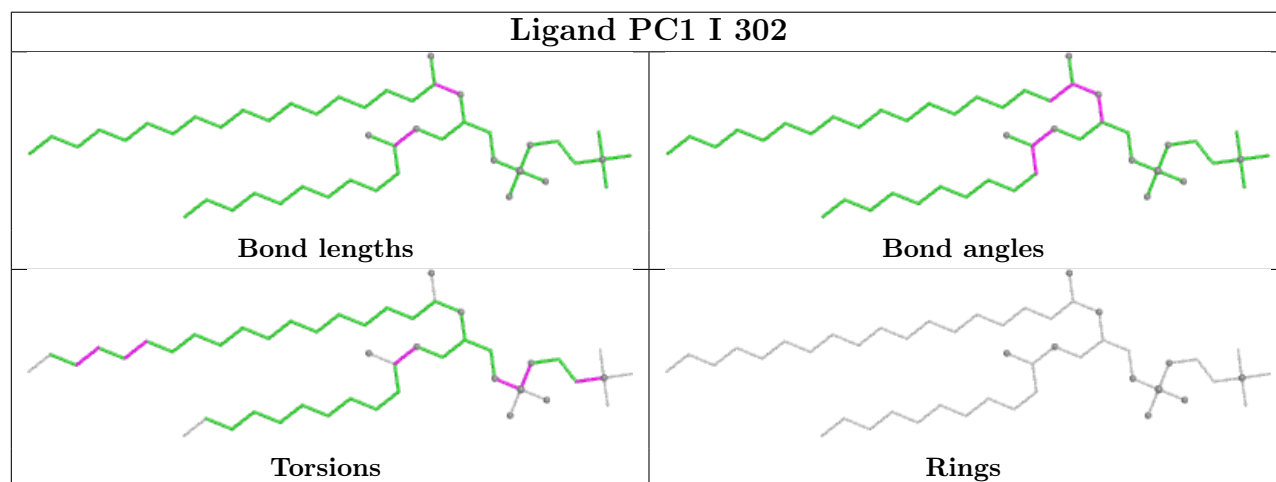
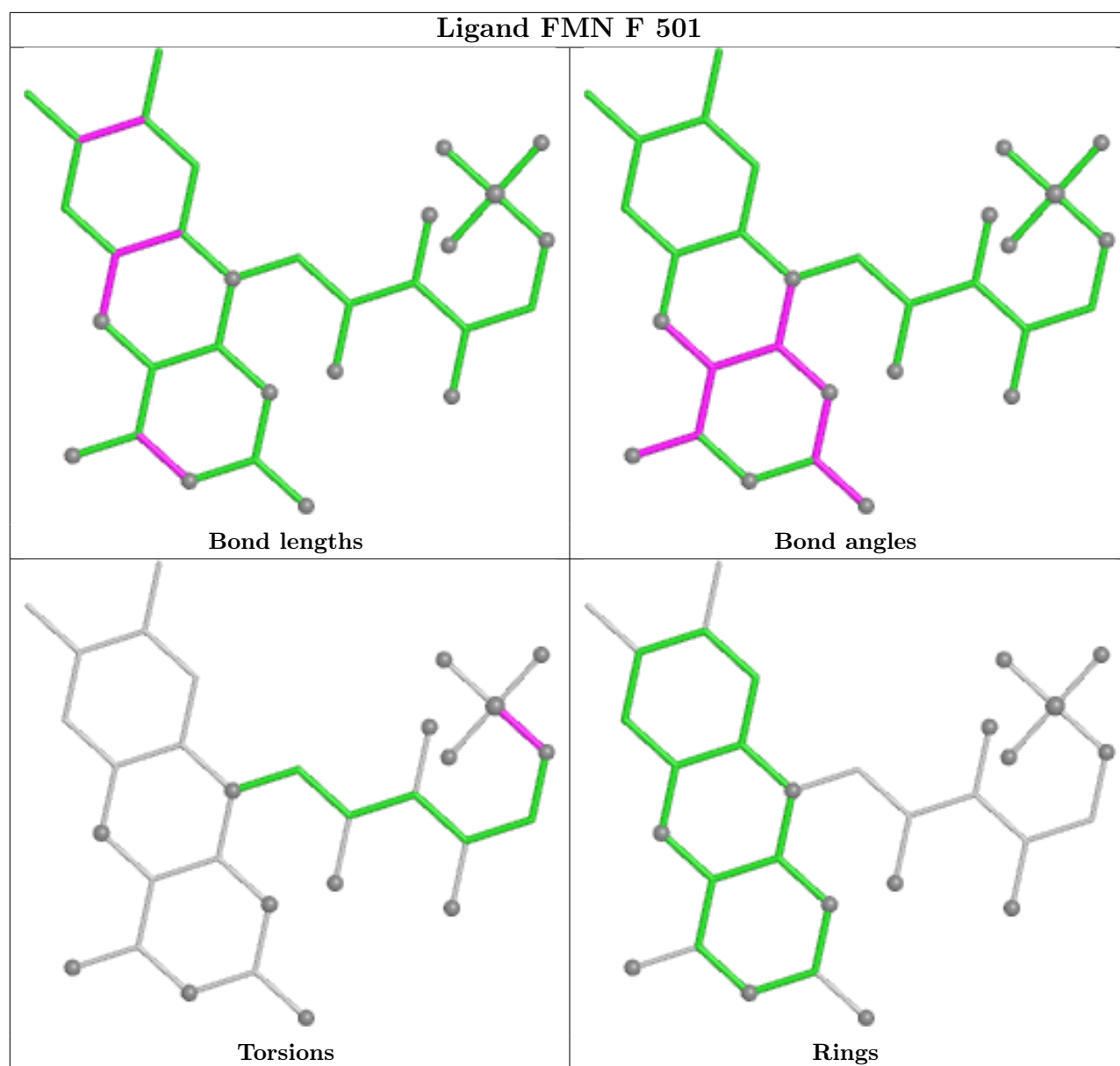
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

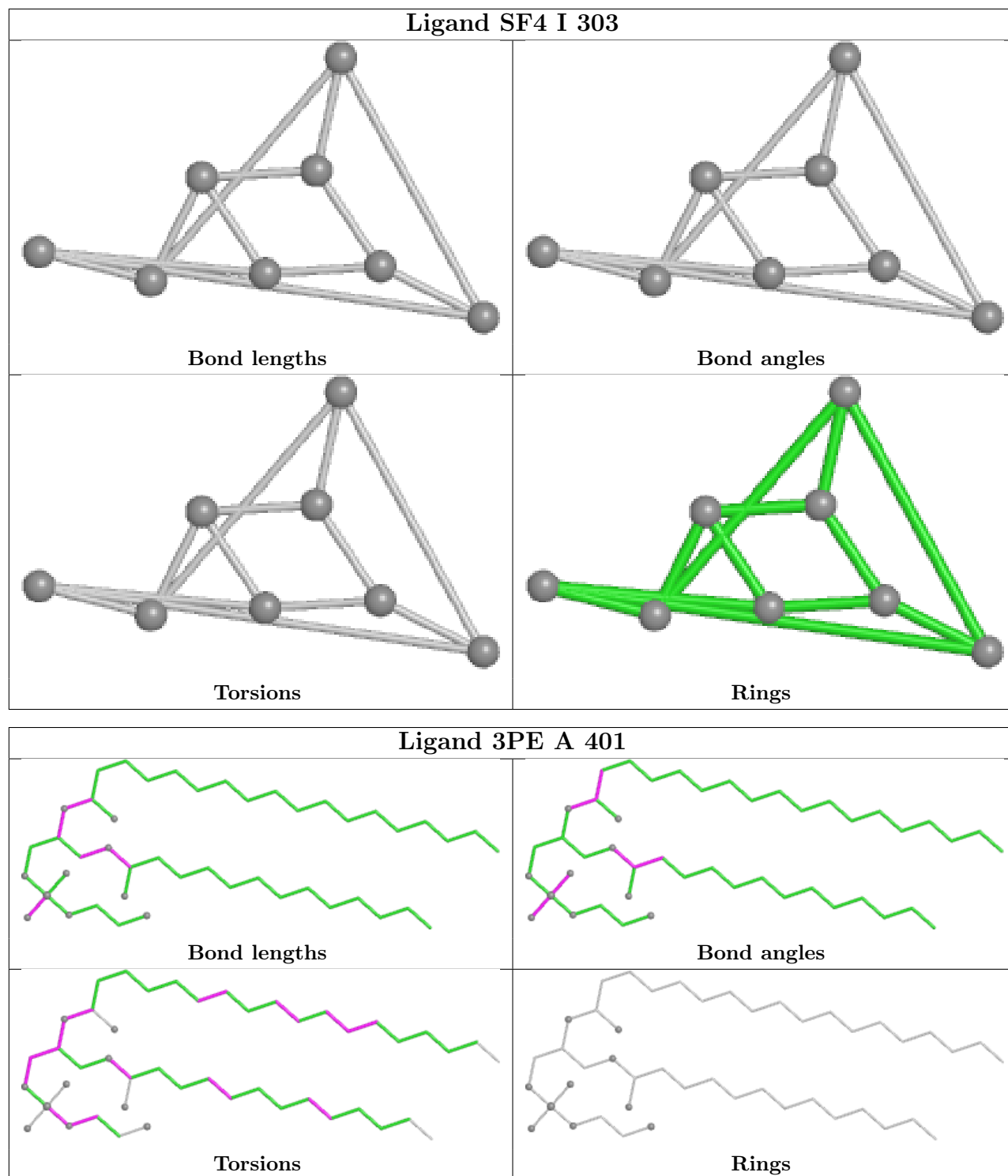


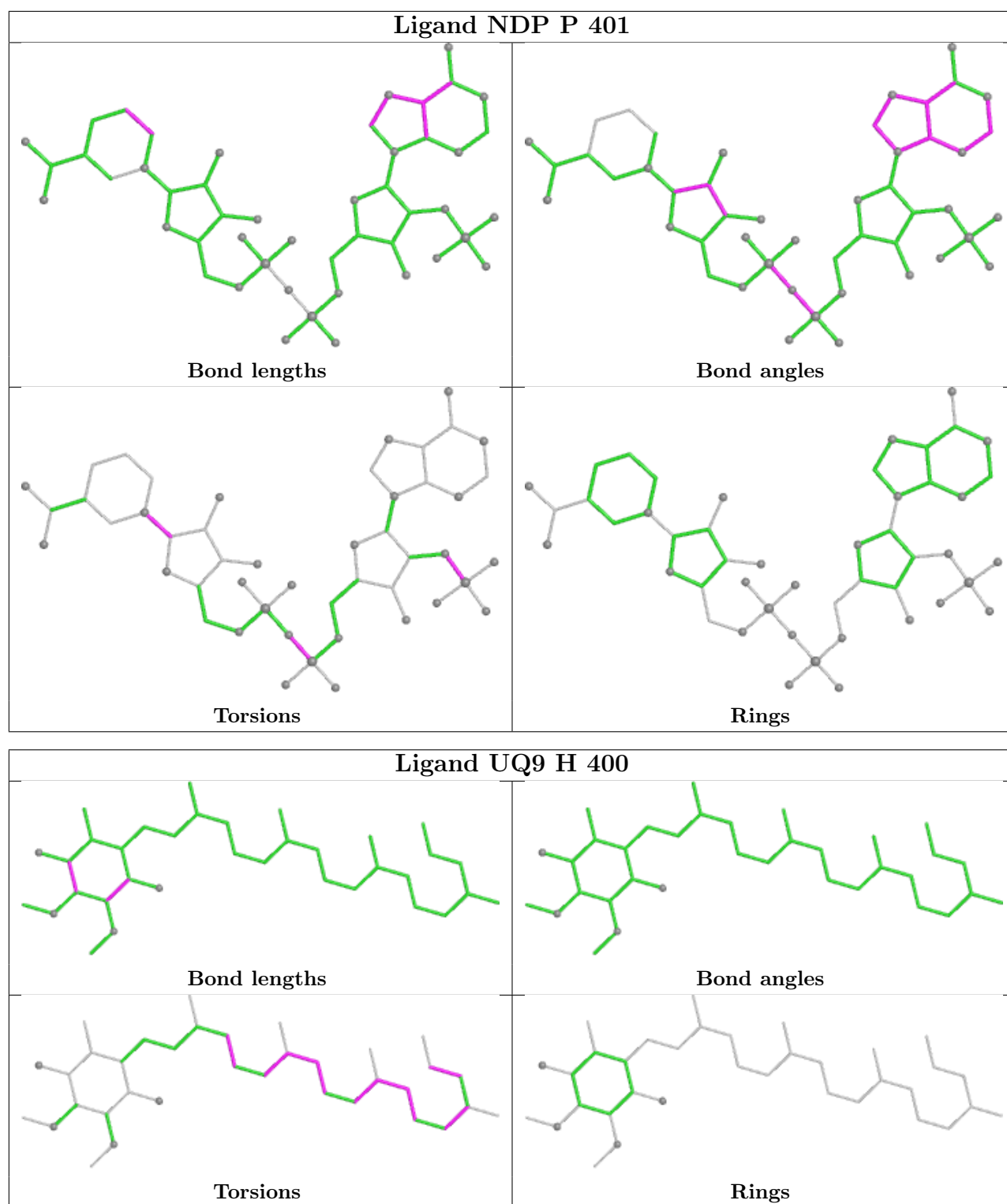




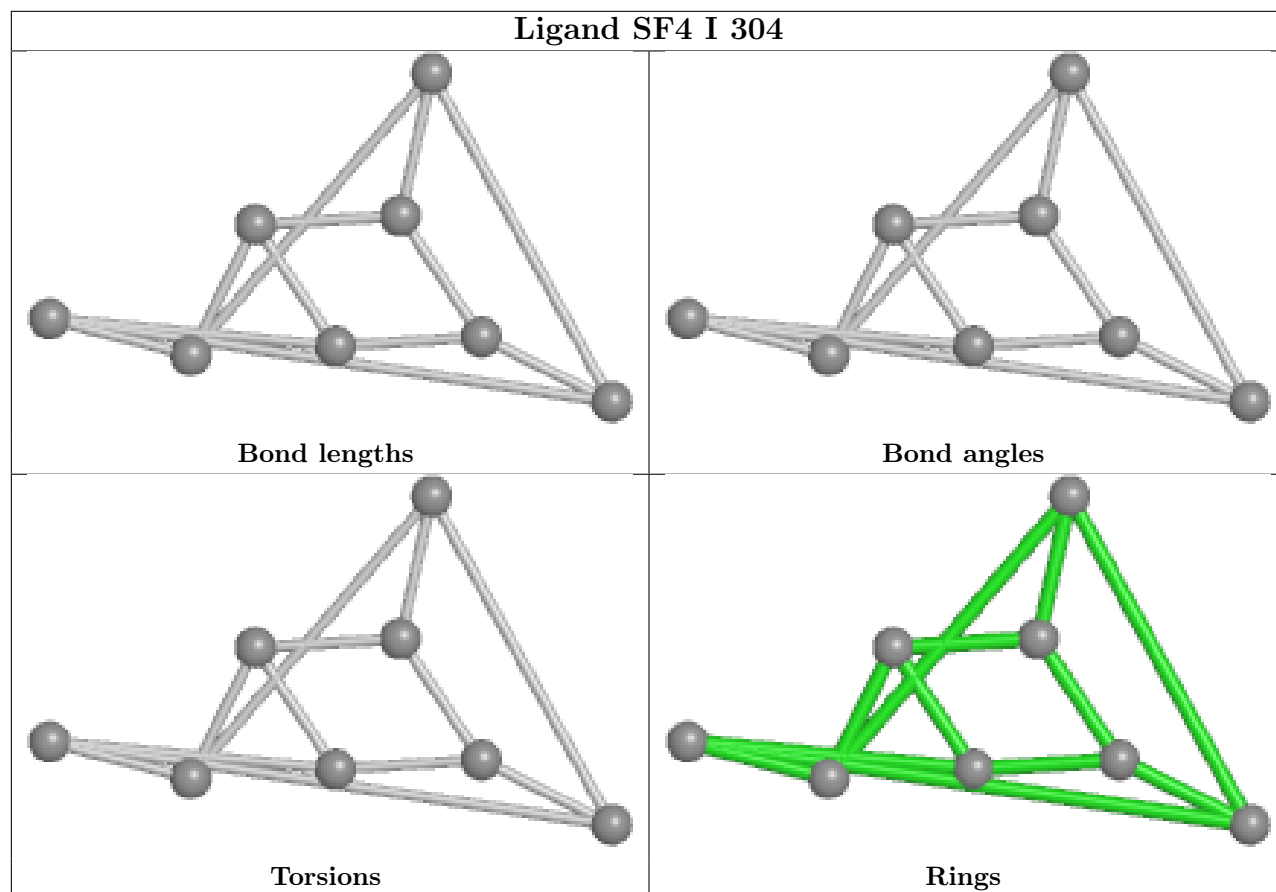




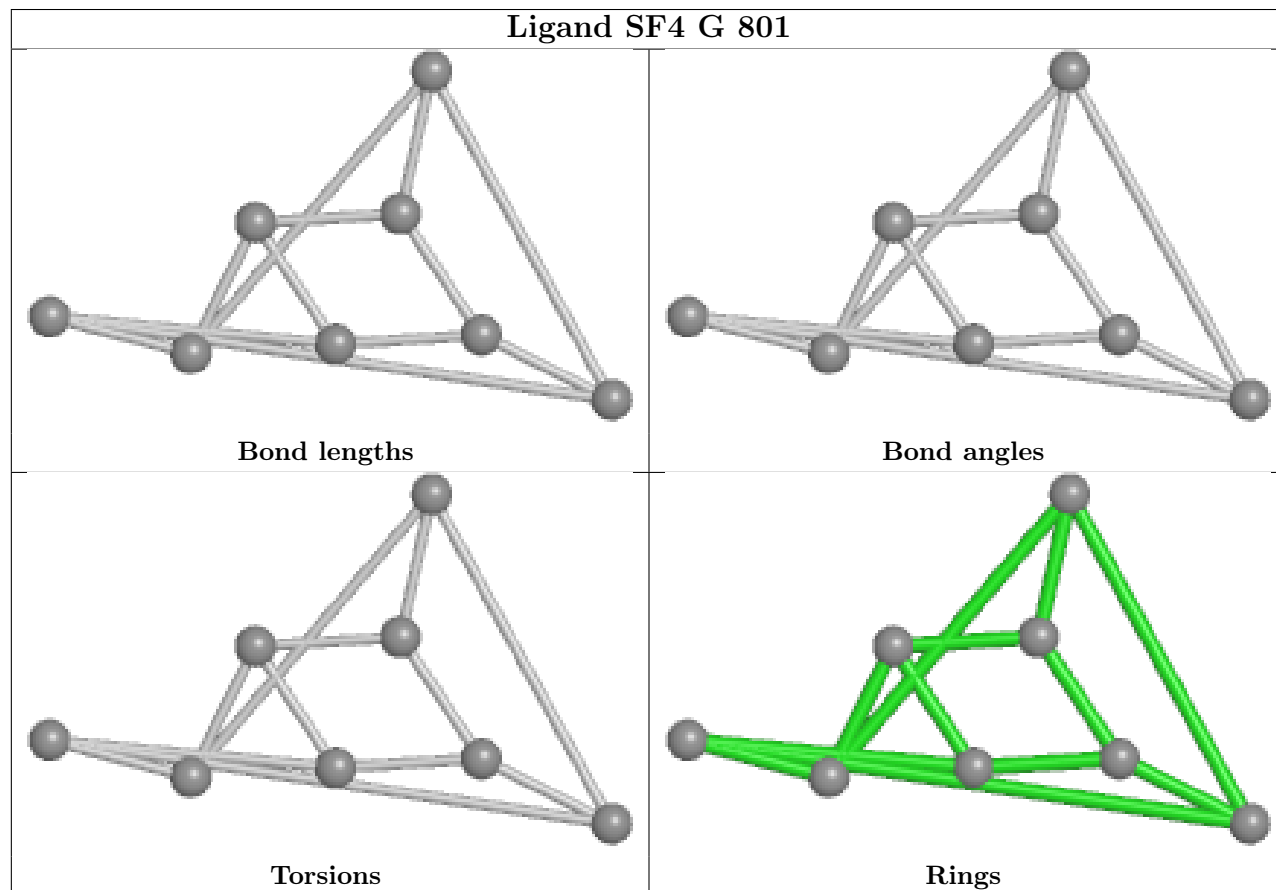


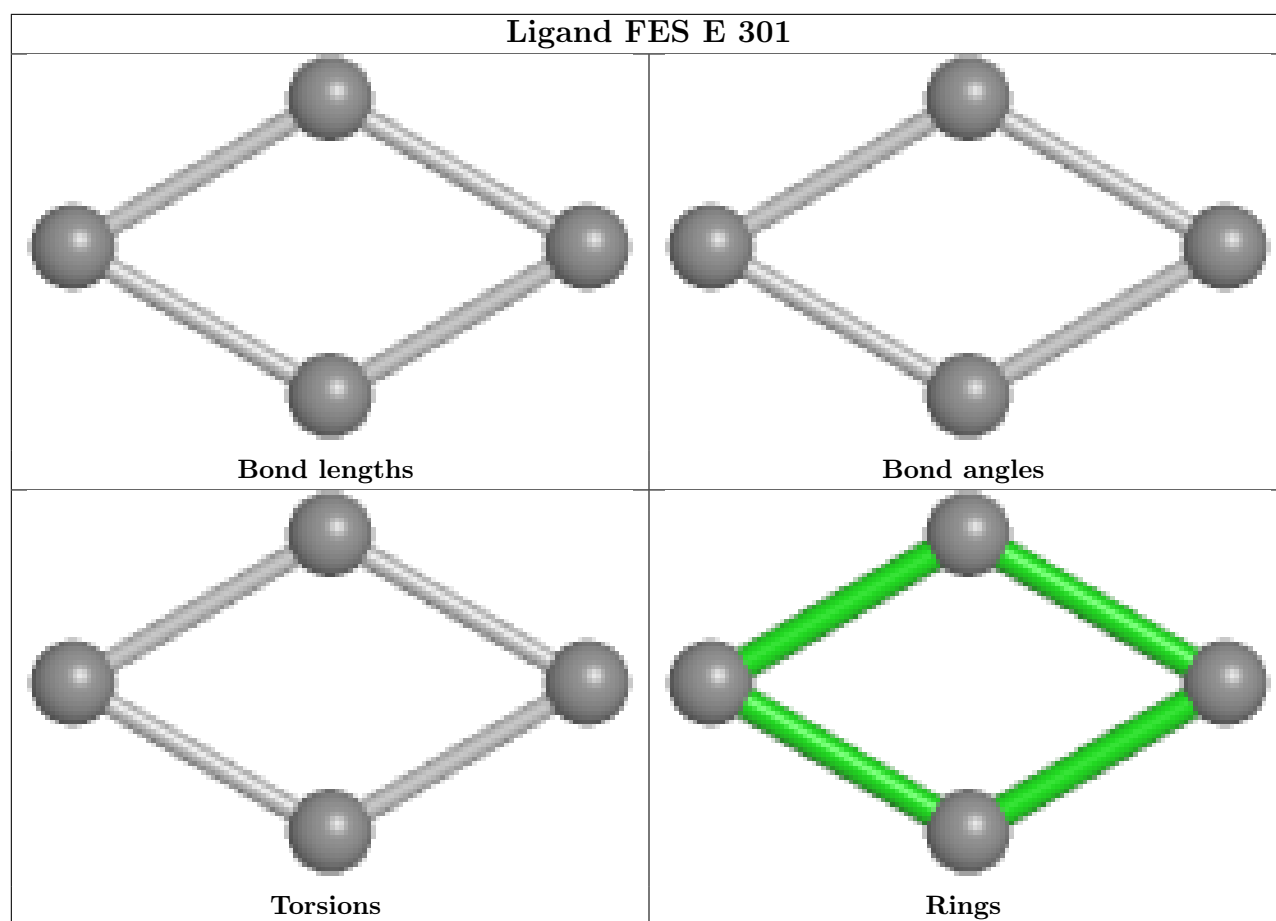


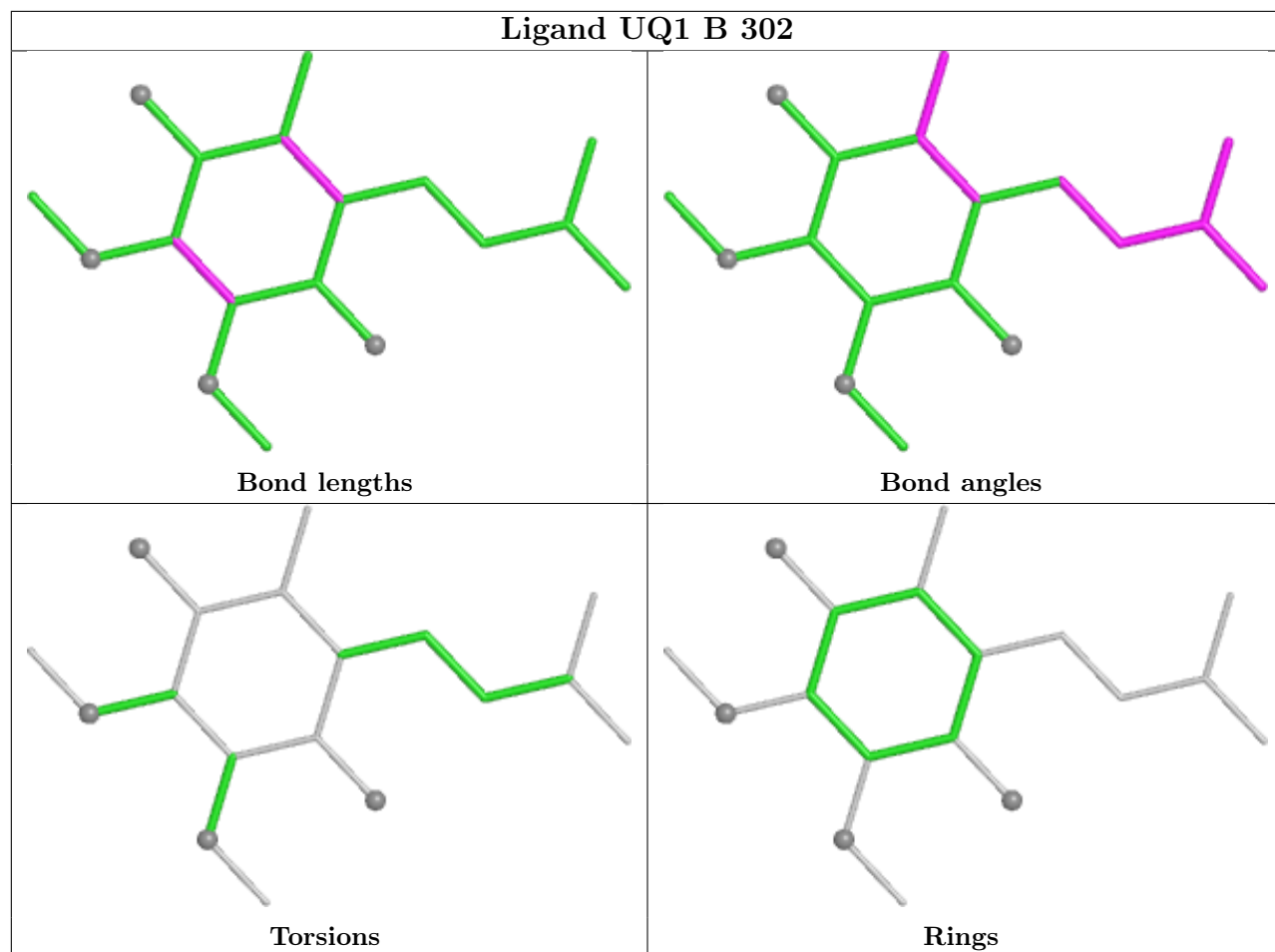
Ligand SF4 I 304

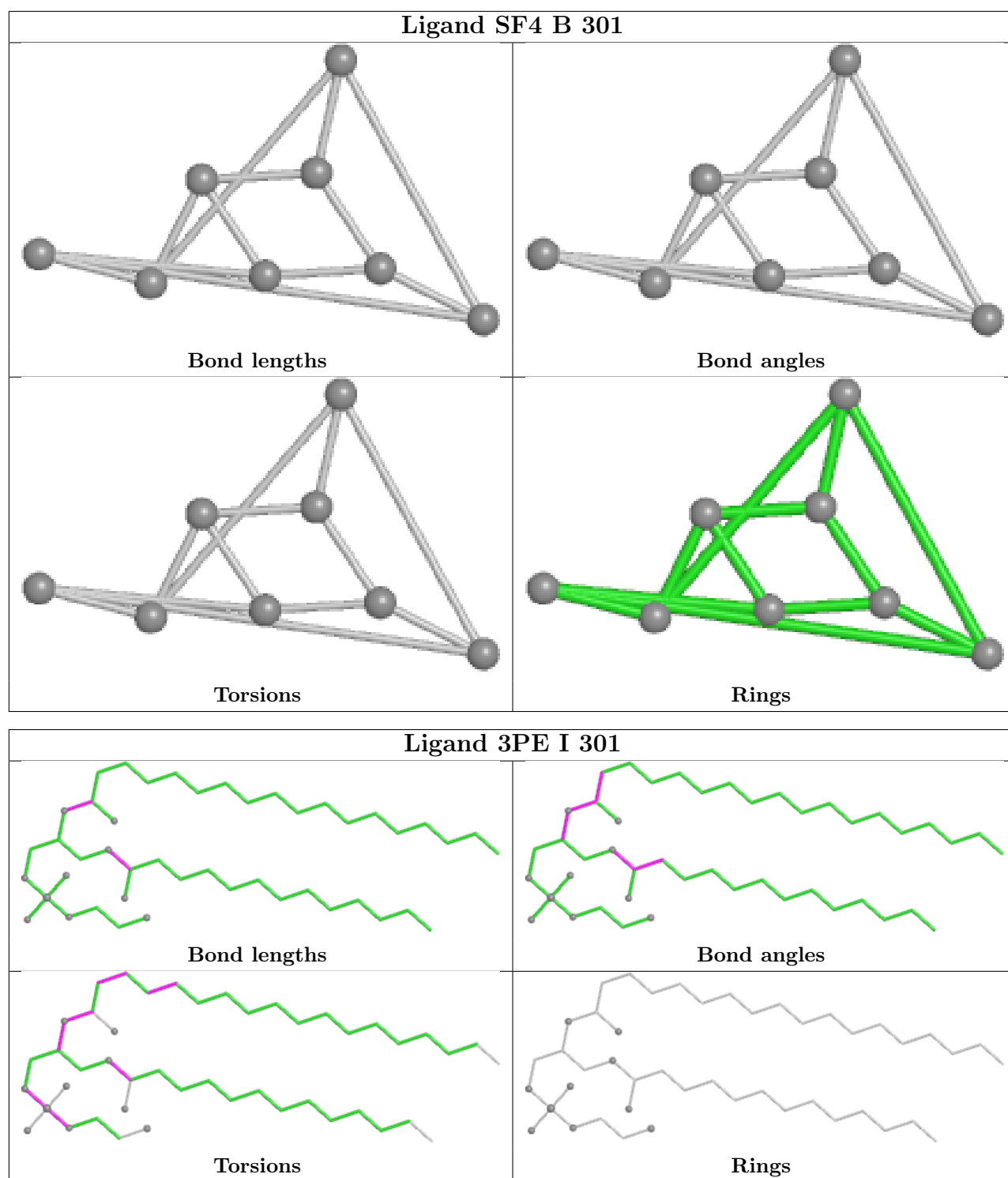


Ligand SF4 G 801









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

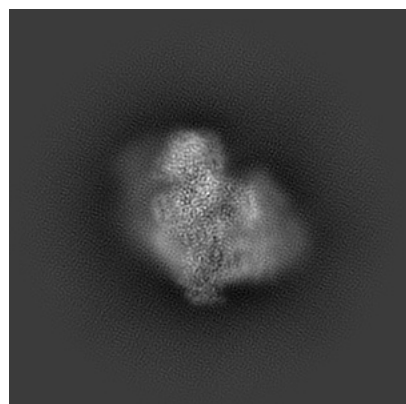
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35337. These allow visual inspection of the internal detail of the map and identification of artifacts.

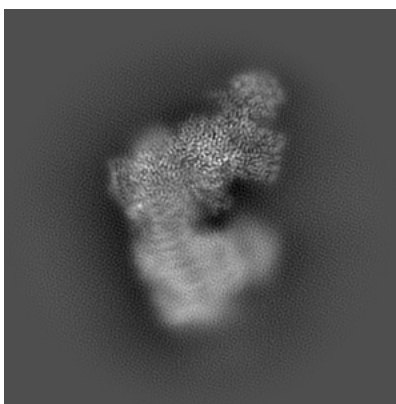
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

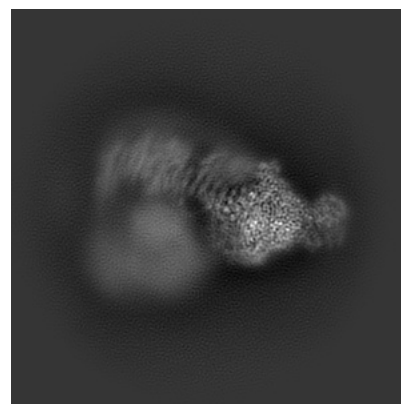
6.1.1 Primary map



X

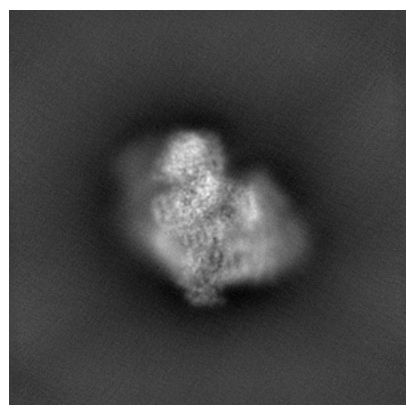


Y

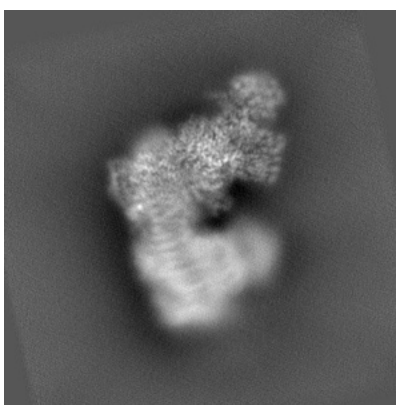


Z

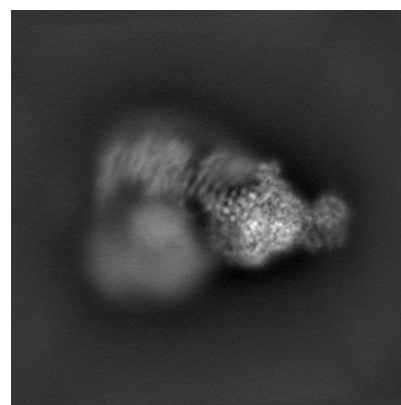
6.1.2 Raw map



X



Y

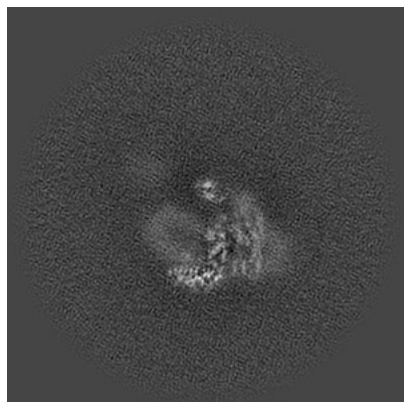


Z

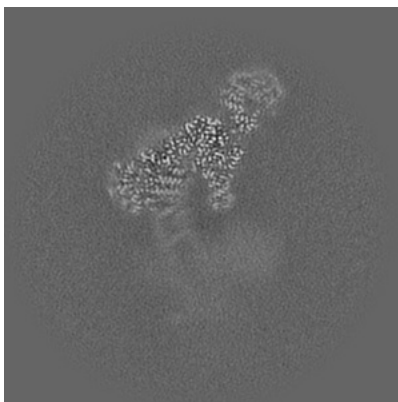
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

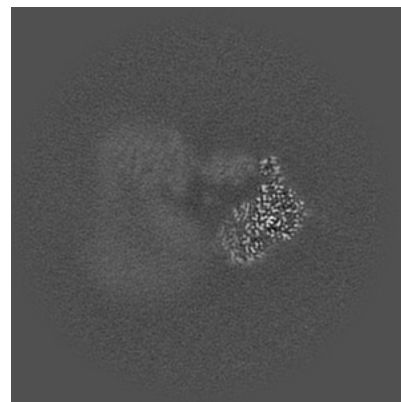
6.2.1 Primary map



X Index: 192

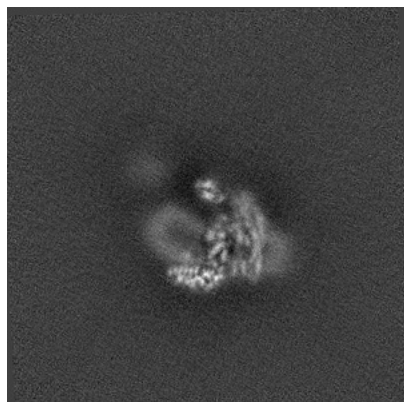


Y Index: 192

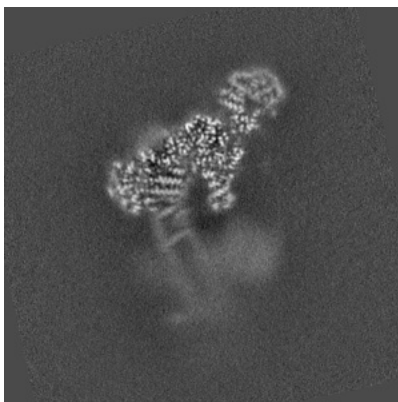


Z Index: 192

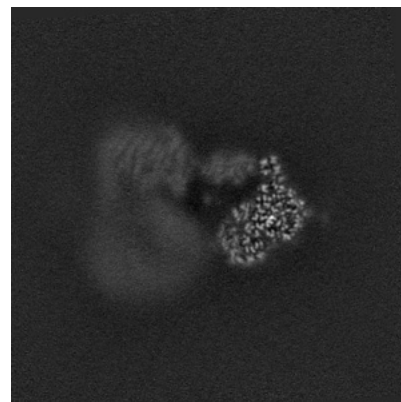
6.2.2 Raw map



X Index: 192



Y Index: 192

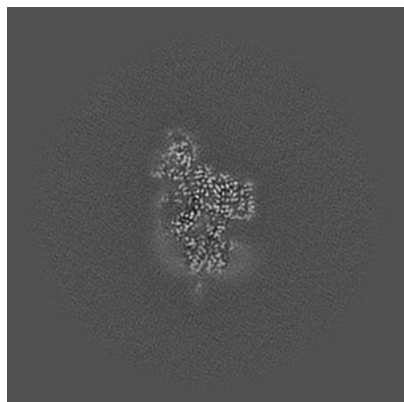


Z Index: 192

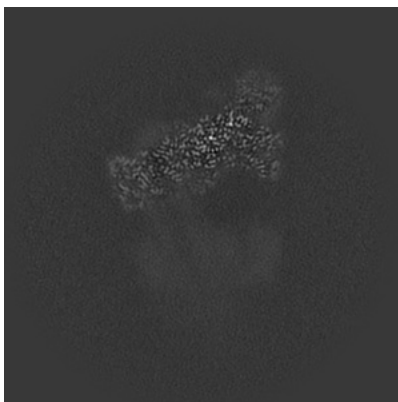
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

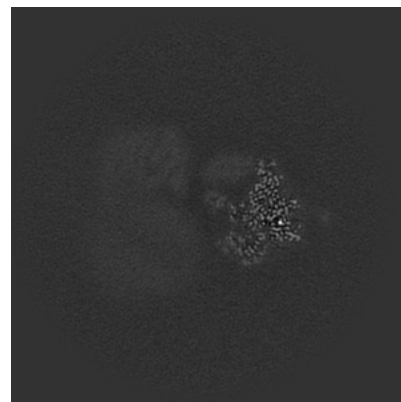
6.3.1 Primary map



X Index: 243

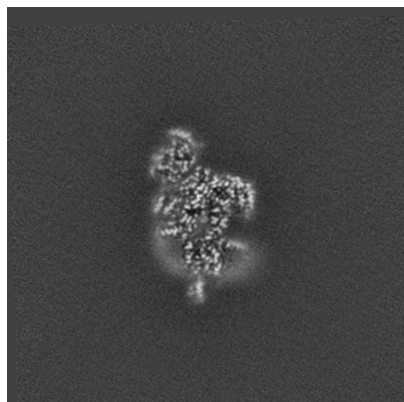


Y Index: 177

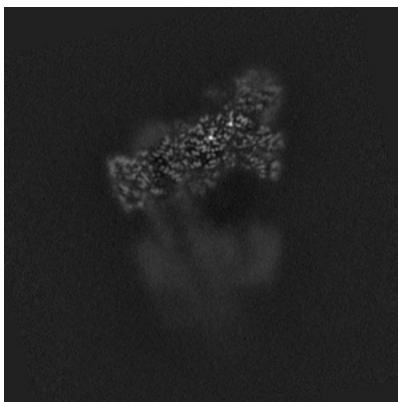


Z Index: 198

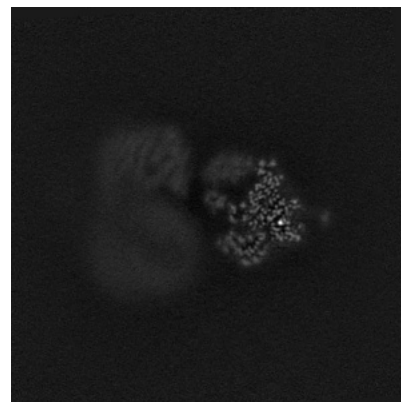
6.3.2 Raw map



X Index: 240



Y Index: 177

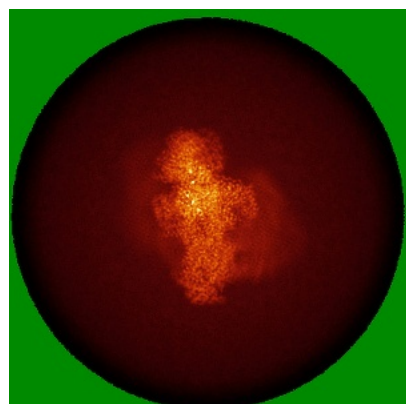


Z Index: 198

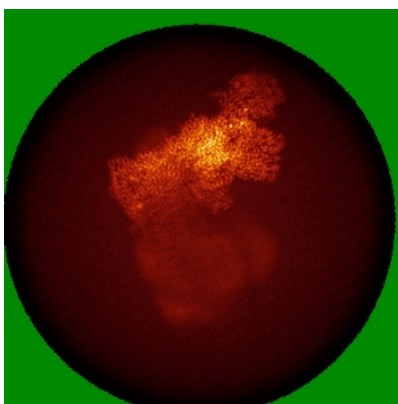
The images above show the largest variance slices of the map in three orthogonal directions.

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

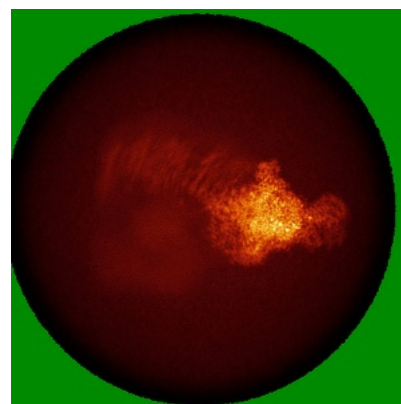
6.4.1 Primary map



X

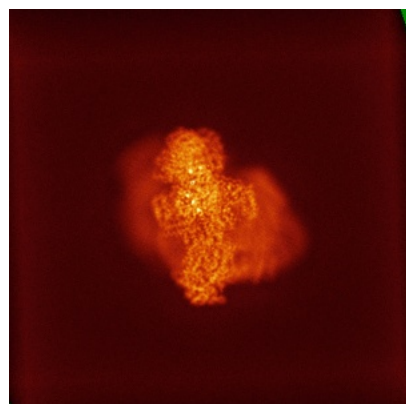


Y

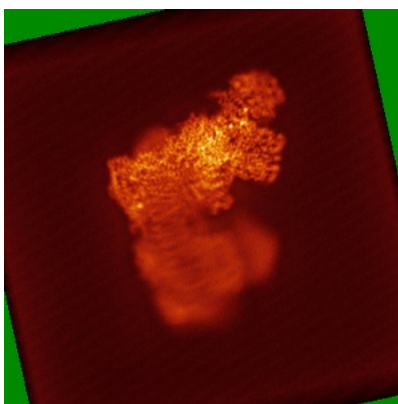


Z

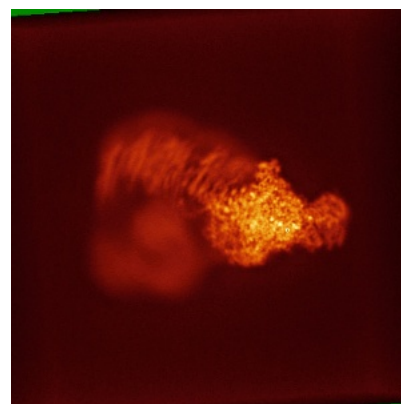
6.4.2 Raw map



X



Y

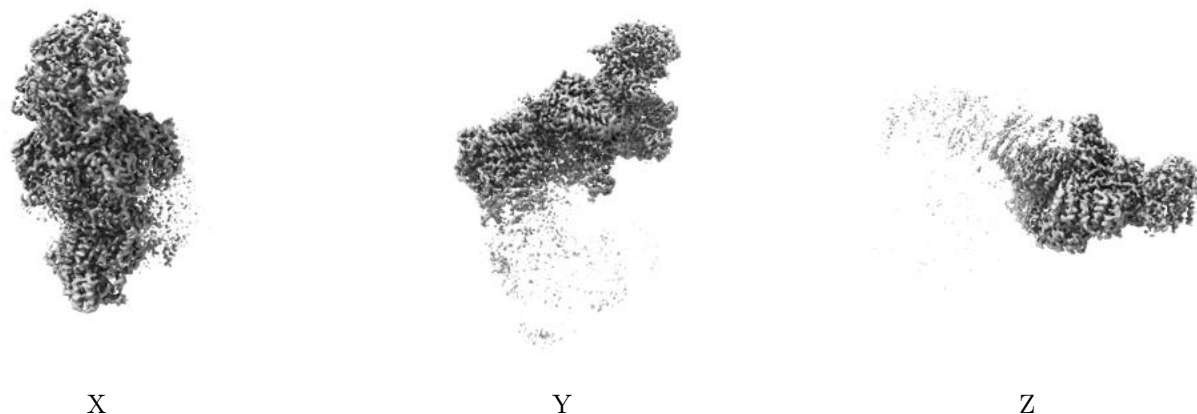


Z

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

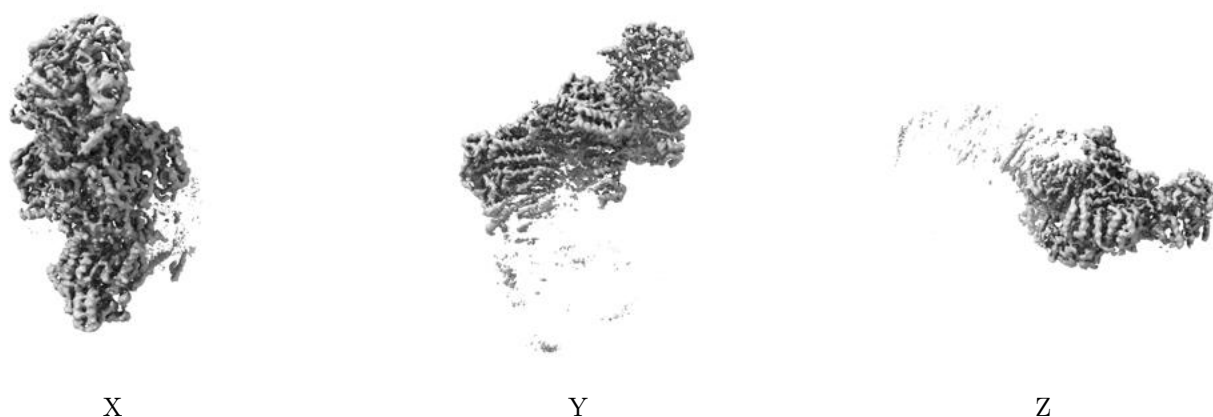
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

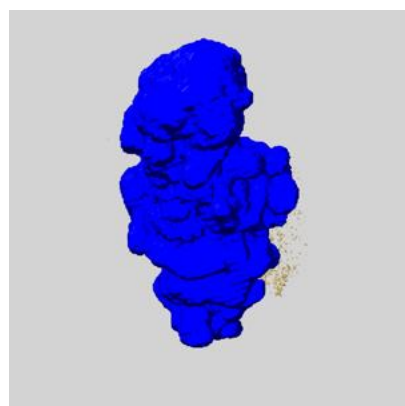
6.6 Mask visualisation [i](#)

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

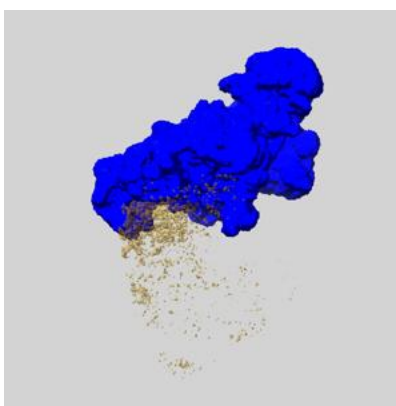
A mask typically either:

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

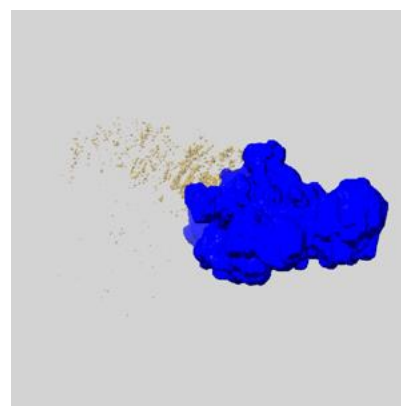
6.6.1 emd_35337_msk_1.map [i](#)



X



Y

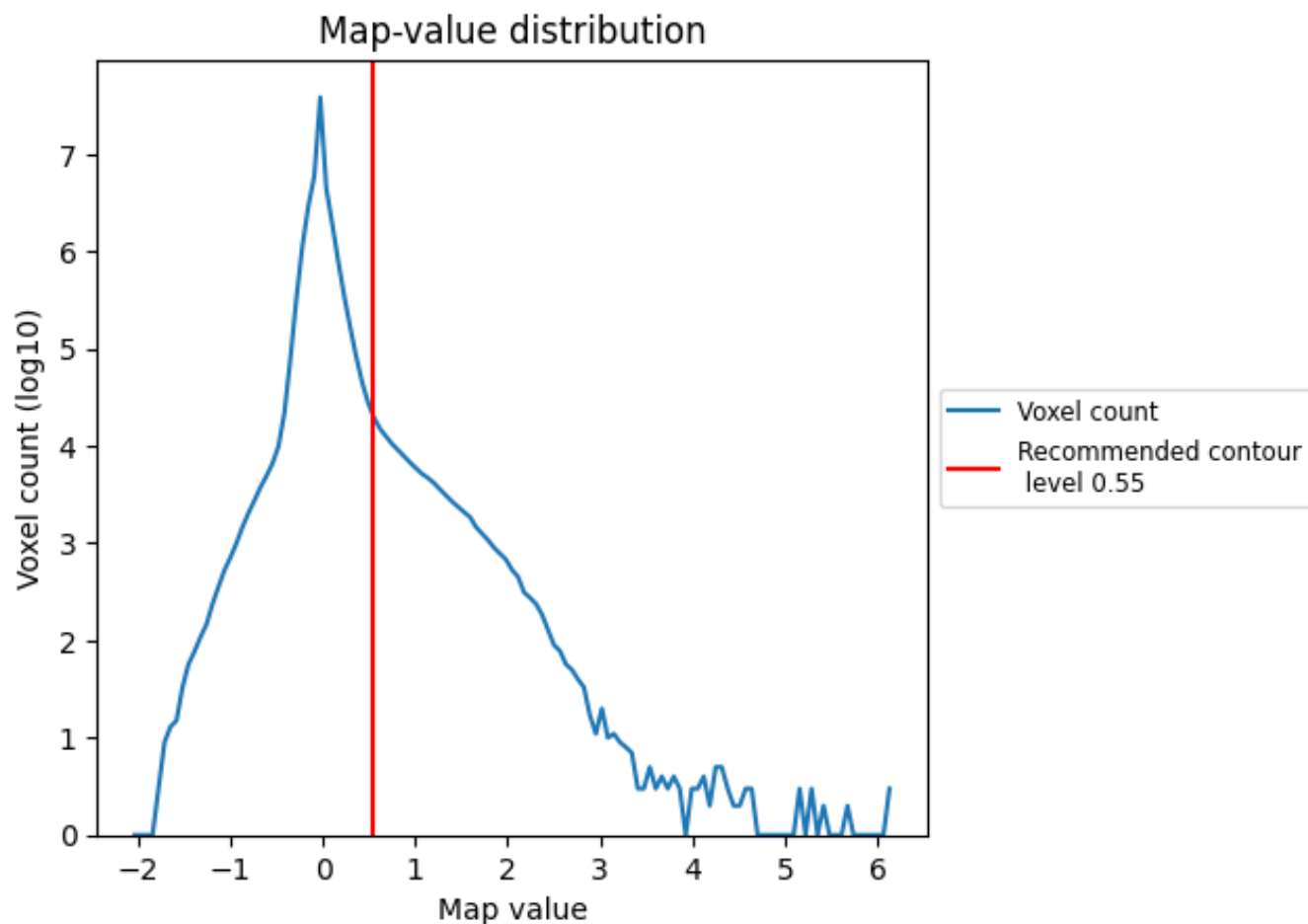


Z

7 Map analysis [i](#)

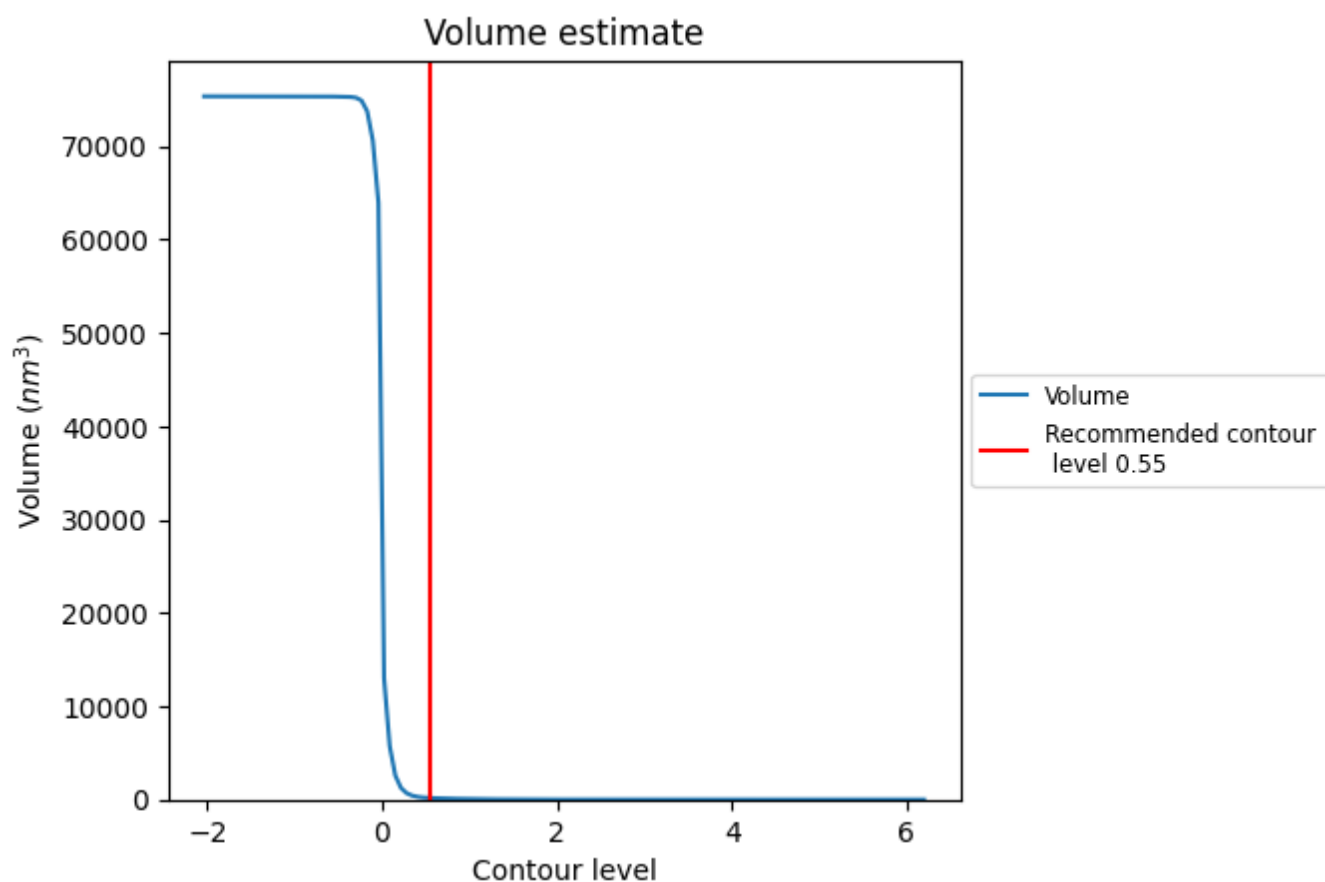
This section contains the results of statistical analysis of the map.

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.

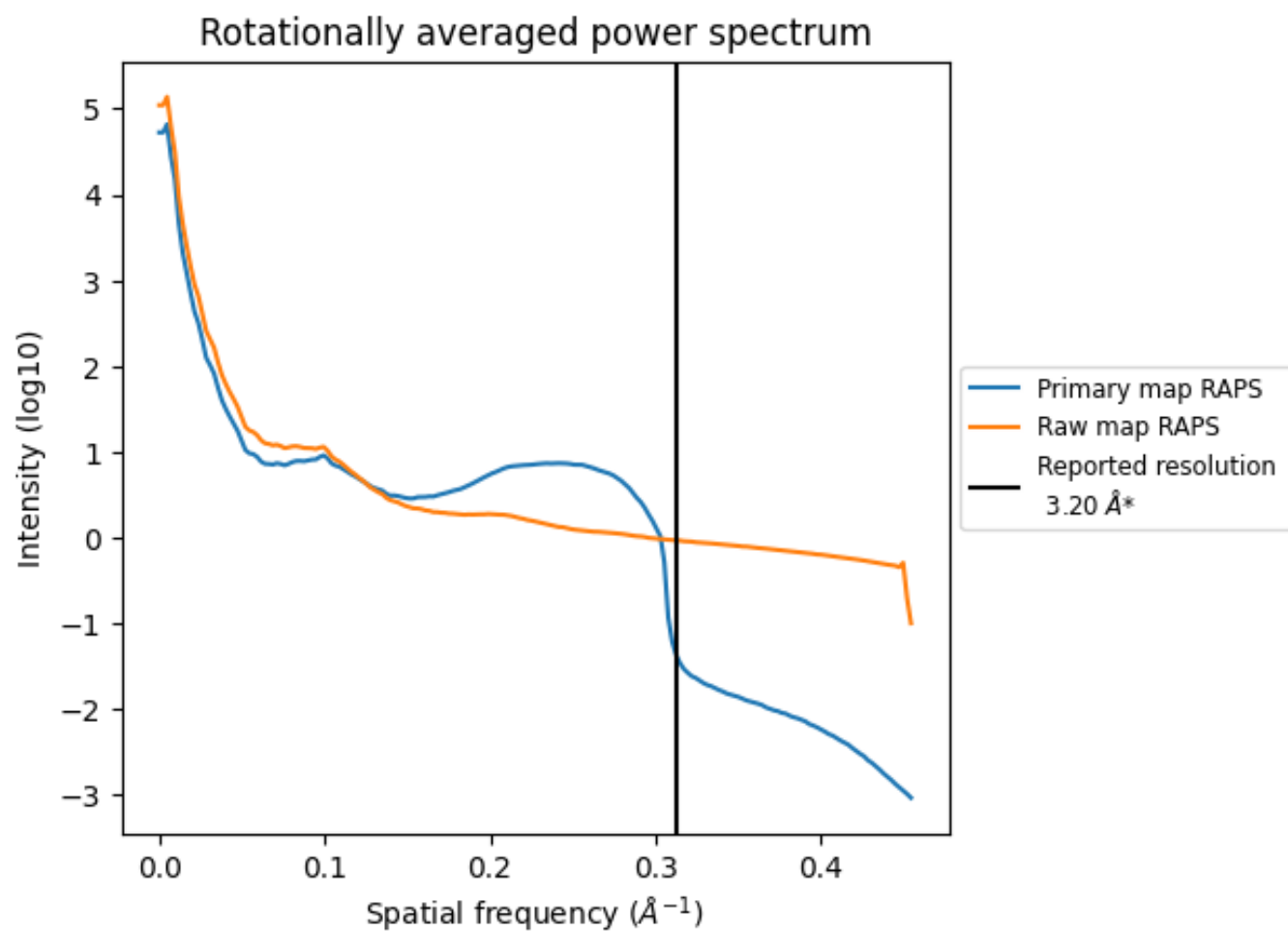
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170 nm^3 ; this corresponds to an approximate mass of 154 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

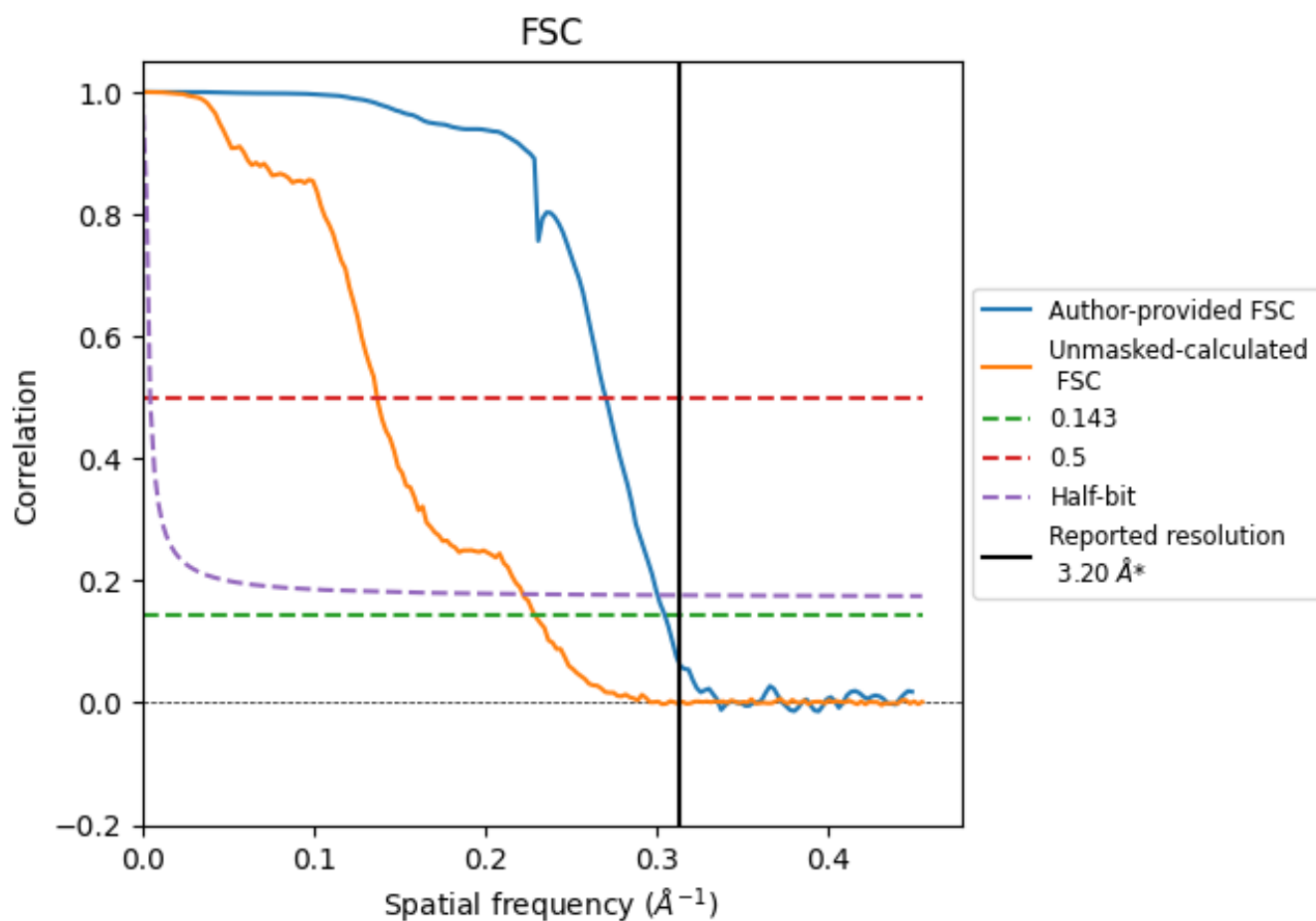


*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

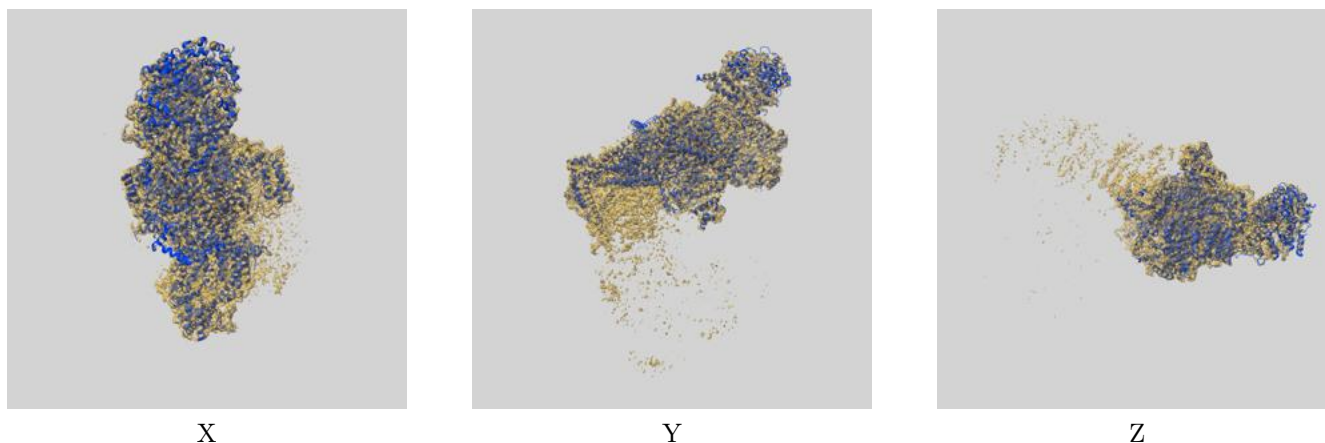
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.28	3.70	3.33
Unmasked-calculated*	4.37	7.30	4.51

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

9 Map-model fit [i](#)

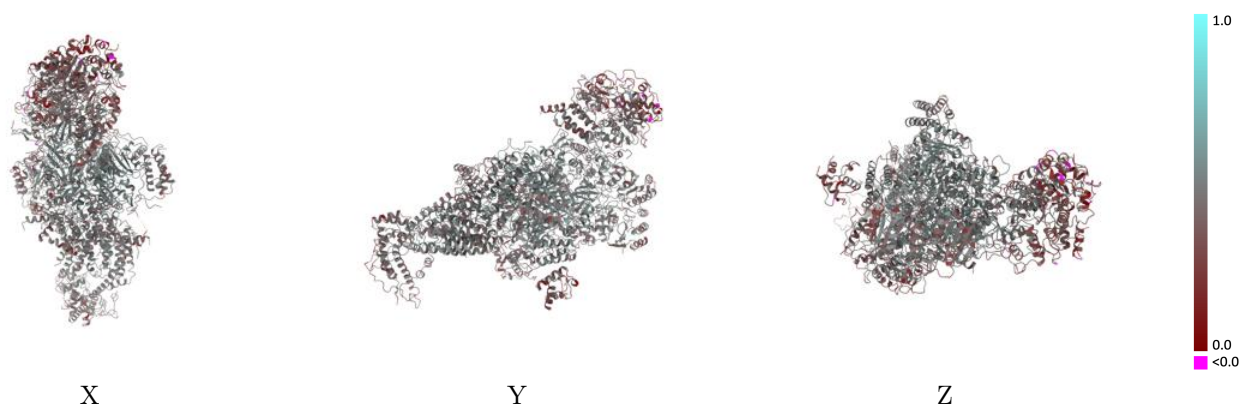
This section contains information regarding the fit between EMDB map EMD-35337 and PDB model 8IBA. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



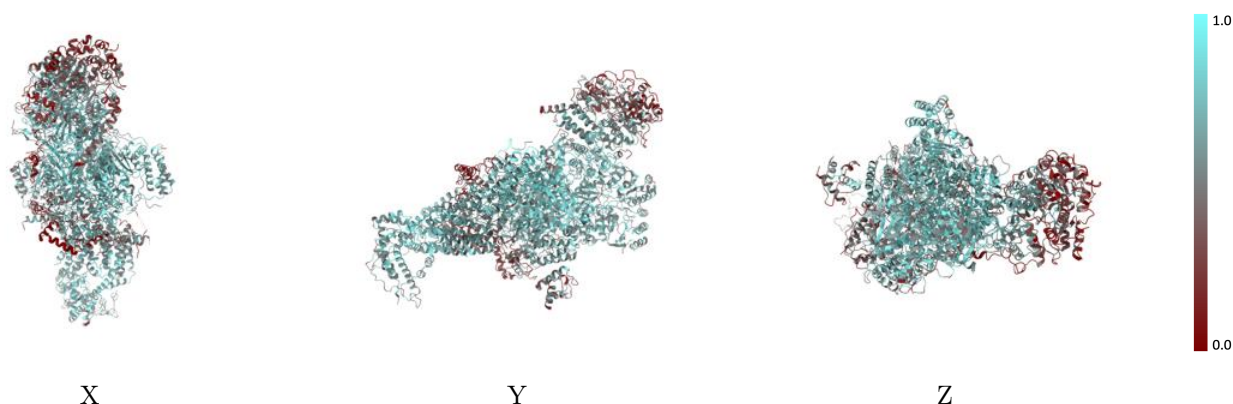
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



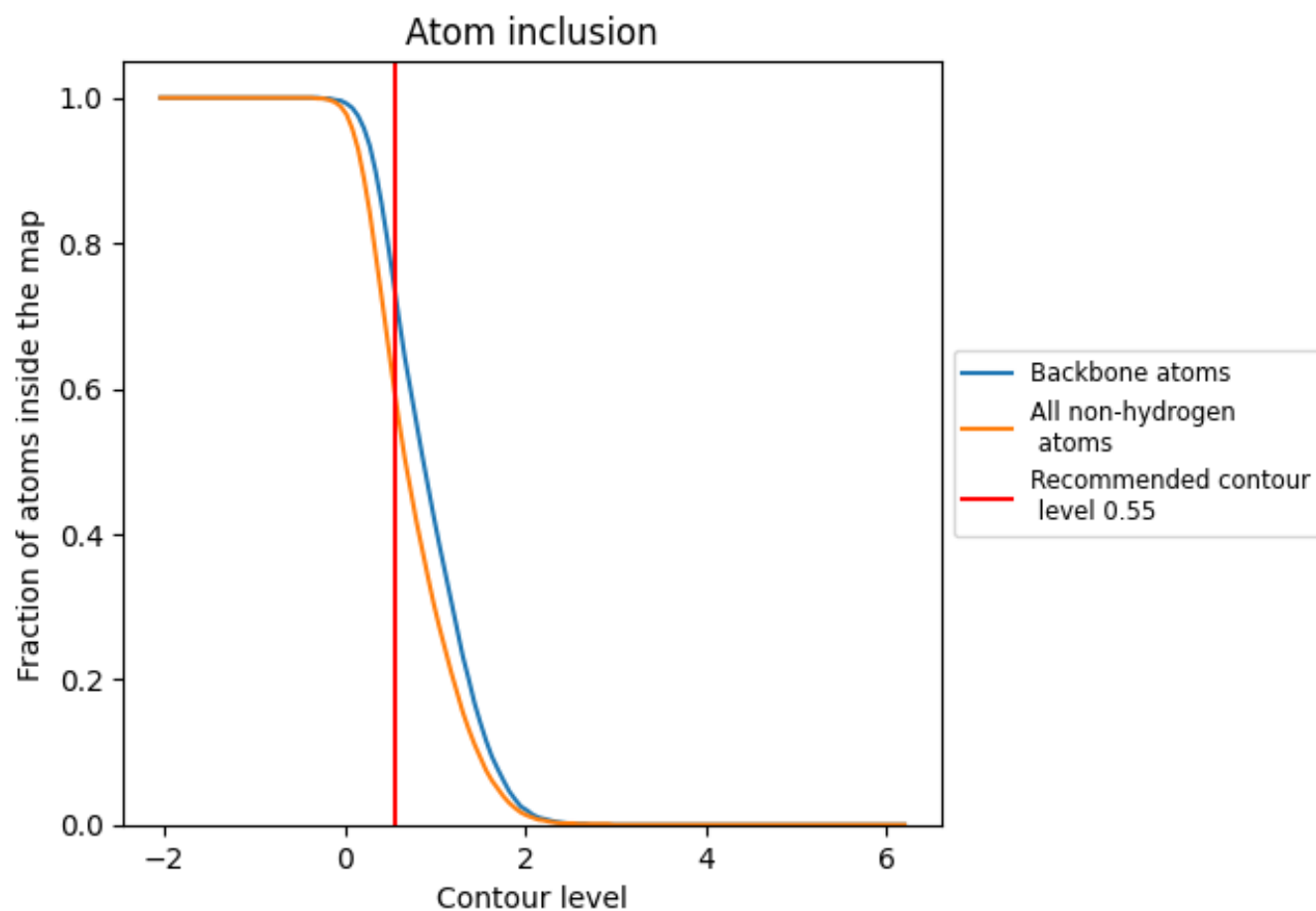
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.5990	 0.4370
A	 0.5650	 0.4640
B	 0.7370	 0.4980
C	 0.7680	 0.5140
D	 0.7580	 0.5070
E	 0.3540	 0.3420
F	 0.4400	 0.3620
G	 0.6890	 0.4530
H	 0.6620	 0.4670
I	 0.7400	 0.4870
P	 0.5020	 0.4000
Q	 0.6180	 0.4630
R	 0.2920	 0.4040
S	 0.6510	 0.4240
T	 0.4260	 0.3170
V	 0.6780	 0.4370
W	 0.6240	 0.4760
X	 0.6490	 0.4060
Z	 0.6430	 0.4130
a	 0.6810	 0.4630
b	 0.5870	 0.4180
q	 0.2640	 0.3900
r	 0.3270	 0.3930
s	 0.0450	 0.3360

