



Full wwPDB EM Validation Report ⓘ

Aug 7, 2026 – 03:44 AM JST

PDB ID : 8XNR / pdb_00008xnr
EMDB ID : EMD-38512
Title : Respiratory complex Peripheral Arm of CI, close form A, focus-refined map of type IB, Wild type mouse under Cold Acclimation
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-12-30
Resolution : 3.30 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:

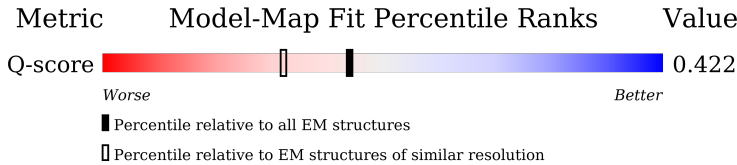
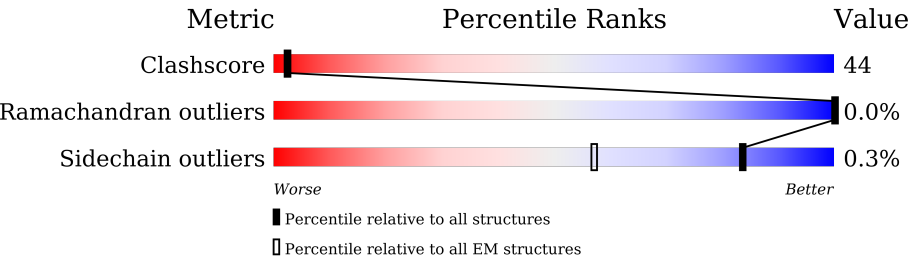
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 3.30 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	15087 (2.80 - 3.80)

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

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

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

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

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

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

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 33911 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	312	Total	C	N	O	S	0	0
			2495	1679	378	416	22		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

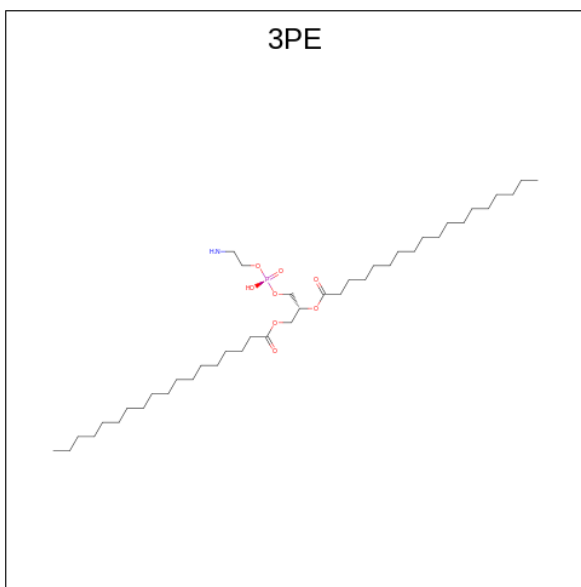
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

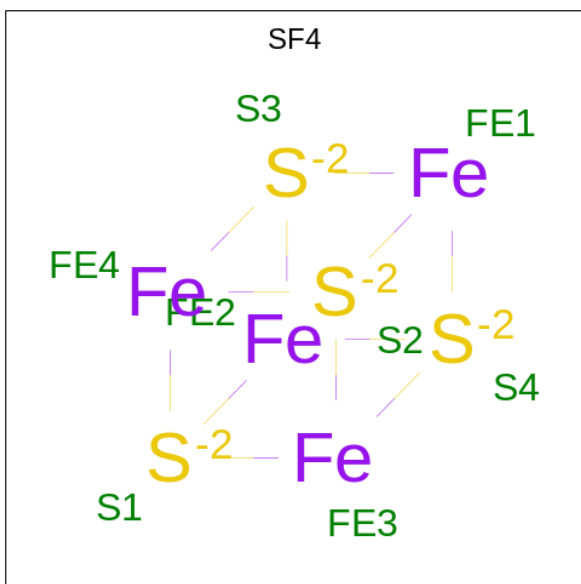
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	26	Total	C	N	O	0	0
			226	147	38	41		

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



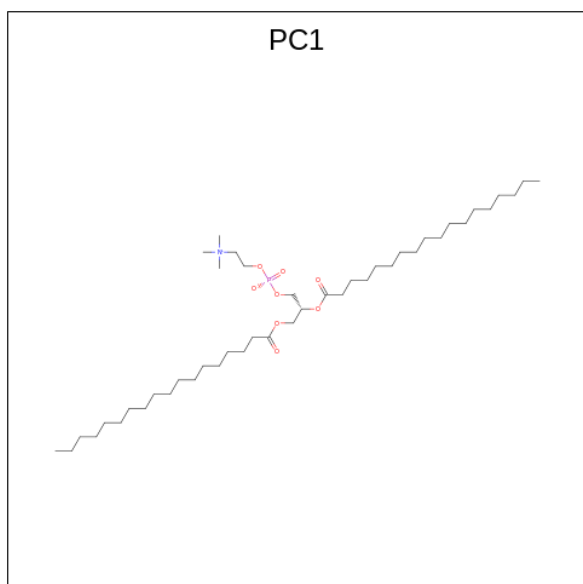
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	b	1	Total	C	N	O	P	0
			46	36	1	8	1	

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



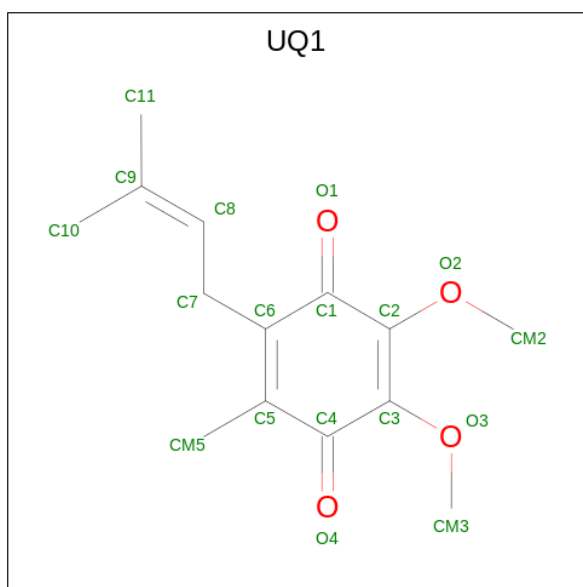
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	Fe	S	0
			8	4	4	
25	F	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	

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



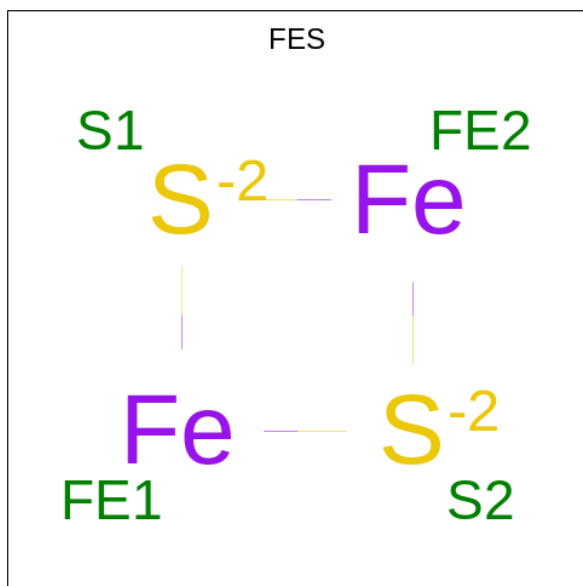
Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
26	I	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 27 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



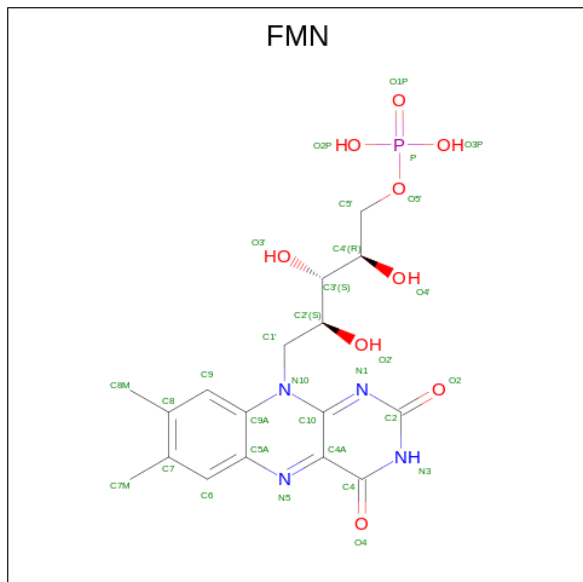
Mol	Chain	Residues	Atoms			AltConf
27	D	1	Total	C	O	0
			18	14	4	

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

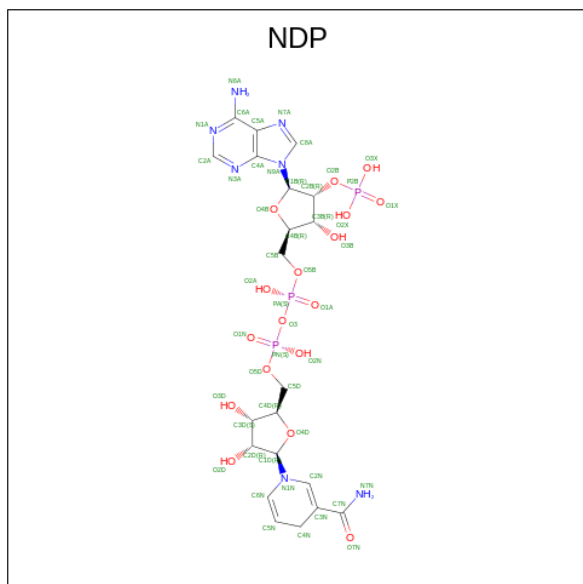


Mol	Chain	Residues	Atoms			AltConf
28	E	1	Total	Fe	S	0
			4	2	2	
28	G	1	Total	Fe	S	0
			4	2	2	

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



- 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).

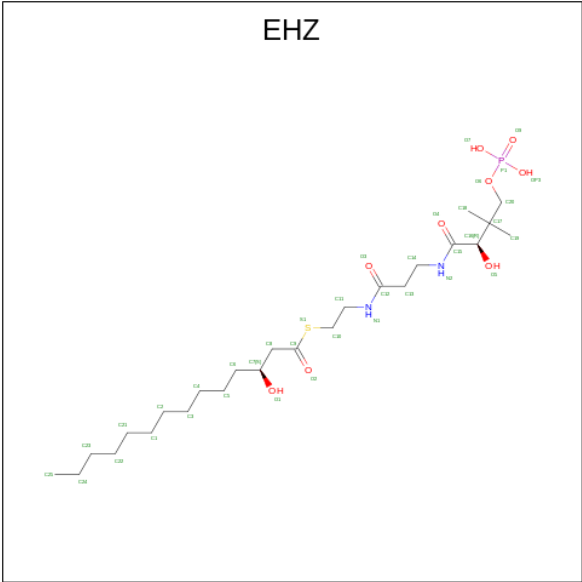


Mol	Chain	Residues	Atoms					AltConf
31	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

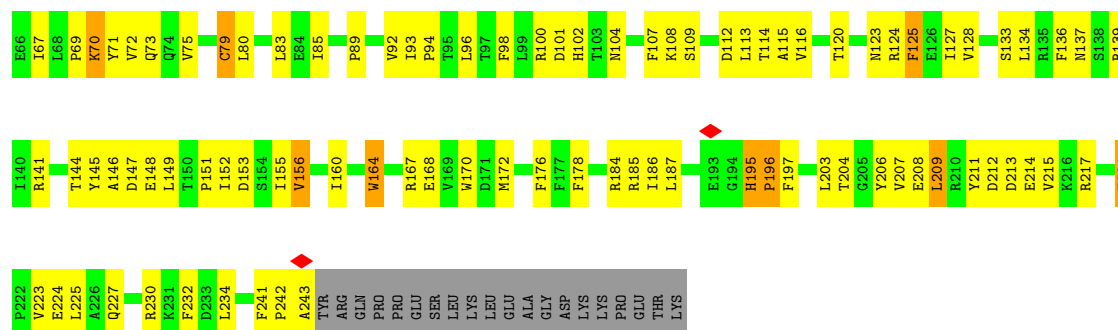
- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

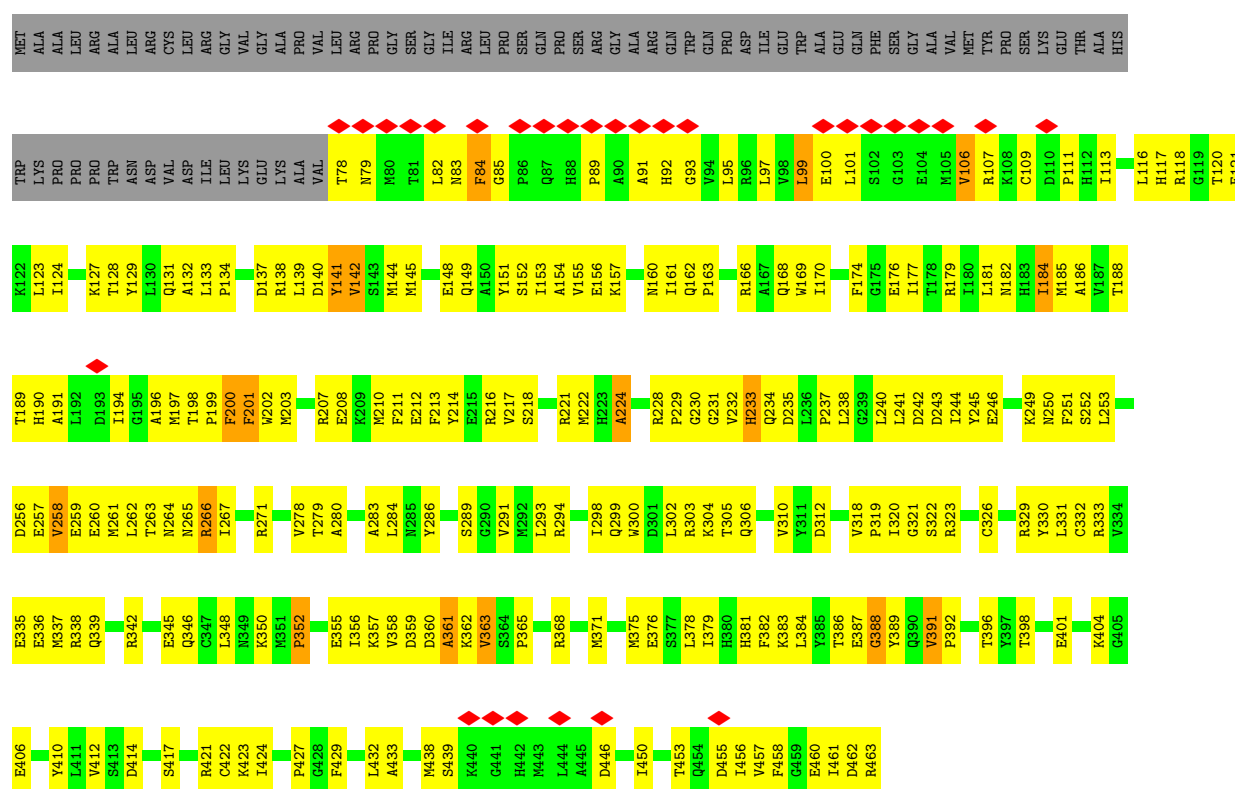
- Molecule 33 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EH3) (formula: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



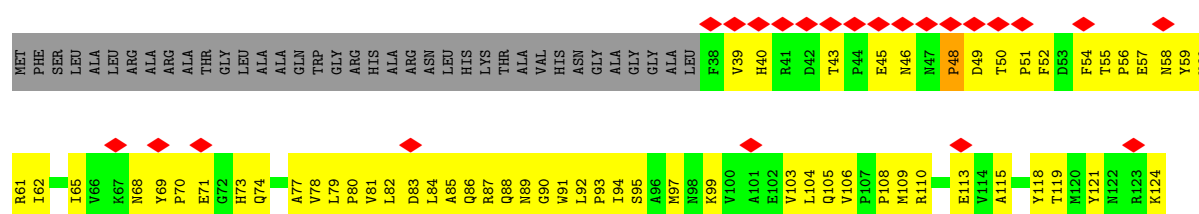
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
33	W	1	32	19	2	9	1	1	0

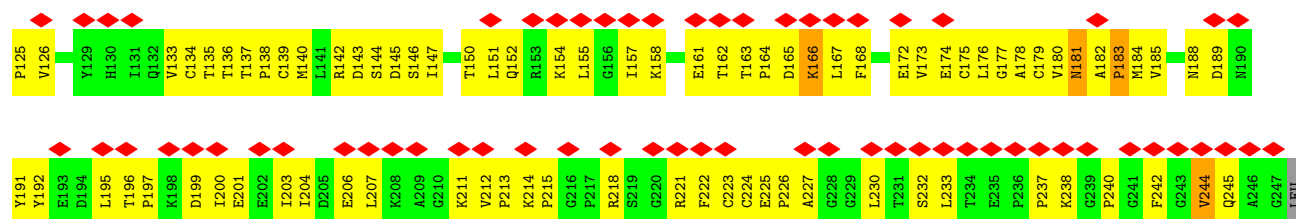


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

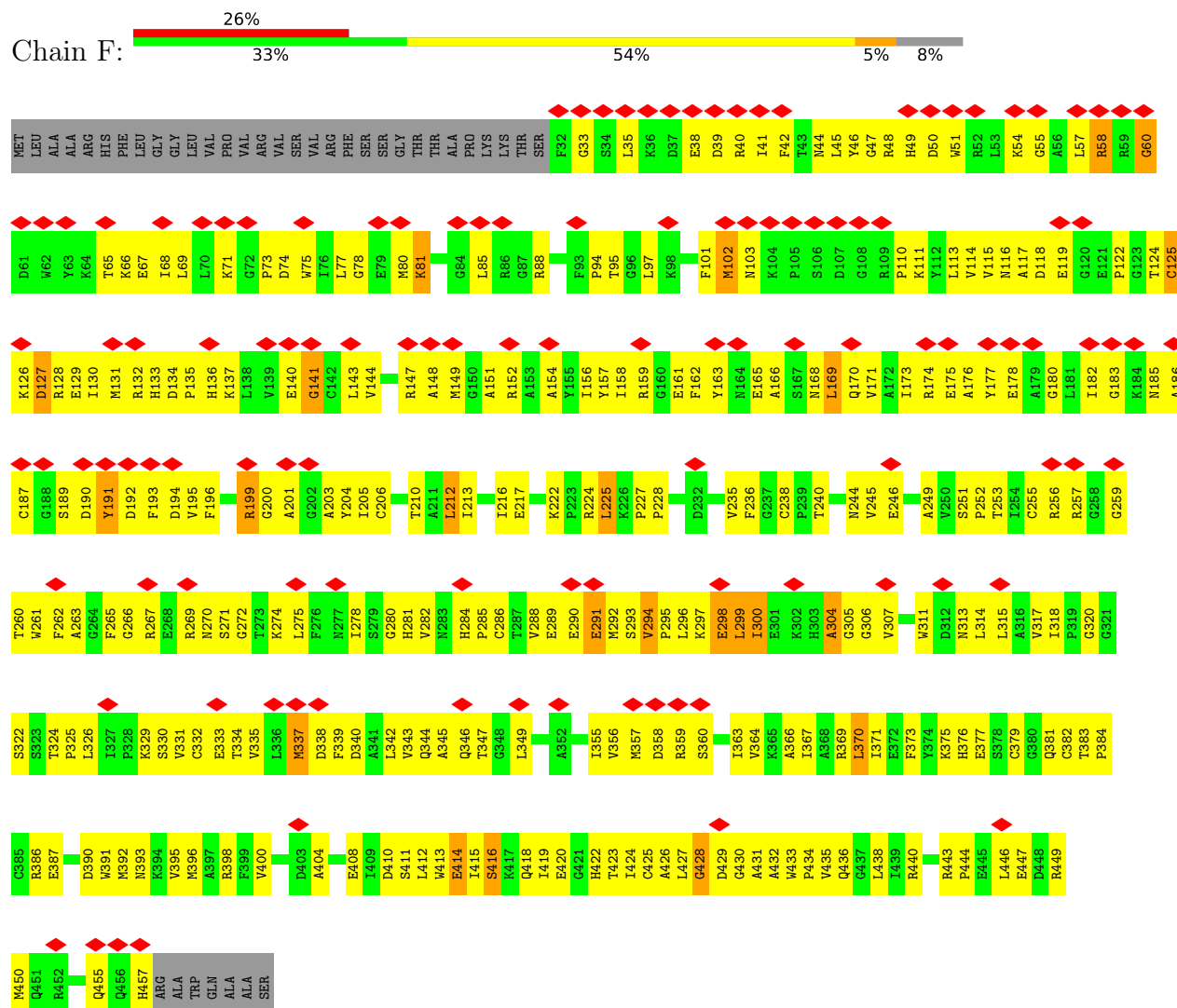


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

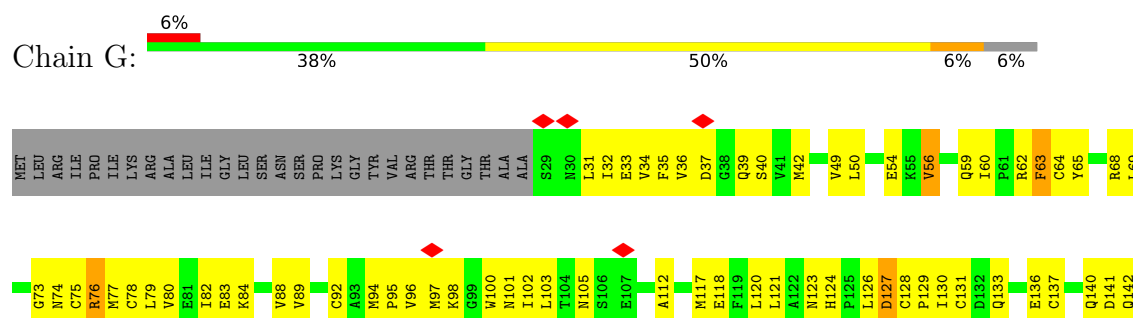


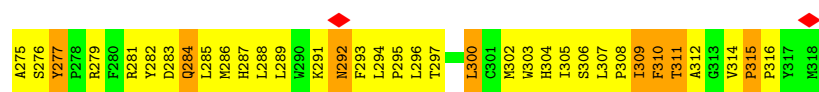


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

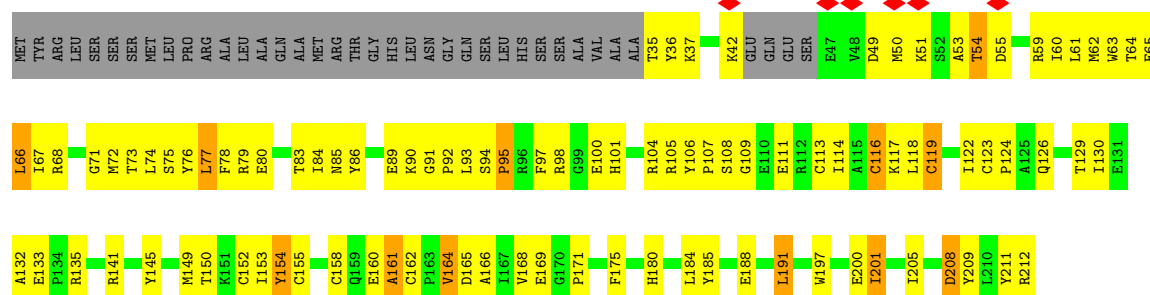


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

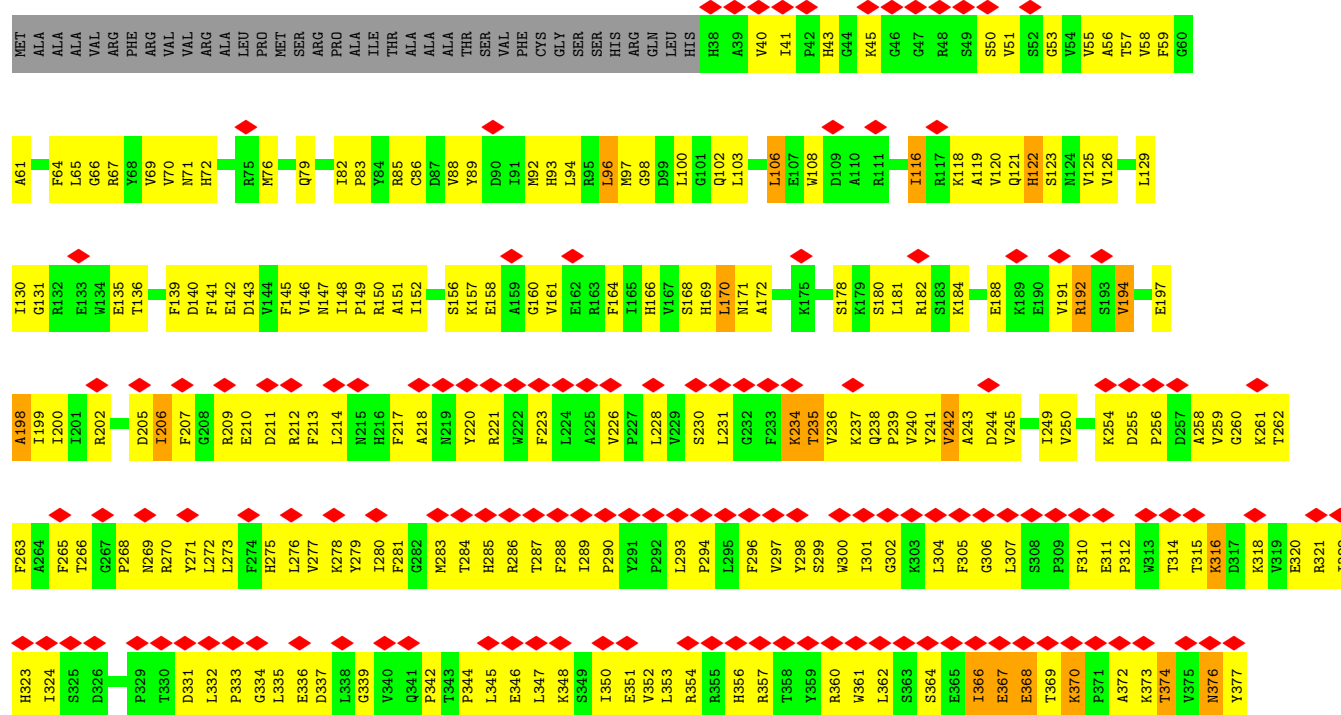




- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

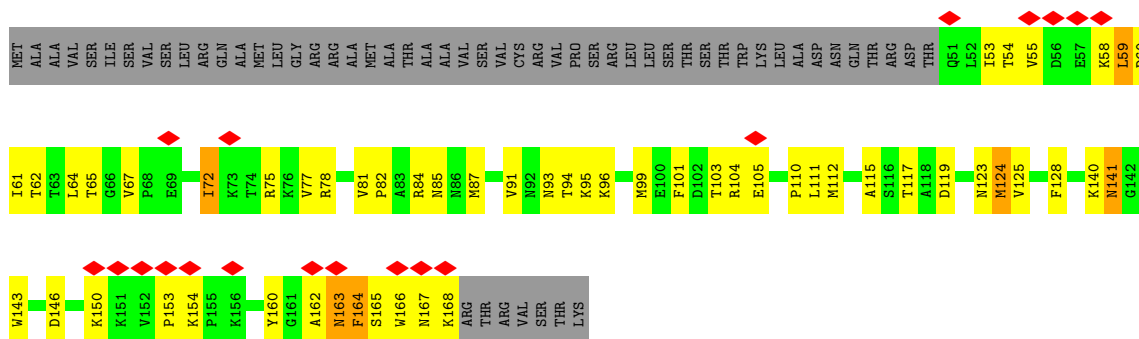


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

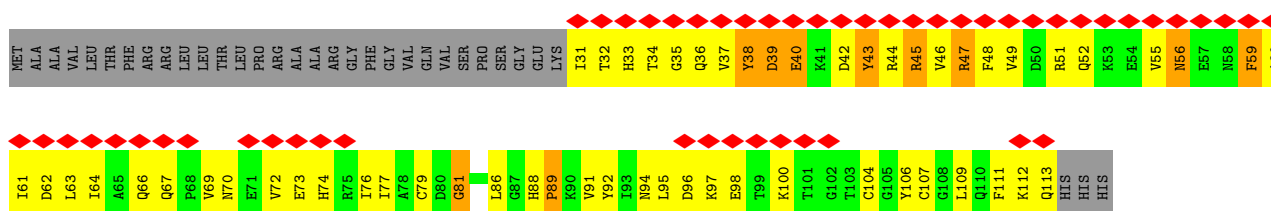
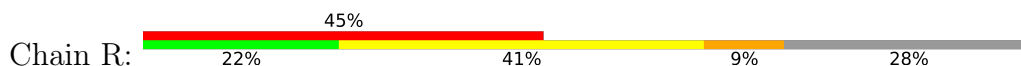


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

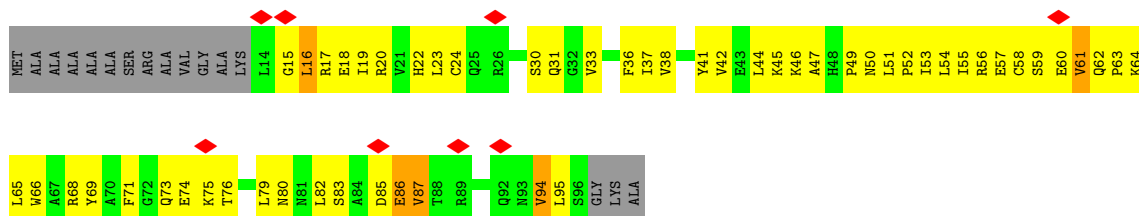




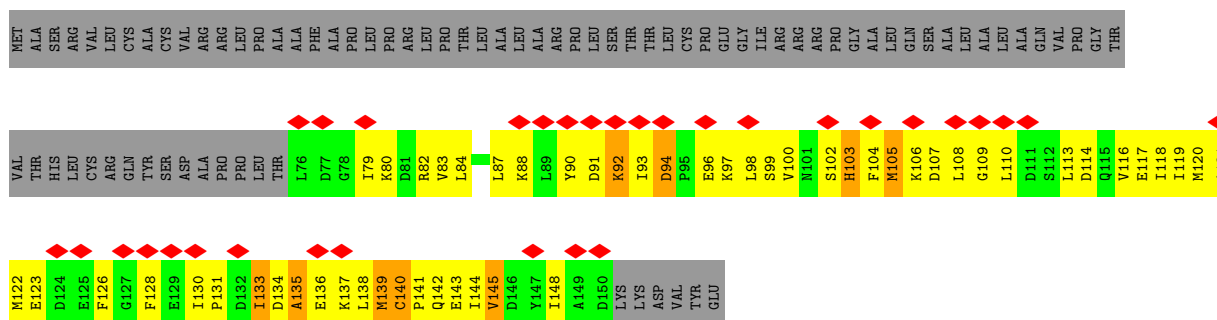
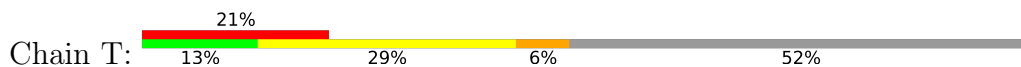
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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

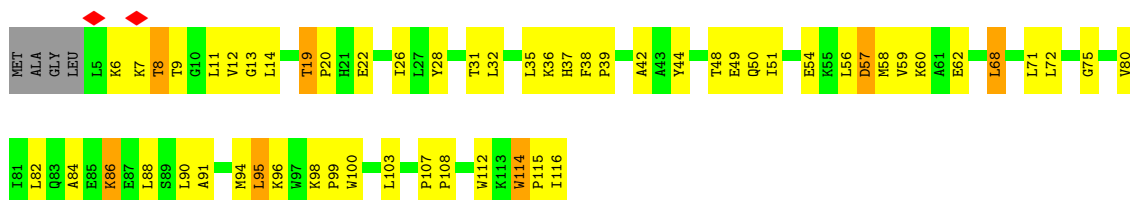


- Molecule 14: Acyl carrier protein, mitochondrial

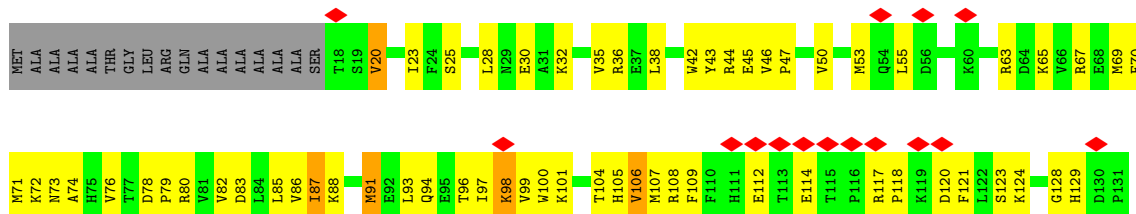


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

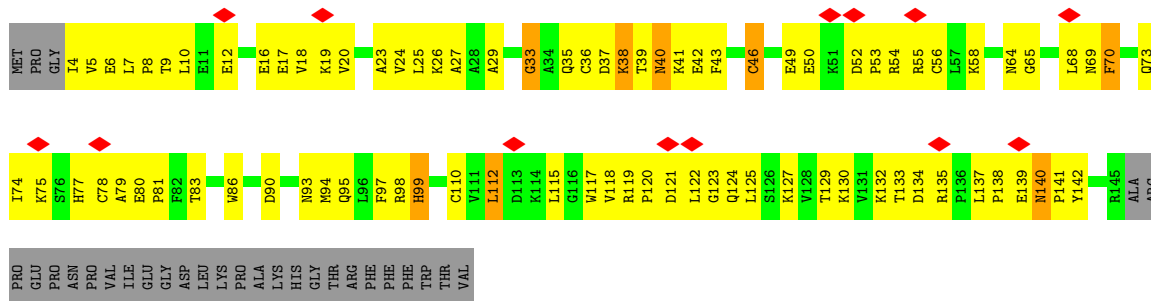




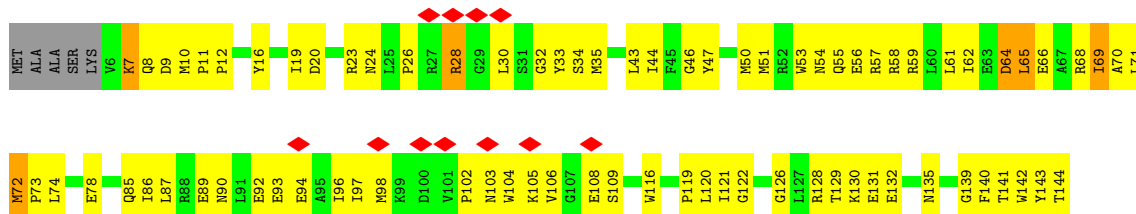
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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



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



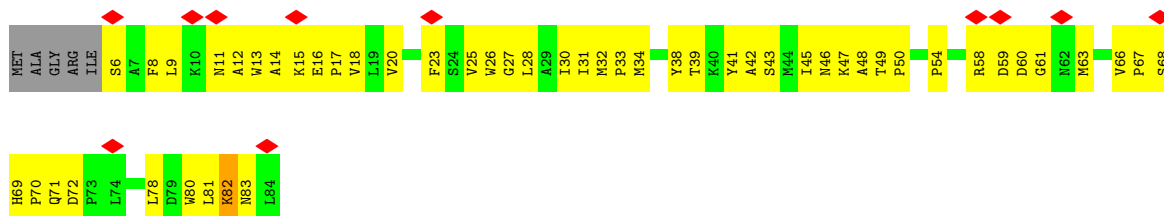
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



ASN
ILE
ASP

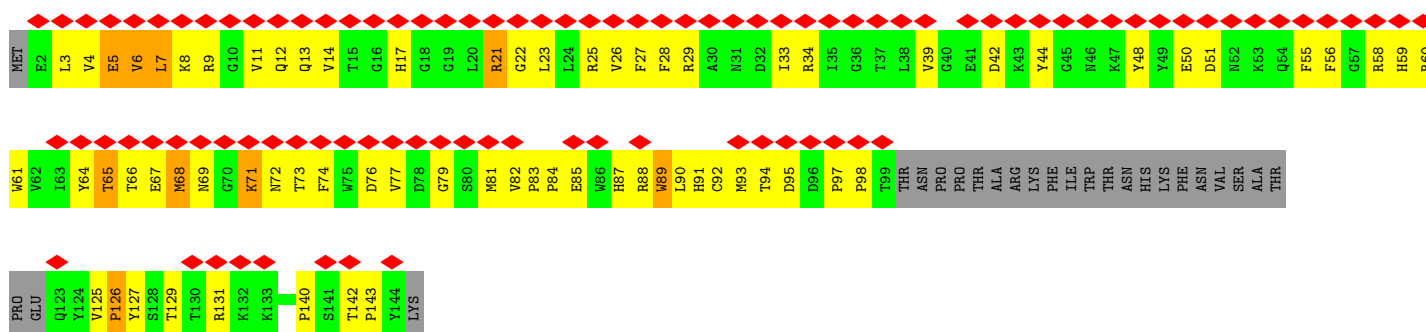
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b: 



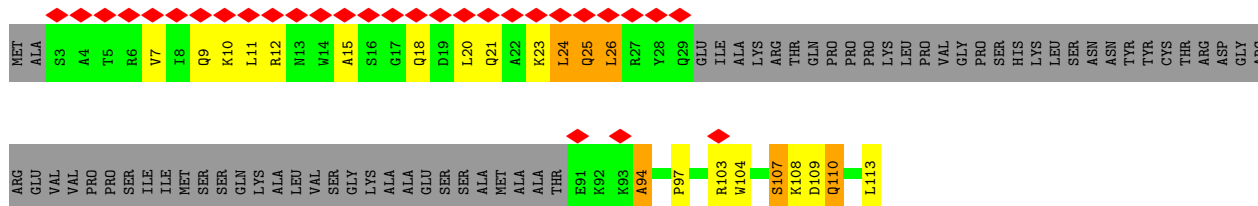
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q: 



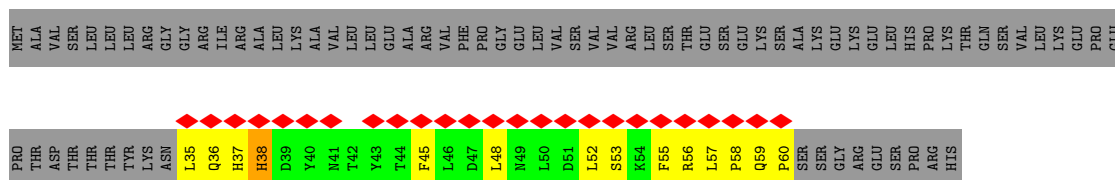
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r: 



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

Chain s: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48863	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	5.454	Depositor
Minimum map value	-1.421	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.087	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: PC1, ZN, UQ9, SF4, NDP, UQ1, FMN, FES, 3PE, EHZ

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	0.82	0/782	1.19	6/1066 (0.6%)
2	B	0.97	1/1278 (0.1%)	1.37	13/1730 (0.8%)
3	C	0.90	1/1687 (0.1%)	1.30	14/2297 (0.6%)
4	D	0.95	5/3169 (0.2%)	1.33	25/4286 (0.6%)
5	E	0.77	1/1675 (0.1%)	1.17	9/2282 (0.4%)
6	F	0.87	2/3363 (0.1%)	1.43	47/4543 (1.0%)
7	G	0.89	6/5374 (0.1%)	1.58	102/7281 (1.4%)
8	H	0.92	1/2570 (0.0%)	1.48	53/3509 (1.5%)
9	I	0.90	0/1427	1.52	19/1927 (1.0%)
10	P	0.77	1/2804 (0.0%)	1.22	27/3802 (0.7%)
11	Q	0.87	1/980 (0.1%)	1.28	12/1324 (0.9%)
12	R	0.87	4/671 (0.6%)	1.34	11/903 (1.2%)
13	S	0.85	0/678	1.44	10/915 (1.1%)
14	T	0.92	0/613	1.51	10/826 (1.2%)
15	V	0.86	0/937	1.46	14/1270 (1.1%)
16	W	0.84	1/993 (0.1%)	1.15	8/1335 (0.6%)
17	X	0.78	0/1191	1.34	18/1605 (1.1%)
18	Z	0.78	0/1183	1.22	13/1597 (0.8%)
19	a	0.87	0/553	1.21	4/745 (0.5%)
20	b	0.75	0/643	0.95	1/884 (0.1%)
21	q	0.88	1/1037 (0.1%)	1.34	15/1408 (1.1%)
22	r	0.88	1/421 (0.2%)	1.38	8/566 (1.4%)
23	s	0.43	0/233	0.75	1/317 (0.3%)
All	All	0.87	26/34262 (0.1%)	1.37	440/46418 (0.9%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	W	106	VAL	C-N	-8.76	1.22	1.34
12	R	39	ASP	CA-C	7.92	1.64	1.53
11	Q	53	ILE	C-O	7.84	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	40	GLU	N-CA	7.74	1.56	1.46
7	G	203	ASP	CA-C	6.74	1.62	1.52
7	G	600	GLU	CA-C	6.55	1.61	1.52
4	D	106	VAL	C-N	-6.46	1.24	1.33
4	D	266	ARG	C-O	-6.31	1.16	1.24
7	G	127	ASP	CA-C	6.26	1.62	1.52
7	G	76	ARG	CA-C	6.11	1.61	1.53
2	B	110	PRO	C-O	-6.07	1.16	1.24
5	E	93	PRO	N-CD	-5.91	1.39	1.47
7	G	361	VAL	CA-C	5.86	1.60	1.52
22	r	25	GLN	CA-C	5.81	1.60	1.52
8	H	60	PRO	N-CD	5.80	1.55	1.47
6	F	225	LEU	C-O	5.76	1.31	1.23
12	R	59	PHE	CA-C	-5.70	1.45	1.52
4	D	392	PRO	C-O	-5.56	1.20	1.24
4	D	107	ARG	C-N	5.54	1.40	1.33
6	F	414	GLU	C-O	-5.51	1.17	1.24
7	G	683	PRO	N-CD	-5.42	1.40	1.47
21	q	126	PRO	N-CD	5.37	1.55	1.47
10	P	235	THR	CA-C	5.30	1.59	1.53
4	D	266	ARG	CA-C	-5.22	1.45	1.52
12	R	89	PRO	N-CD	-5.03	1.40	1.47
3	C	61	GLY	C-N	-5.01	1.27	1.33

All (440) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	174	THR	N-CA-C	-16.86	89.01	114.64
6	F	125	CYS	N-CA-C	-15.61	93.50	113.17
7	G	251	ILE	N-CA-C	13.34	126.85	108.17
7	G	77	MET	N-CA-C	-13.06	97.32	113.38
7	G	500	ILE	N-CA-C	-12.52	98.76	110.53
10	P	106	LEU	N-CA-C	12.19	128.70	109.07
6	F	171	VAL	N-CA-C	-11.85	99.39	110.53
6	F	449	ARG	N-CA-C	-11.63	98.68	111.36
7	G	204	MET	N-CA-C	-11.61	91.48	109.25
11	Q	60	ASP	N-CA-C	-11.32	90.34	109.24
7	G	599	THR	N-CA-C	11.27	126.12	112.38
16	W	87	ILE	N-CA-C	-11.10	99.76	110.42
15	V	57	ASP	N-CA-C	-11.00	99.30	111.07
8	H	259	PHE	N-CA-C	-11.00	99.37	111.36
9	I	164	VAL	N-CA-C	-10.58	100.20	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	77	LEU	N-CA-C	-10.51	99.62	111.71
14	T	139	MET	N-CA-C	-10.40	97.45	113.89
2	B	195	PRO	N-CA-C	-10.35	98.07	110.70
7	G	280	ASP	N-CA-C	10.32	122.53	111.28
4	D	337	MET	N-CA-C	-10.18	100.18	111.07
10	P	366	ILE	N-CA-C	10.16	120.99	110.62
19	a	4	GLU	N-CA-C	10.15	124.77	112.38
7	G	414	PHE	N-CA-C	-10.11	101.44	113.88
9	I	161	ALA	N-CA-C	10.11	122.30	111.28
14	T	135	ALA	N-CA-C	-10.06	100.31	111.28
7	G	325	ARG	N-CA-C	-9.85	100.24	110.97
9	I	166	ALA	N-CA-C	-9.84	100.81	113.12
6	F	178	GLU	N-CA-C	-9.82	99.32	111.11
6	F	103	ASN	N-CA-C	-9.80	101.01	113.16
6	F	141	GLY	N-CA-C	-9.77	101.17	112.50
6	F	144	VAL	N-CA-C	-9.73	101.39	110.53
7	G	654	VAL	N-CA-C	9.73	123.25	111.09
7	G	337	ALA	N-CA-C	-9.59	100.78	114.12
8	H	52	ALA	N-CA-C	-9.58	100.82	111.07
6	F	418	GLN	N-CA-C	-9.58	100.80	111.14
17	X	70	PHE	N-CA-C	-9.51	99.70	111.11
12	R	38	TYR	N-CA-C	-9.45	96.35	110.24
4	D	427	PRO	N-CA-C	-9.42	95.70	110.50
17	X	112	LEU	N-CA-C	-9.41	100.98	111.14
14	T	133	ILE	N-CA-C	9.29	119.83	110.82
7	G	692	LYS	N-CA-C	-9.29	100.52	112.23
7	G	694	PHE	N-CA-C	9.29	121.40	111.28
10	P	367	GLU	N-CA-C	9.26	122.56	111.82
10	P	369	THR	N-CA-CB	9.24	123.48	110.17
18	Z	69	ILE	N-CA-C	-9.20	100.70	110.36
7	G	640	ASP	N-CA-C	-9.18	101.35	111.36
7	G	389	THR	N-CA-C	-9.14	96.25	109.96
5	E	85	ALA	N-CA-C	-9.11	101.43	111.36
19	a	57	VAL	N-CA-C	-9.00	105.16	113.71
7	G	133	GLN	N-CA-CB	8.80	121.55	110.45
7	G	212	LYS	N-CA-C	-8.79	94.58	108.90
8	H	60	PRO	N-CA-CB	8.67	108.55	102.65
8	H	200	LEU	N-CA-C	-8.67	103.55	114.56
9	I	154	TYR	N-CA-CB	-8.67	99.22	111.62
7	G	365	ASN	N-CA-C	-8.66	102.26	112.92
16	W	20	VAL	N-CA-C	8.66	120.75	108.36
10	P	96	LEU	N-CA-C	8.65	121.66	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	142	VAL	N-CA-C	-8.55	102.08	110.72
10	P	373	LYS	N-CA-C	8.50	121.91	110.35
3	C	70	LYS	N-CA-C	8.50	121.61	111.33
13	S	18	GLU	N-CA-C	8.49	123.24	109.40
13	S	86	GLU	N-CA-C	-8.49	102.11	111.36
16	W	100	TRP	N-CA-C	-8.46	99.86	112.04
8	H	141	SER	N-CA-C	-8.44	102.03	111.07
3	C	108	LYS	N-CA-C	8.40	120.06	111.07
17	X	99	HIS	N-CA-C	-8.38	102.23	111.36
7	G	452	LEU	N-CA-C	-8.31	102.22	111.28
11	Q	54	THR	N-CA-C	8.31	123.25	109.46
7	G	558	GLN	N-CA-C	-8.26	102.23	111.07
8	H	311	THR	N-CA-C	-8.24	102.53	112.59
8	H	196	ALA	N-CA-C	8.20	127.94	109.81
6	F	298	GLU	N-CA-C	8.20	120.21	111.28
3	C	196	PRO	N-CA-C	8.17	124.88	113.53
7	G	691	ILE	N-CA-C	8.16	123.65	111.89
16	W	96	THR	N-CA-C	-8.16	102.33	111.14
6	F	191	TYR	N-CA-C	8.15	121.73	110.24
7	G	534	VAL	N-CA-C	-8.13	104.67	111.91
1	A	64	LEU	N-CA-C	-8.13	102.38	111.07
7	G	484	ASP	N-CA-C	8.10	121.02	111.71
15	V	86	LYS	N-CA-C	-8.08	102.42	111.14
13	S	76	THR	N-CA-C	8.05	122.02	108.90
7	G	500	ILE	N-CA-CB	8.04	120.86	110.57
9	I	201	ILE	N-CA-C	-8.02	102.62	110.72
16	W	98	LYS	N-CA-C	-8.00	101.56	113.72
17	X	43	PHE	N-CA-C	-8.00	102.51	111.07
2	B	110	PRO	N-CA-C	7.99	124.44	113.65
8	H	271	LEU	N-CA-C	-7.99	102.51	111.14
1	A	9	ILE	N-CA-C	-7.98	102.48	110.62
21	q	67	GLU	CB-CA-C	-7.96	99.57	112.06
17	X	46	CYS	N-CA-C	-7.95	102.69	111.36
7	G	651	PRO	CB-CA-C	-7.94	98.46	111.56
10	P	206	ILE	N-CA-C	7.93	120.93	108.87
15	V	6	LYS	N-CA-C	-7.87	100.14	110.53
8	H	311	THR	N-CA-CB	7.84	123.47	110.92
9	I	160	GLU	N-CA-C	7.83	124.21	111.37
7	G	270	VAL	N-CA-CB	-7.82	100.69	110.31
10	P	235	THR	CB-CA-C	-7.82	100.03	112.07
7	G	389	THR	N-CA-CB	7.80	121.48	109.85
17	X	58	LYS	N-CA-C	-7.80	102.73	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	74	LEU	N-CA-C	-7.76	102.82	111.28
8	H	253	GLU	N-CA-C	7.72	121.96	112.54
12	R	47	ARG	N-CA-C	7.71	120.66	111.33
6	F	58	ARG	N-CA-C	-7.68	102.99	111.36
21	q	44	TYR	N-CA-C	-7.68	98.92	110.28
21	q	89	TRP	N-CA-C	-7.65	102.88	111.14
2	B	153	PRO	CB-CA-C	-7.63	98.96	111.56
7	G	56	VAL	N-CA-C	-7.61	103.03	110.72
4	D	361	ALA	N-CA-C	-7.61	103.10	112.38
7	G	569	GLN	N-CA-C	7.57	121.94	108.24
12	R	74	HIS	N-CA-C	7.54	121.13	110.50
6	F	171	VAL	N-CA-CB	7.54	120.22	110.57
9	I	119	CYS	N-CA-C	-7.52	103.16	111.36
7	G	277	MET	N-CA-C	7.51	120.64	109.59
7	G	467	LYS	N-CA-C	-7.49	102.27	111.33
2	B	183	ARG	N-CA-C	-7.49	104.39	113.97
8	H	223	PHE	CB-CA-C	-7.48	99.14	110.88
9	I	158	CYS	N-CA-C	-7.47	103.14	111.28
7	G	510	TRP	N-CA-CB	7.42	120.91	109.85
4	D	350	LYS	CB-CA-C	-7.42	100.94	111.85
6	F	430	GLY	N-CA-C	7.40	121.61	112.73
4	D	99	LEU	N-CA-C	7.39	120.97	109.07
7	G	303	THR	N-CA-C	7.37	122.98	113.18
12	R	39	ASP	N-CA-C	7.36	121.26	110.59
15	V	57	ASP	N-CA-CB	7.35	120.67	110.01
8	H	309	ILE	N-CA-C	7.33	117.41	110.30
13	S	94	VAL	N-CA-C	7.30	117.43	110.42
7	G	384	ASN	N-CA-C	-7.29	103.36	111.82
7	G	661	GLU	N-CA-C	7.29	118.91	110.97
3	C	195	HIS	CB-CA-C	7.27	117.36	110.17
8	H	50	ALA	N-CA-C	7.26	118.84	111.07
7	G	374	THR	CB-CA-C	-7.25	99.83	111.28
10	P	370	LYS	N-CA-C	7.25	119.31	109.24
14	T	105	MET	N-CA-C	7.24	119.25	111.36
8	H	139	THR	N-CA-CB	7.20	120.45	110.01
8	H	254	LEU	N-CA-C	-7.16	103.52	111.82
15	V	68	LEU	N-CA-C	-7.13	103.51	111.28
7	G	497	VAL	N-CA-C	-7.13	103.35	110.62
6	F	81	LYS	N-CA-C	-7.12	103.59	111.36
7	G	461	SER	N-CA-C	7.12	119.94	111.33
6	F	73	PRO	N-CA-C	-7.11	103.87	113.40
7	G	465	VAL	N-CA-CB	7.10	118.39	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	217	GLU	N-CA-C	-7.09	101.69	110.41
7	G	150	ARG	N-CA-C	7.06	119.66	109.14
11	Q	162	ALA	N-CA-C	7.05	118.97	111.28
7	G	148	SER	N-CA-C	7.05	120.89	109.40
6	F	169	LEU	N-CA-C	7.04	118.95	111.28
6	F	455	GLN	N-CA-C	7.04	118.60	111.07
10	P	235	THR	CA-C-O	7.04	128.21	121.67
15	V	95	LEU	N-CA-C	-7.03	103.62	111.28
6	F	78	GLY	N-CA-C	-7.02	104.30	112.73
8	H	176	LEU	CA-C-N	-6.99	113.60	120.52
8	H	176	LEU	C-N-CA	-6.99	113.60	120.52
2	B	166	ASN	N-CA-C	-6.98	103.36	110.97
7	G	294	TYR	N-CA-C	-6.97	104.59	113.23
12	R	45	ARG	N-CA-C	-6.96	104.65	113.01
18	Z	34	SER	N-CA-C	-6.96	103.62	111.07
6	F	428	GLY	N-CA-C	-6.95	103.87	112.77
6	F	418	GLN	N-CA-CB	6.94	120.14	110.07
7	G	582	VAL	N-CA-C	6.92	118.44	108.48
5	E	152	GLN	N-CA-C	-6.91	103.67	111.07
6	F	103	ASN	N-CA-CB	6.91	121.02	110.44
6	F	148	ALA	N-CA-C	-6.91	103.83	111.36
16	W	87	ILE	N-CA-CB	6.91	118.63	110.55
8	H	292	ASN	N-CA-C	6.90	118.88	111.36
6	F	246	GLU	N-CA-C	-6.89	103.77	111.28
18	Z	28	ARG	N-CA-C	6.87	119.72	108.52
7	G	362	ASP	N-CA-C	6.87	125.44	110.80
14	T	145	VAL	N-CA-C	-6.87	103.79	110.72
7	G	300	GLN	N-CA-CB	6.86	122.44	112.08
8	H	300	LEU	N-CA-C	-6.86	104.17	112.54
7	G	268	GLY	N-CA-C	6.82	124.77	115.30
7	G	133	GLN	N-CA-C	-6.80	101.23	110.68
8	H	305	ILE	N-CA-C	-6.78	103.43	113.39
12	R	56	ASN	N-CA-C	6.77	119.94	108.90
6	F	244	ASN	N-CA-C	-6.75	100.99	110.50
15	V	114	TRP	N-CA-CB	6.73	120.33	110.30
8	H	8	THR	N-CA-C	-6.73	101.20	110.35
7	G	434	SER	N-CA-C	-6.72	101.01	110.29
9	I	208	ASP	N-CA-C	6.72	121.63	113.17
15	V	8	THR	N-CA-C	6.70	119.05	108.79
3	C	79	CYS	N-CA-C	-6.68	101.68	110.43
4	D	184	ILE	N-CA-C	-6.67	103.82	110.62
16	W	105	HIS	N-CA-C	-6.66	104.97	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	93	HIS	CB-CA-C	6.65	117.86	108.76
3	C	125	PHE	N-CA-CB	-6.64	100.61	110.17
7	G	640	ASP	N-CA-CB	6.63	119.98	110.16
17	X	129	THR	N-CA-C	6.63	120.85	110.17
7	G	601	GLY	N-CA-C	6.63	124.84	115.30
10	P	116	ILE	N-CA-C	-6.62	104.03	110.72
3	C	69	PRO	N-CA-C	-6.62	104.33	113.53
8	H	267	SER	N-CA-C	-6.59	104.17	111.36
15	V	86	LYS	N-CA-CB	6.59	119.62	110.07
7	G	287	SER	N-CA-C	6.58	119.21	110.53
11	Q	141	ASN	N-CA-CB	6.57	120.77	110.46
4	D	388	GLY	N-CA-C	6.55	119.69	110.38
8	H	182	ALA	N-CA-C	-6.55	104.06	111.07
18	Z	65	LEU	N-CA-C	-6.55	104.22	111.36
7	G	435	PRO	N-CA-C	-6.54	100.23	110.50
2	B	97	LEU	N-CA-C	-6.53	101.47	110.35
17	X	98	ARG	N-CA-C	6.52	120.49	112.54
8	H	223	PHE	N-CA-C	-6.48	104.14	111.07
7	G	605	GLN	N-CA-C	6.47	119.07	108.52
7	G	250	SER	N-CA-C	6.46	116.81	108.34
9	I	66	LEU	N-CA-C	-6.46	104.32	111.36
22	r	24	LEU	N-CA-C	6.46	119.61	110.50
13	S	16	LEU	N-CA-C	-6.46	98.38	108.90
8	H	255	TYR	N-CA-CB	6.45	119.37	110.01
4	D	141	TYR	N-CA-C	6.44	120.97	113.18
4	D	84	PHE	N-CA-C	-6.43	104.32	111.71
7	G	95	PRO	N-CA-C	-6.42	101.11	110.80
15	V	49	GLU	N-CA-C	-6.42	104.29	111.28
8	H	177	PRO	N-CA-C	-6.40	101.59	111.13
3	C	125	PHE	N-CA-C	6.40	119.53	110.50
6	F	178	GLU	N-CA-CB	6.40	119.48	109.94
6	F	370	LEU	N-CA-C	-6.40	104.39	111.36
12	R	81	GLY	N-CA-C	-6.40	106.89	115.21
8	H	271	LEU	N-CA-CB	6.37	119.31	110.07
11	Q	59	LEU	N-CA-C	-6.37	100.75	110.30
9	I	205	ILE	N-CA-C	-6.37	104.29	110.72
7	G	273	ILE	N-CA-C	-6.36	98.36	107.77
15	V	71	LEU	N-CA-C	6.34	118.19	111.28
21	q	28	PHE	N-CA-C	6.33	117.85	111.07
15	V	91	ALA	N-CA-C	-6.33	104.38	111.28
7	G	176	CYS	N-CA-C	6.33	119.66	110.42
6	F	144	VAL	N-CA-CB	6.31	118.64	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	GLY	N-CA-C	-6.28	105.21	112.50
7	G	383	SER	N-CA-C	-6.28	106.83	114.75
17	X	99	HIS	N-CA-CB	6.27	119.43	110.16
7	G	356	ASP	N-CA-CB	6.25	119.31	110.12
4	D	233	HIS	N-CA-C	6.25	119.03	111.40
11	Q	141	ASN	N-CA-C	-6.25	105.66	113.28
2	B	113	ASP	N-CA-CB	6.24	119.51	109.28
8	H	52	ALA	N-CA-CB	6.23	119.05	110.01
6	F	101	PHE	N-CA-C	6.22	118.86	111.33
8	H	269	THR	N-CA-C	6.20	118.03	111.28
19	a	26	ILE	N-CA-C	-6.19	104.65	113.07
21	q	69	ASN	N-CA-CB	6.19	121.32	111.66
10	P	368	GLU	N-CA-CB	6.19	119.84	110.30
18	Z	69	ILE	N-CA-CB	6.19	117.38	110.51
7	G	451	ILE	N-CA-C	-6.19	104.96	113.00
22	r	26	LEU	N-CA-CB	-6.19	101.13	110.35
7	G	420	LYS	N-CA-C	6.18	118.81	111.33
6	F	192	ASP	N-CA-C	6.17	119.00	109.07
4	D	352	PRO	N-CA-C	6.17	118.22	110.70
13	S	61	VAL	N-CA-C	-6.17	99.60	108.42
4	D	291	VAL	N-CA-C	-6.14	103.41	111.09
8	H	76	THR	N-CA-C	-6.14	104.58	111.28
10	P	118	LYS	N-CA-C	6.13	118.94	111.82
7	G	418	ILE	N-CA-C	-6.13	103.46	112.04
6	F	212	LEU	N-CA-C	-6.11	104.61	111.28
8	H	276	SER	N-CA-C	6.11	118.91	111.82
7	G	325	ARG	N-CA-CB	6.11	118.83	109.91
18	Z	44	ILE	N-CA-C	-6.11	104.79	110.53
6	F	415	ILE	N-CA-C	-6.11	104.39	110.62
8	H	185	TRP	N-CA-C	-6.09	103.99	112.45
13	S	87	VAL	N-CA-C	-6.06	104.44	110.62
7	G	353	ALA	N-CA-C	-6.04	104.63	112.23
7	G	508	ALA	N-CA-C	6.03	117.86	111.28
22	r	108	LYS	N-CA-C	6.03	117.94	111.36
18	Z	65	LEU	N-CA-CB	6.02	119.07	110.16
8	H	24	GLU	N-CA-C	-6.02	104.08	112.45
8	H	7	LEU	N-CA-C	-6.02	104.35	111.03
7	G	638	THR	N-CA-C	-6.00	100.17	109.24
18	Z	72	MET	CA-C-N	-6.00	113.00	119.24
18	Z	72	MET	C-N-CA	-6.00	113.00	119.24
4	D	258	VAL	N-CA-C	-5.97	104.02	110.23
8	H	103	LEU	N-CA-C	-5.97	104.86	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	196	PRO	N-CA-C	-5.96	101.85	111.03
6	F	291	GLU	N-CA-C	5.94	118.21	110.43
8	H	315	PRO	O-C-N	5.93	123.94	121.15
7	G	387	LEU	CB-CA-C	-5.91	101.76	111.68
17	X	38	LYS	N-CA-C	-5.91	104.75	111.07
6	F	127	ASP	N-CA-C	5.90	118.49	111.71
17	X	97	PHE	N-CA-C	5.89	118.65	111.82
9	I	116	CYS	N-CA-C	-5.87	105.61	112.89
10	P	122	HIS	N-CA-C	5.87	120.14	112.92
14	T	94	ASP	N-CA-CB	-5.85	105.16	111.66
21	q	65	THR	N-CA-C	5.84	119.20	110.14
15	V	19	THR	N-CA-CB	5.84	120.77	110.37
3	C	209	LEU	N-CA-CB	-5.83	100.68	110.83
8	H	116	ILE	N-CA-C	-5.83	104.82	110.42
7	G	639	LEU	N-CA-C	5.83	118.58	111.82
13	S	86	GLU	N-CA-CB	5.83	118.79	110.16
6	F	255	CYS	N-CA-C	-5.82	104.53	111.69
2	B	135	GLY	CA-C-O	-5.82	117.93	122.52
6	F	102	MET	CB-CA-C	-5.81	101.35	110.94
7	G	480	ALA	N-CA-C	-5.81	105.03	111.36
21	q	7	LEU	N-CA-C	-5.81	104.86	111.07
10	P	367	GLU	CB-CA-C	-5.81	99.52	110.67
11	Q	164	PHE	N-CA-CB	5.80	119.81	110.42
7	G	672	ALA	N-CA-C	-5.80	104.96	111.28
12	R	34	THR	N-CA-C	-5.79	106.83	112.97
8	H	252	PRO	N-CA-CB	-5.78	97.96	103.51
17	X	36	CYS	CB-CA-C	-5.78	102.56	111.74
10	P	234	LYS	CB-CA-C	-5.76	103.40	111.80
1	A	105	GLU	N-CA-C	-5.75	105.01	111.28
4	D	414	ASP	N-CA-C	-5.73	101.47	110.36
6	F	393	ASN	N-CA-C	-5.72	104.95	111.07
7	G	289	LYS	N-CA-C	5.71	117.51	111.28
13	S	73	GLN	N-CA-C	-5.71	100.39	109.59
6	F	299	LEU	N-CA-C	5.71	118.44	111.82
10	P	272	LEU	N-CA-C	-5.71	101.83	110.28
12	R	35	GLY	N-CA-C	5.70	121.80	113.48
5	E	119	THR	N-CA-C	-5.69	105.83	112.89
6	F	176	ALA	N-CA-C	5.69	118.21	111.33
10	P	119	ALA	N-CA-C	-5.68	105.00	111.14
11	Q	124	MET	CA-C-N	-5.68	114.91	122.98
11	Q	124	MET	C-N-CA	-5.68	114.91	122.98
8	H	126	LYS	N-CA-C	5.67	117.46	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	59	GLN	N-CA-C	5.65	118.00	107.99
12	R	52	GLN	N-CA-C	5.65	117.99	110.53
6	F	457	HIS	N-CA-CB	-5.65	100.90	110.50
7	G	540	ASN	CA-C-N	-5.65	114.56	120.38
7	G	540	ASN	C-N-CA	-5.65	114.56	120.38
6	F	416	SER	N-CA-C	5.64	117.88	111.11
7	G	599	THR	CA-C-N	-5.63	114.16	122.83
7	G	599	THR	C-N-CA	-5.63	114.16	122.83
2	B	112	TYR	N-CA-C	5.61	122.75	110.80
9	I	191	LEU	N-CA-C	-5.60	105.25	111.36
6	F	304	ALA	CB-CA-C	-5.60	110.10	116.54
18	Z	64	ASP	N-CA-C	5.60	119.83	112.89
21	q	142	THR	N-CA-CB	5.60	119.92	109.68
17	X	40	ASN	N-CA-C	-5.59	104.87	110.97
5	E	183	PRO	N-CA-C	-5.58	102.17	111.26
6	F	294	VAL	CA-C-N	-5.57	114.02	119.76
6	F	294	VAL	C-N-CA	-5.57	114.02	119.76
2	B	201	LEU	N-CA-C	-5.57	105.11	111.07
22	r	94	ALA	N-CA-C	-5.56	101.62	109.96
7	G	530	TYR	N-CA-C	-5.55	102.06	110.28
6	F	118	ASP	N-CA-C	-5.54	102.09	110.28
21	q	68	MET	N-CA-C	5.53	119.29	112.54
4	D	200	PHE	CA-CB-CG	5.53	119.33	113.80
7	G	615	LEU	N-CA-C	-5.53	106.31	113.16
19	a	25	TYR	N-CA-C	-5.50	107.82	114.75
4	D	132	ALA	N-CA-C	-5.50	106.57	113.72
7	G	313	LEU	N-CA-C	5.48	118.49	109.72
21	q	71	LYS	N-CA-C	5.48	119.96	113.16
4	D	231	GLY	N-CA-C	-5.47	103.04	110.43
10	P	86	CYS	N-CA-C	-5.47	103.16	110.55
7	G	127	ASP	CA-C-O	5.47	128.95	121.89
7	G	363	SER	N-CA-C	-5.47	100.27	109.07
8	H	141	SER	N-CA-CB	5.46	117.93	110.01
7	G	150	ARG	N-CA-CB	-5.45	102.79	111.62
2	B	98	ALA	CB-CA-C	-5.45	108.70	115.89
14	T	135	ALA	N-CA-CB	5.43	118.10	110.12
17	X	27	ALA	N-CA-C	-5.41	105.03	111.69
7	G	420	LYS	N-CA-CB	-5.41	101.95	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
18	Z	55	GLN	N-CA-C	-5.41	105.39	111.28
7	G	404	GLY	N-CA-C	5.40	121.37	113.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	391	VAL	CA-C-N	-5.39	115.78	119.66
4	D	391	VAL	C-N-CA	-5.39	115.78	119.66
18	Z	50	MET	N-CA-C	-5.39	105.40	111.28
10	P	374	THR	N-CA-C	5.38	117.50	108.73
7	G	510	TRP	N-CA-C	-5.38	101.89	109.96
14	T	92	LYS	N-CA-C	-5.37	106.31	112.92
11	Q	163	ASN	CB-CA-C	-5.36	99.29	109.95
4	D	201	PHE	N-CA-C	-5.35	105.53	111.36
5	E	48	PRO	N-CA-C	5.35	120.80	113.84
8	H	252	PRO	CA-N-CD	5.34	119.47	112.00
8	H	284	GLN	N-CA-C	-5.32	105.56	111.36
6	F	199	ARG	N-CA-C	5.32	117.41	109.59
7	G	362	ASP	CA-CB-CG	5.32	117.92	112.60
8	H	94	PRO	N-CA-C	5.32	118.66	111.22
21	q	131	ARG	N-CA-C	5.31	117.68	110.35
9	I	54	THR	N-CA-C	-5.30	104.91	111.33
10	P	339	GLY	N-CA-C	5.30	122.63	115.00
8	H	310	PHE	N-CA-C	5.29	119.36	113.01
11	Q	164	PHE	N-CA-C	-5.28	106.81	113.20
7	G	356	ASP	N-CA-C	-5.27	105.53	111.28
5	E	74	GLN	N-CA-C	-5.27	107.50	114.04
9	I	160	GLU	N-CA-CB	-5.27	100.76	109.72
4	D	363	VAL	N-CA-C	5.26	116.34	111.81
6	F	300	ILE	N-CA-CB	5.25	119.32	110.56
7	G	277	MET	N-CA-CB	-5.24	101.64	109.71
15	V	84	ALA	N-CA-C	5.24	116.67	111.07
21	q	6	VAL	CB-CA-C	-5.23	105.08	112.14
10	P	260	GLY	N-CA-C	-5.23	108.40	115.36
22	r	25	GLN	N-CA-C	5.23	118.92	112.54
5	E	48	PRO	CB-CA-C	-5.23	104.43	111.85
7	G	600	GLU	CB-CA-C	-5.23	102.96	111.06
8	H	46	LEU	N-CA-C	-5.22	106.69	113.16
17	X	33	GLY	N-CA-C	-5.22	107.84	114.16
7	G	435	PRO	CB-CA-C	-5.22	105.87	111.56
11	Q	72	ILE	N-CA-C	-5.21	108.42	113.53
7	G	63	PHE	CA-C-O	-5.21	115.02	121.06
3	C	164	TRP	N-CA-C	5.21	117.04	111.36
10	P	316	LYS	N-CA-C	-5.21	104.86	111.11
13	S	85	ASP	N-CA-C	5.21	117.86	111.82
22	r	107	SER	N-CA-C	-5.20	102.16	109.96
8	H	101	GLY	N-CA-C	5.20	118.53	112.50
21	q	21	ARG	N-CA-C	5.20	117.62	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	713	ALA	N-CA-C	-5.19	105.52	111.07
8	H	146	MET	N-CA-C	-5.19	105.52	111.07
10	P	194	VAL	N-CA-CB	5.19	118.36	110.58
4	D	391	VAL	N-CA-C	5.18	113.84	109.02
7	G	556	THR	N-CA-C	-5.18	101.54	109.41
7	G	458	GLY	N-CA-C	-5.16	108.20	115.32
7	G	172	ILE	N-CA-C	-5.16	98.61	109.34
22	r	110	GLN	CA-C-N	-5.16	113.61	118.97
22	r	110	GLN	C-N-CA	-5.16	113.61	118.97
10	P	198	ALA	N-CA-C	-5.15	100.12	108.52
7	G	569	GLN	CB-CA-C	-5.15	104.22	112.05
8	H	277	TYR	N-CA-C	5.14	117.96	110.10
20	b	82	LYS	N-CA-C	-5.14	103.75	110.53
3	C	156	VAL	N-CA-C	-5.13	104.09	111.17
1	A	2	ASN	CA-C-N	-5.13	113.01	120.29
1	A	2	ASN	C-N-CA	-5.13	113.01	120.29
7	G	387	LEU	N-CA-C	-5.12	98.35	107.98
2	B	98	ALA	N-CA-C	5.12	117.62	109.02
8	H	196	ALA	CA-C-N	-5.12	113.48	119.32
8	H	196	ALA	C-N-CA	-5.12	113.48	119.32
16	W	91	MET	N-CA-C	-5.12	105.88	111.82
21	q	5	GLU	N-CA-C	5.11	116.54	111.07
6	F	60	GLY	N-CA-C	-5.11	106.00	114.48
5	E	181	ASN	N-CA-C	-5.11	99.47	108.20
4	D	224	ALA	N-CA-C	5.10	117.23	111.11
9	I	95	PRO	N-CA-C	5.10	121.20	113.81
3	C	109	SER	N-CA-C	5.09	118.10	109.76
23	s	38	HIS	N-CA-C	5.09	118.59	112.38
5	E	166	LYS	N-CA-C	-5.08	104.63	111.54
17	X	140	ASN	CA-C-N	-5.08	114.55	119.78
17	X	140	ASN	C-N-CA	-5.08	114.55	119.78
3	C	221	GLU	N-CA-C	-5.07	102.37	108.25
7	G	393	GLY	N-CA-C	-5.07	107.76	115.66
21	q	140	PRO	N-CA-C	-5.07	102.29	110.55
17	X	112	LEU	N-CA-CB	5.06	117.41	110.07
8	H	254	LEU	N-CA-CB	5.06	118.12	110.28
10	P	376	ASN	CB-CA-C	-5.06	102.25	110.85
7	G	280	ASP	N-CA-CB	-5.05	102.69	110.12
8	H	90	PRO	CA-C-O	-5.05	117.49	121.38
4	D	224	ALA	CA-C-O	-5.05	115.50	120.90
12	R	43	TYR	N-CA-CB	-5.04	103.19	110.70
10	P	170	LEU	N-CA-C	5.03	117.02	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	140	CYS	CB-CA-C	-5.02	104.12	109.85
18	Z	130	LYS	N-CA-C	-5.02	105.70	111.07
9	I	160	GLU	CB-CA-C	5.02	119.17	110.84
14	T	140	CYS	N-CA-C	5.01	116.66	109.04
3	C	208	GLU	CA-C-O	-5.01	115.73	121.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	762	0	823	73	0
2	B	1247	0	1258	154	0
3	C	1641	0	1596	138	0
4	D	3095	0	3066	313	0
5	E	1635	0	1626	173	0
6	F	3288	0	3243	343	0
7	G	5287	0	5323	550	0
8	H	2495	0	2582	347	0
9	I	1398	0	1359	164	0
10	P	2730	0	2747	224	0
11	Q	957	0	949	84	0
12	R	660	0	639	87	0
13	S	667	0	683	72	0
14	T	604	0	596	90	0
15	V	915	0	954	87	0
16	W	970	0	991	89	0
17	X	1164	0	1154	97	0
18	Z	1152	0	1148	101	0
19	a	540	0	550	44	0
20	b	620	0	617	87	0
21	q	1004	0	962	83	0
22	r	413	0	429	42	0
23	s	226	0	214	14	0
24	A	46	0	69	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	H	46	0	69	12	0
24	b	46	0	69	12	0
25	B	8	0	0	4	0
25	F	8	0	0	10	0
25	G	16	0	0	5	0
25	I	16	0	0	16	0
26	B	35	0	44	3	0
26	I	47	0	71	7	0
27	D	18	0	18	18	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
All	All	33911	0	33937	2951	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (2951) 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: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
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.40	1.18
15:V:44:TYR:CE1	15:V:48:THR:HG21	1.77	1.18
6:F:382:CYS:SG	25:F:502:SF4:FE3	1.38	1.12
9:I:123:CYS:SG	25:I:302:SF4:FE1	1.40	1.11
4:D:92:HIS:HA	27:D:501:UQ1:C3	1.80	1.11
2:B:122:ARG:NH1	27:D:501:UQ1:H113	1.64	1.11
6:F:379:CYS:SG	25:F:502:SF4:FE4	1.43	1.09
17:X:4:ILE:HG22	17:X:5:VAL:H	0.96	1.09
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.08
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.08
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.08
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.27	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:88:HIS:CB	12:R:89:PRO:HD2	1.84	1.07
12:R:88:HIS:HB2	12:R:89:PRO:HD2	1.08	1.07
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.07
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.07
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.07
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.07
11:Q:160:TYR:CZ	11:Q:164:PHE:HZ	1.72	1.06
14:T:138:LEU:HD12	14:T:138:LEU:O	1.55	1.06
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.06
9:I:152:CYS:SG	25:I:302:SF4:FE2	1.46	1.06
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.05
13:S:23:LEU:HD12	13:S:23:LEU:O	1.54	1.05
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.31	1.05
15:V:44:TYR:CE1	15:V:48:THR:CG2	2.39	1.05
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.33	1.05
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.05
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.92	1.04
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.37	1.04
2:B:82:ILE:HG23	8:H:57:MET:SD	1.97	1.04
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
4:D:185:MET:CE	4:D:207:ARG:HH12	1.70	1.04
6:F:266:GLY:CA	6:F:271:SER:HA	1.86	1.04
2:B:122:ARG:HH11	27:D:501:UQ1:H113	0.88	1.03
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.03
8:H:142:TYR:CD1	8:H:289:LEU:HD12	1.94	1.03
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.03
9:I:208:ASP:O	9:I:208:ASP:OD1	1.75	1.02
3:C:102:HIS:HE1	15:V:48:THR:HG22	1.22	1.02
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.02
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.22	1.02
16:W:32:LYS:HG2	33:W:201:EHZ:C19	1.90	1.01
21:q:66:THR:HG22	21:q:74:PHE:HB2	1.39	1.01
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
9:I:152:CYS:HG	25:I:302:SF4:FE2	0.70	1.00
11:Q:160:TYR:CZ	11:Q:164:PHE:CZ	2.49	1.00
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
9:I:155:CYS:SG	25:I:302:SF4:FE4	1.52	1.00
2:B:105:MET:HE2	4:D:200:PHE:HE2	1.23	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	1.00
15:V:44:TYR:CZ	15:V:48:THR:HG21	1.97	0.99
6:F:266:GLY:HA3	6:F:271:SER:CA	1.90	0.99
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.99
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.99
2:B:82:ILE:HG12	8:H:57:MET:CE	1.93	0.98
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	0.98
5:E:179:CYS:HG	28:E:301:FES:FE2	0.69	0.98
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.98
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	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
17:X:4:ILE:HG22	17:X:5:VAL:N	1.77	0.98
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.78	0.98
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.98
4:D:185:MET:HE3	4:D:207:ARG:HH12	1.28	0.98
6:F:379:CYS:HG	25:F:502:SF4:FE4	0.74	0.97
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.47	0.97
7:G:92:CYS:SG	28:G:803:FES:S1	2.62	0.97
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.46	0.96
4:D:185:MET:HE3	4:D:207:ARG:NH1	1.80	0.96
4:D:185:MET:HE3	4:D:207:ARG:NH2	1.79	0.96
11:Q:160:TYR:CE2	11:Q:164:PHE:CE2	2.53	0.96
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.96
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.96
10:P:376:ASN:OD1	10:P:377:TYR:N	1.98	0.96
5:E:240:PRO:HA	6:F:60:GLY:HA3	1.44	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
4:D:185:MET:HE3	4:D:207:ARG:HH22	1.28	0.95
13:S:16:LEU:HD11	13:S:51:LEU:HD11	1.46	0.95
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.95
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.95
12:R:38:TYR:HE2	21:q:127:TYR:HB2	1.30	0.95
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.44	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.94
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.48	0.94
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.94
9:I:113:CYS:SG	25:I:303:SF4:FE3	1.59	0.94
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.94
8:H:224:PHE:CE2	30:H:401:UQ9:H13	2.02	0.94
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.32	0.93
10:P:333:PRO:HB2	10:P:337:ASP:HB2	1.47	0.93
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.93
10:P:262:THR:H	10:P:332:LEU:HD12	1.34	0.93
11:Q:160:TYR:CE2	11:Q:164:PHE:HE2	1.86	0.93
10:P:93:HIS:CD2	10:P:94:LEU:CD1	2.52	0.92
18:Z:86:ILE:HG23	18:Z:128:ARG:HE	1.33	0.92
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.92
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.92
4:D:185:MET:CE	4:D:207:ARG:HH22	1.82	0.92
12:R:88:HIS:HB2	12:R:89:PRO:CD	1.97	0.92
17:X:4:ILE:CG2	17:X:5:VAL:H	1.82	0.92
22:r:9:GLN:HA	22:r:12:ARG:HD3	1.50	0.92
2:B:122:ARG:HH11	27:D:501:UQ1:C11	1.81	0.92
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.91
15:V:75:GLY:HA2	22:r:103:ARG:HD2	1.51	0.91
17:X:37:ASP:OD2	20:b:70:PRO:HD3	1.69	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	0.91
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.91
10:P:93:HIS:NE2	10:P:94:LEU:CD1	2.35	0.90
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.90
7:G:176:CYS:HG	25:G:802:SF4:FE4	0.62	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
6:F:425:CYS:HG	25:F:502:SF4:FE1	0.62	0.89
4:D:185:MET:HE3	4:D:207:ARG:CZ	2.03	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
6:F:110:PRO:HB3	6:F:152:ARG:CZ	2.03	0.89
6:F:266:GLY:HA3	6:F:271:SER:HA	0.94	0.89
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.88	0.89
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:226:CYS:HG	25:G:802:SF4:FE1	0.75	0.88
2:B:81:LEU:HG	8:H:53:MET:HE1	1.53	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.55	0.88
6:F:382:CYS:HG	25:F:502:SF4:FE3	0.61	0.88
4:D:99:LEU:CD2	4:D:109:CYS:SG	2.62	0.88
13:S:16:LEU:HD22	13:S:19:ILE:HD11	1.53	0.88
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.88
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.88
10:P:96:LEU:HD12	10:P:97:MET:N	1.88	0.87
7:G:32:ILE:HG23	7:G:98:LYS:HD2	1.54	0.87
7:G:97:MET:HB2	7:G:100:TRP:CD1	2.09	0.87
10:P:192:ARG:HH22	10:P:198:ALA:HB3	1.36	0.87
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.09	0.87
20:b:60:ASP:OD1	20:b:61:GLY:N	2.07	0.87
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.87
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.86
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.56	0.86
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.86
13:S:16:LEU:HD12	13:S:16:LEU:O	1.76	0.86
16:W:55:LEU:HD22	16:W:107:MET:HE2	1.57	0.86
14:T:79:ILE:HB	14:T:145:VAL:HG13	1.55	0.86
7:G:78:CYS:SG	28:G:803:FES:FE2	1.68	0.86
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.86
6:F:292:MET:HG2	6:F:338:ASP:OD1	1.75	0.86
9:I:162:CYS:SG	25:I:303:SF4:FE4	1.68	0.85
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.85
4:D:99:LEU:HD23	4:D:109:CYS:HA	1.57	0.85
17:X:53:PRO:HD2	18:Z:116:TRP:CD1	2.11	0.85
6:F:44:ASN:HD21	6:F:51:TRP:HA	1.41	0.85
10:P:206:ILE:H	31:P:401:NDP:H71N	1.25	0.85
4:D:266:ARG:HB2	9:I:65:GLU:OE2	1.77	0.85
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.59	0.85
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.95	0.85
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.85
9:I:162:CYS:HG	25:I:303:SF4:FE4	0.54	0.85
7:G:126:LEU:CD1	12:R:89:PRO:HB2	2.07	0.84
4:D:92:HIS:CD2	27:D:501:UQ1:O2	2.30	0.84
10:P:192:ARG:NH2	10:P:198:ALA:HB3	1.92	0.84
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.59	0.84
15:V:56:LEU:HD12	15:V:57:ASP:N	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:32:THR:HG22	12:R:36:GLN:H	1.40	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.07	0.84
6:F:300:ILE:HD13	6:F:307:VAL:H	1.41	0.84
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.84
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.84
8:H:224:PHE:CE2	30:H:401:UQ9:C13	2.60	0.84
2:B:105:MET:CE	4:D:200:PHE:HE2	1.90	0.84
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.84
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	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	0.83
3:C:172:MET:CE	3:C:187:LEU:HB2	2.09	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
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.83
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.83
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.79	0.83
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.60	0.83
7:G:78:CYS:HG	28:G:803:FES:FE2	0.52	0.83
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.82
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.92	0.82
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.82
8:H:183:MET:HE2	26:I:301:PC1:H2A1	1.61	0.82
2:B:89:SER:O	8:H:54:LYS:HD3	1.79	0.82
3:C:217:ARG:NH1	16:W:112:GLU:HB2	1.95	0.82
6:F:117:ALA:HB1	6:F:131:MET:SD	2.19	0.82
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.82
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.82
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.45	0.82
7:G:401:LEU:CD1	7:G:466:LEU:HD21	2.09	0.82
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.82
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.82
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
12:R:51:ARG:HH21	21:q:125:VAL:HG12	1.44	0.81
16:W:55:LEU:CD2	16:W:107:MET:HE2	2.09	0.81
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.81
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.81
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.81
21:q:71:LYS:O	21:q:72:ASN:OD1	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.81
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.81
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.96	0.81
9:I:123:CYS:HG	25:I:302:SF4:FE1	0.52	0.81
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.11	0.81
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.81
8:H:311:THR:HB	18:Z:51:MET:SD	2.21	0.81
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.80
6:F:342:LEU:HB3	6:F:347:THR:HG23	1.63	0.80
20:b:20:VAL:HA	24:b:201:3PE:H282	1.64	0.80
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.80
2:B:89:SER:O	8:H:54:LYS:CD	2.29	0.80
2:B:105:MET:HE2	4:D:200:PHE:CE2	2.14	0.80
13:S:36:PHE:HZ	13:S:44:LEU:HD11	1.45	0.80
1:A:25:PRO:HG3	8:H:60:PRO:HD3	1.63	0.80
7:G:73:GLY:HA2	28:G:803:FES:S1	2.21	0.80
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.62	0.80
8:H:251:LEU:O	8:H:251:LEU:CD1	2.27	0.80
6:F:154:ALA:CB	6:F:193:PHE:HZ	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
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.63	0.80
14:T:87:LEU:HD21	14:T:104:PHE:HZ	1.47	0.80
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.80
6:F:174:ARG:HA	23:s:52:LEU:HD21	1.64	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.46	0.79
14:T:93:ILE:HG21	14:T:110:LEU:HD22	1.63	0.79
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.79
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	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:306:SER:OG	8:H:310:PHE:CE2	2.36	0.79
16:W:42:TRP:CZ2	16:W:93:LEU:HB2	2.17	0.79
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.65	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
8:H:17:MET:SD	8:H:229:THR:OG1	2.41	0.79
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.79
4:D:280:ALA:CB	15:V:11:LEU:HG	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.78
21:q:55:PHE:CD1	22:r:26:LEU:HD22	2.17	0.78
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.78
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.78
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.65	0.78
14:T:113:LEU:HD22	16:W:71:MET:HE2	1.63	0.78
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.63	0.78
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.23	0.78
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.65	0.78
13:S:20:ARG:HG3	13:S:54:LEU:HB2	1.65	0.78
14:T:87:LEU:HD22	14:T:104:PHE:CE1	2.19	0.78
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.18	0.78
3:C:102:HIS:CE1	15:V:48:THR:HG22	2.14	0.78
20:b:66:VAL:HG13	20:b:72:ASP:HB2	1.65	0.78
14:T:83:VAL:CG2	14:T:126:PHE:HZ	1.97	0.78
21:q:9:ARG:HA	21:q:12:GLN:HG2	1.65	0.78
4:D:92:HIS:HA	27:D:501:UQ1:O3	1.83	0.78
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.78
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.77
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.66	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.32	0.77
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.77
5:E:178:ALA:HA	6:F:125:CYS:SG	2.24	0.77
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.77
9:I:155:CYS:HG	25:I:302:SF4:FE4	1.02	0.77
2:B:96:GLY:HA2	2:B:101:ALA:HB2	1.67	0.77
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
9:I:113:CYS:HG	25:I:303:SF4:FE3	0.49	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	1.66	0.77
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.77
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.50	0.77
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.00	0.77
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	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	1.66	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77
4:D:99:LEU:HD22	4:D:109:CYS:SG	2.24	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.76
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.50	0.76
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.76
3:C:217:ARG:HH12	16:W:112:GLU:HB2	1.50	0.76
17:X:20:VAL:HG22	17:X:24:VAL:HG21	1.66	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
10:P:143:ASP:HA	10:P:147:ASN:HB2	1.67	0.76
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.67	0.76
14:T:93:ILE:HG23	14:T:110:LEU:HD13	1.66	0.76
4:D:185:MET:CE	4:D:207:ARG:NH1	2.43	0.76
5:E:189:ASP:CG	6:F:163:TYR:HB3	2.11	0.76
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
16:W:42:TRP:CD2	16:W:93:LEU:HD12	2.21	0.76
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.67	0.76
4:D:185:MET:HE1	4:D:207:ARG:HH12	1.50	0.76
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
13:S:51:LEU:HD13	13:S:95:LEU:HD21	1.68	0.76
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.68	0.76
26:B:302:PC1:H371	8:H:49:PHE:HB3	1.66	0.76
4:D:271:ARG:HD2	8:H:279:ARG:O	1.85	0.76
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.76
11:Q:160:TYR:CD2	11:Q:164:PHE:HE2	2.03	0.76
4:D:371:MET:SD	4:D:381:HIS:CD2	2.79	0.75
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.75
7:G:651:PRO:HG3	13:S:57:GLU:H	1.51	0.75
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.75
3:C:102:HIS:HE1	15:V:48:THR:CG2	1.99	0.75
8:H:91:MET:O	8:H:92:PRO:C	2.26	0.75
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.75
12:R:89:PRO:HG3	12:R:106:TYR:CE1	2.20	0.75
13:S:19:ILE:HG13	13:S:95:LEU:HD11	1.69	0.75
17:X:29:ALA:HB2	18:Z:71:LEU:HD11	1.67	0.75
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.75
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.67	0.75
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.52	0.75
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:167:ASN:O	11:Q:168:LYS:CD	2.35	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.75
16:W:28:LEU:HG	16:W:32:LYS:HE3	1.69	0.75
4:D:99:LEU:HD21	4:D:109:CYS:SG	2.26	0.75
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.75
20:b:23:PHE:HD2	24:b:201:3PE:H281	1.51	0.75
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.74
14:T:117:GLU:HA	14:T:120:MET:HE3	1.67	0.74
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.74
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.88	0.74
1:A:4:TYR:CE2	24:A:401:3PE:H231	2.22	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.74
10:P:336:GLU:HG3	10:P:342:PRO:HD3	1.67	0.74
20:b:20:VAL:HG13	24:b:201:3PE:H2A1	1.69	0.74
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.74
7:G:674:LEU:HD11	13:S:46:LYS:HE2	1.69	0.74
16:W:55:LEU:HB3	16:W:107:MET:HE2	1.66	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
14:T:94:ASP:HB3	14:T:98:LEU:HB2	1.68	0.74
21:q:56:PHE:HD1	21:q:59:HIS:HE2	1.35	0.74
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.69	0.74
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.74
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.74
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.03	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
8:H:180:PRO:HD3	18:Z:43:LEU:HD21	1.70	0.74
2:B:91:TRP:CZ3	30:H:401:UQ9:H1M	2.22	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73
2:B:112:TYR:OH	9:I:91:GLY:CA	2.29	0.73
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.68	0.73
6:F:210:THR:HB	6:F:224:ARG:HB2	1.70	0.73
6:F:425:CYS:SG	25:F:502:SF4:FE1	1.78	0.73
14:T:103:HIS:CG	14:T:106:LYS:HD2	2.23	0.73
5:E:240:PRO:HG3	6:F:57:LEU:O	1.88	0.73
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.28	0.73
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.70	0.73
14:T:88:LYS:HG3	14:T:98:LEU:HD22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:93:GLU:O	18:Z:97:ILE:HG13	1.88	0.73
20:b:23:PHE:HE1	24:b:201:3PE:H371	1.53	0.73
7:G:176:CYS:SG	25:G:802:SF4:FE4	1.78	0.73
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.73
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.73
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.73
16:W:32:LYS:HE2	33:W:201:EHZ:C19	2.18	0.73
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.73
20:b:69:HIS:HD2	20:b:70:PRO:HD2	1.54	0.73
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.70	0.73
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.54	0.73
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.73
11:Q:167:ASN:O	11:Q:168:LYS:HD2	1.88	0.73
12:R:89:PRO:HG3	12:R:106:TYR:CZ	2.23	0.73
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.73
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.73
18:Z:65:LEU:O	18:Z:69:ILE:HG12	1.89	0.73
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.87	0.73
5:E:39:VAL:HG11	7:G:163:LYS:NZ	2.04	0.72
1:A:21:ALA:O	1:A:25:PRO:HD3	1.88	0.72
5:E:232:SER:HB3	6:F:288:VAL:HG23	1.69	0.72
10:P:169:HIS:H	10:P:184:LYS:HE3	1.54	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
21:q:56:PHE:HA	21:q:59:HIS:CD2	2.24	0.72
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.72
4:D:375:MET:HE1	7:G:126:LEU:HA	1.71	0.72
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.72
12:R:89:PRO:CG	12:R:106:TYR:CZ	2.72	0.72
2:B:94:THR:OG1	27:D:501:UQ1:C10	2.37	0.72
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.72
16:W:101:LYS:NZ	16:W:109:PHE:CE2	2.58	0.72
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.70	0.71
4:D:266:ARG:CB	9:I:65:GLU:OE2	2.39	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.71
8:H:113:VAL:HG22	8:H:136:VAL:HG23	1.72	0.71
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	0.71
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.71	0.71
14:T:120:MET:HG2	16:W:44:ARG:HH11	1.54	0.71
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.71	0.71
8:H:183:MET:HE2	26:I:301:PC1:H271	1.72	0.71
9:I:200:GLU:OE2	21:q:93:MET:SD	2.48	0.71
10:P:192:ARG:NH1	10:P:192:ARG:HA	2.05	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
5:E:240:PRO:CA	6:F:60:GLY:HA3	2.20	0.71
9:I:53:ALA:HB1	20:b:14:ALA:HB2	1.71	0.71
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.71
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.24	0.71
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.71
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.55	0.71
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
8:H:311:THR:O	18:Z:51:MET:HG3	1.91	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
8:H:23:VAL:HG11	19:a:9:LEU:HD21	1.72	0.71
26:I:301:PC1:H2D1	26:I:301:PC1:H291	1.71	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
12:R:67:GLN:HG2	12:R:109:LEU:CD2	2.21	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.71
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.55	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.26	0.71
10:P:170:LEU:O	10:P:171:ASN:OD1	2.09	0.71
2:B:116:ARG:O	8:H:39:ILE:HG22	1.91	0.70
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.70
18:Z:69:ILE:HG23	20:b:54:PRO:HD3	1.73	0.70
4:D:142:VAL:HB	4:D:182:ASN:HD22	1.54	0.70
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.74	0.70
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.73	0.70
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	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
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.27	0.70
6:F:314:LEU:HB3	6:F:329:LYS:HD3	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.70
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.70
2:B:89:SER:O	8:H:54:LYS:CE	2.40	0.70
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.55	0.70
7:G:127:ASP:HA	12:R:106:TYR:OH	1.90	0.70
2:B:95:PHE:HE2	2:B:131:MET:SD	2.15	0.70
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.22	0.70
14:T:100:VAL:HB	14:T:142:GLN:HB2	1.74	0.70
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.70
15:V:56:LEU:HD12	15:V:56:LEU:C	2.16	0.70
4:D:202:TRP:CZ3	4:D:261:MET:HG3	2.27	0.69
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.69
16:W:32:LYS:CG	33:W:201:EHZ:C19	2.69	0.69
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.69
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.73	0.69
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.69
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.69
18:Z:86:ILE:HG23	18:Z:128:ARG:NE	2.06	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.21	0.69
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.58	0.69
10:P:171:ASN:OD1	10:P:171:ASN:O	2.11	0.69
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.74	0.69
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.74	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.74	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: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
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.74	0.69
11:Q:160:TYR:CE2	11:Q:164:PHE:CZ	2.80	0.69
14:T:87:LEU:HD22	14:T:104:PHE:HE1	1.58	0.69
8:H:187:ILE:HD12	24:H:402:3PE:H242	1.73	0.69
9:I:92:PRO:HA	21:q:91:HIS:O	1.93	0.69
17:X:50:GLU:HG3	17:X:56:CYS:SG	2.33	0.69
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.69
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.23	0.69
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.28	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:33:LEU:HD23	22:r:25:GLN:HG2	1.76	0.68
14:T:138:LEU:HD13	14:T:144:ILE:CG1	2.22	0.68
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.68
3:C:107:PHE:CD1	3:C:133:SER:HB2	2.28	0.68
8:H:85:LEU:HD21	8:H:108:THR:HB	1.74	0.68
20:b:23:PHE:HZ	24:b:201:3PE:H351	1.58	0.68
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.68
10:P:191:VAL:HA	10:P:194:VAL:HG22	1.73	0.68
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.75	0.68
22:r:20:LEU:C	22:r:20:LEU:HD12	2.18	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
4:D:92:HIS:HB3	4:D:458:PHE:HE2	1.59	0.68
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.57	0.68
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.68
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	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
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.68
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.68
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.68
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.75	0.68
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.68
8:H:224:PHE:CZ	30:H:401:UQ9:H13	2.28	0.68
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.76	0.68
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.08	0.68
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.76	0.68
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.58	0.68
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.68
6:F:228:PRO:HG3	11:Q:160:TYR:HD2	1.59	0.68
8:H:292:ASN:HD21	24:H:402:3PE:H121	1.59	0.68
10:P:192:ARG:NH2	10:P:200:ILE:HD11	2.09	0.68
20:b:23:PHE:HE1	24:b:201:3PE:H3A2	1.59	0.68
7:G:126:LEU:HD11	12:R:89:PRO:HB2	1.75	0.68
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.28	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.67
1:A:105:GLU:CG	1:A:111:LEU:HG	2.25	0.67
2:B:94:THR:HB	2:B:104:MET:HE1	1.75	0.67
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.67
9:I:188:GLU:OE2	12:R:56:ASN:HB2	1.94	0.67
15:V:116:ILE:HG23	15:V:116:ILE:O	1.92	0.67
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.67
10:P:197:GLU:HB3	10:P:259:VAL:CG2	2.24	0.67
17:X:18:VAL:HG21	18:Z:74:LEU:HD11	1.75	0.67
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.67
1:A:3:LEU:HD23	24:A:401:3PE:H251	1.75	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
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.75	0.67
9:I:188:GLU:CD	12:R:56:ASN:HB2	2.19	0.67
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.67
6:F:300:ILE:HD13	6:F:307:VAL:HG23	1.77	0.67
10:P:302:GLY:HA2	10:P:314:THR:HG23	1.77	0.67
4:D:92:HIS:HA	27:D:501:UQ1:C4	2.24	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
6:F:297:LYS:HB2	6:F:333:GLU:HA	1.77	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
13:S:16:LEU:HB3	13:S:69:TYR:HD1	1.58	0.67
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.67
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.67
9:I:54:THR:HG21	18:Z:33:TYR:CZ	2.29	0.67
10:P:192:ARG:HH22	10:P:198:ALA:CB	2.07	0.67
10:P:94:LEU:HA	10:P:97:MET:HE3	1.77	0.66
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.05	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.25	0.66
14:T:130:ILE:HG23	14:T:131:PRO:HD2	1.77	0.66
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.77	0.66
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.09	0.66
3:C:141:ARG:NH1	4:D:410:TYR:HE1	1.93	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
14:T:87:LEU:CD2	14:T:104:PHE:CZ	2.78	0.66
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.74	0.66
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.76	0.66
6:F:41:ILE:HG23	6:F:253:THR:HG21	1.76	0.66
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.66
3:C:98:PHE:CA	15:V:90:LEU:HD11	2.19	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
4:D:92:HIS:CA	27:D:501:UQ1:O3	2.42	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.77	0.66
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.66
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.66
12:R:42:ASP:HB3	12:R:44:ARG:HH11	1.61	0.66
13:S:24:CYS:SG	13:S:61:VAL:O	2.53	0.66
8:H:283:ASP:OD1	8:H:284:GLN:N	2.29	0.66
16:W:121:PHE:HA	16:W:124:LYS:HE2	1.75	0.66
1:A:8:PHE:HE1	24:A:401:3PE:H2C1	1.60	0.66
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.30	0.66
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.74	0.66
9:I:80:GLU:OE2	22:r:26:LEU:CD1	2.44	0.66
10:P:169:HIS:H	10:P:184:LYS:CE	2.09	0.66
9:I:35:THR:CG2	22:r:107:SER:HA	2.26	0.66
14:T:83:VAL:HG22	14:T:126:PHE:CZ	2.31	0.66
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.66
16:W:42:TRP:CH2	16:W:93:LEU:HA	2.31	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
2:B:91:TRP:CH2	30:H:401:UQ9:H1M	2.31	0.65
15:V:44:TYR:CE1	15:V:48:THR:HG23	2.30	0.65
2:B:122:ARG:NH1	27:D:501:UQ1:C11	2.49	0.65
3:C:79:CYS:O	3:C:80:LEU:HB2	1.96	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
10:P:59:PHE:HB2	10:P:130:ILE:HD11	1.78	0.65
13:S:58:CYS:HB2	13:S:61:VAL:HG12	1.78	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.65
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.77	0.65
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.77	0.65
8:H:199:ASP:O	8:H:279:ARG:HD2	1.96	0.65
10:P:199:ILE:HD11	10:P:258:ALA:O	1.96	0.65
13:S:16:LEU:HB3	13:S:69:TYR:CD1	2.32	0.65
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.65
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.65
10:P:236:VAL:CG1	10:P:270:ARG:HH21	2.10	0.65
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.65
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.26	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.65
5:E:79:LEU:HB2	5:E:80:PRO:HD3	1.78	0.65
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.77	0.65
10:P:191:VAL:HG13	10:P:192:ARG:NH2	2.12	0.65
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.78	0.65
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.65
2:B:146:ARG:O	2:B:147:LYS:C	2.39	0.65
2:B:173:TYR:O	3:C:203:LEU:HD22	1.97	0.65
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.65
9:I:79:ARG:HG2	22:r:12:ARG:HH21	1.62	0.65
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.65
14:T:118:ILE:HG23	14:T:122:MET:HE3	1.78	0.65
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.78	0.64
10:P:88:VAL:HG12	10:P:92:MET:HE2	1.80	0.64
17:X:124:GLN:O	20:b:70:PRO:HB2	1.97	0.64
2:B:93:MET:HE1	2:B:131:MET:HE2	1.78	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.78	0.64
10:P:226:VAL:HG21	10:P:281:PHE:CZ	2.32	0.64
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
8:H:33:LEU:CD2	22:r:25:GLN:HG2	2.26	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.33	0.64
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.64
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.79	0.64
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	0.64
11:Q:163:ASN:OD1	11:Q:164:PHE:N	2.31	0.64
4:D:202:TRP:CH2	4:D:261:MET:HG3	2.33	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.64
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.64
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	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
6:F:228:PRO:HG3	11:Q:160:TYR:CD2	2.33	0.64
14:T:138:LEU:O	14:T:138:LEU:CD1	2.40	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.63	0.64
10:P:333:PRO:HB2	10:P:337:ASP:CB	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:37:ASP:OD1	17:X:38:LYS:N	2.31	0.64
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	0.64
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.64
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.64
12:R:32:THR:HG22	12:R:36:GLN:N	2.10	0.64
13:S:16:LEU:HA	13:S:69:TYR:HA	1.79	0.64
2:B:136:THR:CG2	2:B:177:VAL:HG22	2.29	0.63
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.63
10:P:180:SER:O	10:P:184:LYS:HG3	1.98	0.63
13:S:15:GLY:HA3	13:S:17:ARG:HH22	1.63	0.63
14:T:83:VAL:HG23	14:T:126:PHE:HZ	1.62	0.63
14:T:87:LEU:HD21	14:T:104:PHE:CZ	2.32	0.63
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.63
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.63
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.63
17:X:65:GLY:HA2	17:X:68:LEU:HD12	1.78	0.63
2:B:92:PRO:HD2	2:B:120:VAL:HG12	1.80	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
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.63
10:P:284:THR:HG23	10:P:356:HIS:HB2	1.79	0.63
13:S:16:LEU:HD12	13:S:16:LEU:C	2.22	0.63
21:q:6:VAL:HA	21:q:9:ARG:HG2	1.79	0.63
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.63
16:W:55:LEU:CB	16:W:107:MET:CE	2.75	0.63
18:Z:65:LEU:O	18:Z:68:ARG:HG2	1.98	0.63
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.63
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.28	0.63
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.63
16:W:101:LYS:NZ	16:W:109:PHE:HE2	1.94	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.99	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
2:B:70:ARG:HG3	2:B:73:TYR:H	1.63	0.63
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.63
10:P:66:GLY:O	10:P:67:ARG:C	2.42	0.63
14:T:93:ILE:CG2	14:T:110:LEU:HD13	2.28	0.63
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.79	0.63

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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	0.63
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.63
10:P:93:HIS:NE2	10:P:94:LEU:HD11	2.14	0.63
1:A:52:SER:HB2	1:A:54:LYS:HG2	1.79	0.63
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.63
5:E:230:LEU:HD11	6:F:48:ARG:HE	1.64	0.63
6:F:33:GLY:HA2	6:F:291:GLU:CB	2.16	0.63
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.81	0.63
18:Z:58:ARG:NH2	20:b:49:THR:HG21	2.13	0.63
4:D:142:VAL:HG12	4:D:182:ASN:HA	1.81	0.62
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.62
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.80	0.62
12:R:89:PRO:HG2	12:R:106:TYR:CZ	2.33	0.62
16:W:83:ASP:O	16:W:86:VAL:HG22	1.99	0.62
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.34	0.62
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.62
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.62
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.28	0.62
14:T:103:HIS:ND1	14:T:140:CYS:SG	2.73	0.62
16:W:55:LEU:CB	16:W:107:MET:HE2	2.30	0.62
2:B:194:CYS:O	25:B:301:SF4:S2	2.58	0.62
7:G:399:VAL:CG2	7:G:462:PHE:HZ	2.12	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.80	0.62
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.35	0.62
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
10:P:240:VAL:HB	10:P:266:THR:O	2.00	0.62
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.81	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.26	0.62
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.81	0.62
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:651:PRO:CD	13:S:56:ARG:HB3	2.30	0.62
8:H:25:ARG:HD2	30:H:401:UQ9:H10A	1.80	0.62
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.35	0.62
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.29	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.65	0.62
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.34	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.81	0.62
14:T:87:LEU:CD2	14:T:104:PHE:HZ	2.12	0.62
14:T:138:LEU:HD12	14:T:138:LEU:C	2.24	0.62
17:X:69:ASN:O	17:X:73:GLN:HG3	2.00	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.61
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.61
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.61
22:r:20:LEU:HD12	22:r:21:GLN:N	2.14	0.61
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.36	0.61
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.47	0.61
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.81	0.61
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.81	0.61
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.83	0.61
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.61
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.61
7:G:617:ARG:NH1	16:W:129:HIS:HA	2.14	0.61
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.61	0.61
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	0.61
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.61
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.31	0.61
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.30	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
14:T:79:ILE:CB	14:T:145:VAL:HG13	2.28	0.61
20:b:11:ASN:O	20:b:15:LYS:N	2.31	0.61
20:b:23:PHE:CE1	24:b:201:3PE:H3A2	2.35	0.61
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.61
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.82	0.61
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.61
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.61
18:Z:28:ARG:HG3	18:Z:28:ARG:O	1.99	0.61
20:b:23:PHE:CE1	24:b:201:3PE:H371	2.35	0.61
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.63	0.61
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
11:Q:167:ASN:O	11:Q:168:LYS:CG	2.48	0.61
12:R:98:GLU:CD	12:R:98:GLU:H	2.07	0.61
21:q:71:LYS:O	21:q:72:ASN:CG	2.43	0.61
5:E:71:GLU:HB2	23:s:59:GLN:HB3	1.82	0.61
7:G:82:ILE:CG2	7:G:100:TRP:HB3	2.30	0.61
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.61
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.61
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.62	0.61
10:P:191:VAL:HG13	10:P:192:ARG:HH21	1.66	0.61
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.61
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.61
6:F:416:SER:O	6:F:419:ILE:HG22	2.01	0.61
14:T:103:HIS:HB2	14:T:106:LYS:HB2	1.83	0.61
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.61
21:q:3:LEU:O	21:q:6:VAL:HG22	2.01	0.61
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.32	0.61
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.61
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.66	0.61
5:E:182:ALA:O	5:E:183:PRO:C	2.42	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:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.61
8:H:42:PRO:HD2	8:H:45:ILE:HG12	1.83	0.61
10:P:169:HIS:HD2	10:P:181:LEU:HD11	1.65	0.61
10:P:192:ARG:HA	10:P:192:ARG:CZ	2.30	0.61
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.61
21:q:3:LEU:HD12	21:q:6:VAL:HG21	1.81	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.60
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.60
4:D:144:MET:HE3	4:D:222:MET:HB2	1.83	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.02	0.60
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.60
10:P:263:PHE:HD2	10:P:333:PRO:O	1.83	0.60
21:q:34:ARG:NE	21:q:58:ARG:NH2	2.48	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.60
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.60
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.60
12:R:32:THR:HA	12:R:55:VAL:HG23	1.84	0.60
4:D:264:ASN:O	4:D:265:ASN:C	2.45	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
10:P:136:THR:CG2	10:P:139:PHE:HB2	2.31	0.60
10:P:299:SER:HB3	10:P:316:LYS:HE3	1.83	0.60
16:W:42:TRP:CZ2	16:W:93:LEU:CB	2.83	0.60
17:X:133:THR:HG23	20:b:58:ARG:HH12	1.65	0.60
18:Z:143:TYR:O	18:Z:144:THR:C	2.45	0.60
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.60
4:D:142:VAL:CG1	4:D:182:ASN:HA	2.31	0.60
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
12:R:89:PRO:CG	12:R:106:TYR:CE1	2.83	0.60
16:W:53:MET:SD	16:W:106:VAL:HG21	2.42	0.60
2:B:144:ALA:O	2:B:145:LEU:C	2.45	0.60
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.37	0.60
13:S:19:ILE:HG13	13:S:95:LEU:CD1	2.31	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
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.37	0.60
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.60
9:I:80:GLU:OE2	22:r:26:LEU:HD11	2.01	0.60
14:T:83:VAL:HG22	14:T:126:PHE:HZ	1.66	0.60
16:W:97:ILE:HG23	16:W:98:LYS:HG3	1.83	0.60
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.65	0.60
8:H:239:THR:O	8:H:239:THR:HG22	2.01	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
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.37	0.59
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.59
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.59
3:C:70:LYS:O	15:V:103:LEU:HD12	2.02	0.59
12:R:42:ASP:HB3	12:R:44:ARG:NH1	2.17	0.59
4:D:95:LEU:HG	4:D:97:LEU:HG	1.84	0.59
4:D:142:VAL:HG22	4:D:185:MET:SD	2.42	0.59
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
17:X:20:VAL:HG12	17:X:25:LEU:HD21	1.84	0.59
17:X:37:ASP:HA	17:X:40:ASN:HB2	1.84	0.59
20:b:8:PHE:HA	20:b:11:ASN:ND2	2.18	0.59
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.59
7:G:304:GLU:OE2	10:P:41:ILE:HG12	2.01	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.59
8:H:310:PHE:O	20:b:38:TYR:HB2	2.02	0.59
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.02	0.59
18:Z:98:MET:HB2	18:Z:104:TRP:NE1	2.18	0.59
1:A:68:GLU:CD	1:A:98:LEU:HG	2.28	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
8:H:142:TYR:CG	8:H:289:LEU:HD12	2.38	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
10:P:262:THR:N	10:P:332:LEU:HD12	2.12	0.59
4:D:375:MET:HE1	7:G:126:LEU:CA	2.33	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	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
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.84	0.59
10:P:96:LEU:HD12	10:P:96:LEU:C	2.28	0.59
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.32	0.59
2:B:91:TRP:CH2	30:H:401:UQ9:C1M	2.86	0.59
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.36	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
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.59
17:X:78:CYS:SG	17:X:110:CYS:HB3	2.42	0.59
21:q:51:ASP:O	21:q:59:HIS:HB2	2.02	0.59
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.33	0.59
2:B:105:MET:CE	4:D:200:PHE:CE2	2.80	0.59
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.59
4:D:388:GLY:HA3	4:D:417:SER:OG	2.02	0.59
6:F:119:GLU:HB3	6:F:124:THR:CG2	2.32	0.59
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.59
10:P:318:LYS:O	10:P:322:ILE:HG13	2.02	0.59
13:S:47:ALA:O	13:S:49:PRO:HD3	2.03	0.59
14:T:123:GLU:OE1	16:W:44:ARG:NH1	2.36	0.59
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.58
10:P:57:THR:HG23	10:P:123:SER:CB	2.33	0.58
10:P:178:SER:O	10:P:182:ARG:HG2	2.02	0.58
13:S:23:LEU:O	13:S:23:LEU:CD1	2.41	0.58
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.85	0.58
18:Z:122:GLY:O	18:Z:126:GLY:N	2.34	0.58
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	2.01	0.58
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.84	0.58
6:F:44:ASN:HB3	6:F:134:ASP:HB2	1.84	0.58
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	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
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.85	0.58
10:P:122:HIS:CB	12:R:46:VAL:HG12	2.33	0.58
12:R:40:GLU:HA	12:R:45:ARG:CZ	2.32	0.58
6:F:382:CYS:SG	25:F:502:SF4:S1	3.02	0.58
10:P:357:ARG:HD3	10:P:361:TRP:O	2.03	0.58
23:s:57:LEU:HG	23:s:58:PRO:HD2	1.83	0.58
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.58
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.67	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.58
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.58
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.83	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.17	0.58
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.30	0.58
18:Z:62:ILE:HG12	20:b:49:THR:HA	1.85	0.58
4:D:99:LEU:HB3	4:D:101:LEU:CD1	2.34	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
10:P:57:THR:HG23	10:P:123:SER:HB2	1.86	0.58
13:S:16:LEU:O	13:S:16:LEU:CD1	2.51	0.58
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.84	0.58
4:D:99:LEU:CD2	4:D:109:CYS:HA	2.32	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.58
17:X:141:PRO:O	17:X:142:TYR:HB2	2.04	0.58
18:Z:129:THR:HB	18:Z:132:GLU:HG3	1.86	0.58
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.04	0.58
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.04	0.58
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.58
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.86	0.58
17:X:122:LEU:HD23	20:b:82:LYS:HG2	1.85	0.58
23:s:35:LEU:HB3	23:s:38:HIS:HB2	1.85	0.58
2:B:126:ARG:HH12	8:H:61:MET:HB3	1.69	0.58
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.58
10:P:220:TYR:HA	10:P:223:PHE:HD2	1.67	0.58
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.58
20:b:69:HIS:CD2	20:b:70:PRO:HD2	2.36	0.58
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.58
2:B:99:CYS:C	2:B:101:ALA:N	2.59	0.58
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.58
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.86	0.58
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.58
17:X:90:ASP:OD2	19:a:62:VAL:HG11	2.04	0.58
17:X:134:ASP:O	17:X:135:ARG:C	2.45	0.58
4:D:128:THR:H	4:D:131:GLN:NE2	2.00	0.57
6:F:48:ARG:NH1	6:F:48:ARG:HA	2.19	0.57
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.57
8:H:85:LEU:CD2	8:H:108:THR:HB	2.33	0.57
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.57
10:P:245:VAL:O	10:P:249:ILE:HG13	2.04	0.57
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.39	0.57
4:D:89:PRO:O	27:D:501:UQ1:O4	2.22	0.57
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.57
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.39	0.57
14:T:90:TYR:CE2	14:T:92:LYS:HB3	2.39	0.57
2:B:110:PRO:HB3	8:H:33:LEU:O	2.03	0.57
2:B:115:ASP:HA	2:B:119:VAL:O	2.04	0.57
2:B:164:CYS:SG	25:B:301:SF4:S4	3.02	0.57
3:C:186:ILE:HG13	3:C:187:LEU:N	2.18	0.57
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.29	0.57
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.84	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:192:ARG:CZ	10:P:198:ALA:HB3	2.34	0.57
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.57
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.86	0.57
14:T:90:TYR:CE2	14:T:92:LYS:CB	2.87	0.57
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.57
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.86	0.57
8:H:307:LEU:HD11	18:Z:47:TYR:CG	2.39	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
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.84	0.57
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
8:H:42:PRO:HD2	8:H:45:ILE:CG1	2.35	0.57
8:H:142:TYR:CE1	8:H:289:LEU:HD12	2.39	0.57
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.57
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.30	0.57
5:E:164:PRO:C	5:E:166:LYS:H	2.11	0.57
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.86	0.57
12:R:37:VAL:O	12:R:38:TYR:C	2.44	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
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
13:S:16:LEU:HD11	13:S:51:LEU:CD1	2.29	0.57
1:A:60:ILE:O	1:A:61:THR:C	2.46	0.57
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.57
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.57
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.57
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.85	0.57
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.04	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
21:q:129:THR:O	21:q:129:THR:HG22	2.03	0.57
2:B:170:TYR:OH	4:D:131:GLN:O	2.22	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
8:H:69:SER:C	8:H:71:PHE:H	2.12	0.57
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:348:LEU:O	18:Z:11:PRO:HB3	2.05	0.57
7:G:126:LEU:HD12	12:R:89:PRO:HB2	1.84	0.57
9:I:62:MET:SD	18:Z:35:MET:HG2	2.45	0.57
10:P:320:GLU:O	10:P:324:ILE:HG12	2.05	0.57
2:B:153:PRO:HB2	2:B:155:PRO:HD2	1.85	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
4:D:142:VAL:HG13	4:D:185:MET:SD	2.45	0.56
4:D:266:ARG:NH1	9:I:60:ILE:HA	2.20	0.56
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.56
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.88	0.56
9:I:89:GLU:HG3	21:q:61:TRP:HB3	1.87	0.56
16:W:83:ASP:O	16:W:87:ILE:HG12	2.04	0.56
17:X:5:VAL:HG13	17:X:7:LEU:HG	1.87	0.56
18:Z:92:GLU:O	18:Z:96:ILE:HG13	2.05	0.56
2:B:100:CYS:HG	25:B:301:SF4:FE4	1.22	0.56
3:C:80:LEU:HD21	4:D:157:LYS:O	2.05	0.56
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.05	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.56
10:P:188:GLU:O	10:P:192:ARG:HG2	2.05	0.56
16:W:104:THR:O	16:W:108:ARG:HG3	2.05	0.56
17:X:52:ASP:OD2	17:X:55:ARG:HG3	2.03	0.56
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.58	0.56
4:D:259:GLU:O	4:D:260:GLU:C	2.49	0.56
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.87	0.56
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.37	0.56
6:F:293:SER:N	6:F:338:ASP:OD1	2.38	0.56
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.10	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
8:H:312:ALA:HB2	20:b:38:TYR:HB3	1.87	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
12:R:59:PHE:O	12:R:63:LEU:HG	2.06	0.56
14:T:134:ASP:OD1	14:T:134:ASP:O	2.23	0.56
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.87	0.56
6:F:213:ILE:HG23	6:F:235:VAL:HA	1.86	0.56
8:H:51:ASP:OD2	30:H:401:UQ9:H12	2.06	0.56
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.70	0.56
12:R:62:ASP:O	12:R:66:GLN:HG3	2.06	0.56
1:A:105:GLU:HG2	1:A:111:LEU:HG	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.21	0.56
14:T:130:ILE:HD11	14:T:148:ILE:HD11	1.86	0.56
16:W:42:TRP:CZ2	33:W:201:EHZ:O1	2.58	0.56
1:A:113:TRP:HH2	8:H:287:HIS:CD2	2.23	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
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
7:G:401:LEU:HD11	7:G:462:PHE:HE2	1.71	0.56
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.41	0.56
8:H:273:ILE:HD11	24:H:402:3PE:H2A1	1.86	0.56
11:Q:165:SER:HB3	11:Q:168:LYS:O	2.06	0.56
12:R:88:HIS:O	12:R:89:PRO:C	2.45	0.56
17:X:137:LEU:HD23	17:X:138:PRO:O	2.05	0.56
18:Z:7:LYS:HB2	18:Z:7:LYS:NZ	2.20	0.56
1:A:22:PHE:O	1:A:25:PRO:HD2	2.05	0.56
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.40	0.56
4:D:338:ARG:NH1	18:Z:23:ARG:HA	2.21	0.56
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.40	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:600:GLU:OE1	7:G:600:GLU:N	2.39	0.56
10:P:64:PHE:HE1	10:P:209:ARG:O	1.88	0.56
10:P:315:THR:O	10:P:316:LYS:C	2.45	0.56
14:T:90:TYR:HE2	14:T:92:LYS:CB	2.19	0.56
2:B:154:GLU:O	10:P:89:TYR:OH	2.21	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
8:H:19:PHE:HB3	19:a:12:MET:HG3	1.87	0.56
8:H:296:LEU:HD21	24:H:402:3PE:H351	1.87	0.56
16:W:42:TRP:CE2	16:W:93:LEU:HB2	2.41	0.56
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.56
2:B:69:SER:O	2:B:70:ARG:C	2.48	0.56
4:D:92:HIS:CB	27:D:501:UQ1:O3	2.54	0.56
4:D:142:VAL:CB	4:D:182:ASN:HD22	2.17	0.56
4:D:238:LEU:HA	18:Z:9:ASP:HB2	1.86	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
16:W:42:TRP:CZ2	16:W:93:LEU:CA	2.89	0.56
6:F:293:SER:HB3	6:F:338:ASP:OD2	2.06	0.56
7:G:382:ARG:HD2	13:S:56:ARG:CD	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:122:HIS:HB2	12:R:46:VAL:HG12	1.88	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	0.55
2:B:97:LEU:HD21	2:B:141:MET:HG2	1.88	0.55
8:H:175:LEU:HD21	26:I:301:PC1:H2C1	1.88	0.55
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.41	0.55
10:P:140:ASP:OD1	10:P:142:GLU:HB2	2.05	0.55
11:Q:160:TYR:OH	11:Q:164:PHE:HZ	1.89	0.55
11:Q:167:ASN:O	11:Q:168:LYS:HG2	2.04	0.55
4:D:266:ARG:NH2	9:I:59:ARG:O	2.39	0.55
4:D:279:THR:HA	15:V:12:VAL:HG13	1.87	0.55
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.55
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.88	0.55
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.55
17:X:132:LYS:HB3	20:b:59:ASP:HB3	1.87	0.55
18:Z:69:ILE:CG2	20:b:54:PRO:HD3	2.37	0.55
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.71	0.55
3:C:184:ARG:HA	16:W:91:MET:SD	2.46	0.55
7:G:35:PHE:O	7:G:101:ASN:HA	2.07	0.55
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.55
11:Q:110:PRO:HB3	12:R:43:TYR:OH	2.06	0.55
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.06	0.55
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.55
4:D:84:PHE:HB2	4:D:97:LEU:HB2	1.87	0.55
5:E:162:THR:HG22	5:E:166:LYS:HA	1.88	0.55
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.07	0.55
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.55
10:P:98:GLY:HA3	10:P:103:LEU:HG	1.87	0.55
10:P:145:PHE:O	10:P:149:PRO:HG2	2.05	0.55
16:W:23:ILE:HG13	16:W:80:ARG:HG2	1.87	0.55
1:A:102:LEU:CD1	1:A:111:LEU:HD11	2.37	0.55
2:B:95:PHE:CE2	2:B:131:MET:SD	2.99	0.55
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.55
2:B:174:SER:HA	3:C:203:LEU:CD2	2.37	0.55
4:D:142:VAL:HG23	4:D:457:VAL:HG21	1.88	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.46	0.55
14:T:83:VAL:CG2	14:T:126:PHE:CZ	2.83	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:139:CYS:CB	5:E:144:SER:HB3	2.35	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.71	0.55
8:H:249:ILE:HD13	17:X:99:HIS:CG	2.42	0.55
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.71	0.55
17:X:124:GLN:C	17:X:125:LEU:HD12	2.32	0.55
20:b:8:PHE:CG	20:b:9:LEU:N	2.74	0.55
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.89	0.55
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.46	0.55
6:F:67:GLU:O	6:F:71:LYS:HG2	2.06	0.55
6:F:170:GLN:HB3	23:s:48:LEU:HD22	1.89	0.55
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.55
10:P:376:ASN:OD1	10:P:376:ASN:C	2.50	0.55
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.87	0.55
17:X:39:THR:HG23	17:X:40:ASN:N	2.20	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
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
5:E:233:LEU:HD11	6:F:289:GLU:OE2	2.07	0.55
6:F:48:ARG:HA	6:F:48:ARG:HH11	1.72	0.55
6:F:382:CYS:SG	25:F:502:SF4:S4	3.05	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
9:I:75:SER:O	22:r:12:ARG:HG2	2.07	0.55
10:P:236:VAL:HG13	10:P:270:ARG:HH21	1.71	0.55
16:W:53:MET:HB2	16:W:55:LEU:HG	1.89	0.55
18:Z:56:GLU:HA	18:Z:59:ARG:HH11	1.72	0.55
22:r:7:VAL:O	22:r:11:LEU:HG	2.06	0.55
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.55
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.55
10:P:71:ASN:HA	10:P:97:MET:SD	2.47	0.55
16:W:25:SER:HB3	16:W:30:GLU:HB3	1.88	0.55
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.55
5:E:164:PRO:C	5:E:166:LYS:N	2.64	0.55
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.37	0.55
6:F:339:PHE:O	6:F:343:VAL:HG23	2.07	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
8:H:69:SER:C	8:H:71:PHE:N	2.61	0.55
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.55
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.49	0.55
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:128:PHE:CE2	14:T:130:ILE:HG13	2.42	0.54
16:W:35:VAL:HG21	33:W:201:EHZ:N2	2.22	0.54
17:X:64:ASN:O	17:X:68:LEU:HG	2.07	0.54
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.54
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
9:I:123:CYS:SG	25:I:302:SF4:S3	3.06	0.54
19:a:31:ASN:HD21	19:a:36:LYS:HB2	1.71	0.54
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.32	0.54
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.23	0.54
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
5:E:199:ASP:O	5:E:203:ILE:HG13	2.08	0.54
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.54
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.88	0.54
5:E:180:VAL:CG1	5:E:224:CYS:SG	2.96	0.54
6:F:119:GLU:HG3	6:F:127:ASP:OD2	2.07	0.54
7:G:617:ARG:HH12	16:W:128:GLY:C	2.16	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
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
14:T:87:LEU:HD22	14:T:104:PHE:CZ	2.41	0.54
19:a:58:ASN:HB2	19:a:61:TYR:CD2	2.43	0.54
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.54
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.43	0.54
4:D:232:VAL:HG23	4:D:356:ILE:HD13	1.88	0.54
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.37	0.54
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.07	0.54
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.90	0.54
6:F:300:ILE:HD11	6:F:311:TRP:HD1	1.72	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	2.22	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.54
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.54
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:207:PHE:CE1	10:P:214:LEU:HD22	2.43	0.54
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.90	0.54
21:q:17:HIS:NE2	21:q:33:ILE:HG23	2.23	0.54
2:B:126:ARG:HH12	8:H:61:MET:CB	2.21	0.54
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.43	0.54
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
8:H:133:LEU:O	8:H:136:VAL:HG12	2.08	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
10:P:172:ALA:H	10:P:202:ARG:NH2	2.06	0.54
15:V:50:GLN:HE22	22:r:94:ALA:H	1.56	0.54
20:b:8:PHE:O	20:b:9:LEU:C	2.50	0.54
1:A:110:GLY:O	1:A:111:LEU:HB2	2.08	0.54
3:C:217:ARG:HH12	16:W:112:GLU:CB	2.19	0.54
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.33	0.54
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.54
9:I:80:GLU:CB	22:r:26:LEU:HD11	2.38	0.54
10:P:300:TRP:O	10:P:304:LEU:HG	2.08	0.54
10:P:316:LYS:O	10:P:320:GLU:HG2	2.08	0.54
14:T:97:LYS:HG3	14:T:97:LYS:O	2.08	0.54
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.54
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.89	0.54
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.54
8:H:43:TYR:CE2	21:q:27:PHE:HZ	2.26	0.54
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.54
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.23	0.54
4:D:92:HIS:HB3	4:D:458:PHE:CE2	2.41	0.54
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.54
4:D:189:THR:CG2	27:D:501:UQ1:HM33	2.38	0.54
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.90	0.54
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.54
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	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
3:C:80:LEU:HD22	4:D:157:LYS:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.54
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.54
6:F:299:LEU:CD1	6:F:300:ILE:HG23	2.37	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.07	0.54
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.91	0.54
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.37	0.54
8:H:293:PHE:CE1	24:H:402:3PE:H32	2.43	0.54
13:S:16:LEU:HD13	13:S:19:ILE:CD1	2.38	0.54
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.54
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.69	0.53
4:D:253:LEU:HD11	22:r:18:GLN:HG3	1.90	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.52	0.53
9:I:67:ILE:HG13	26:I:301:PC1:H251	1.89	0.53
9:I:109:GLY:O	12:R:63:LEU:HD12	2.08	0.53
10:P:85:ARG:HE	31:P:401:NDP:C2A	2.21	0.53
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.53
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.53
4:D:92:HIS:O	4:D:93:GLY:C	2.50	0.53
4:D:368:ARG:HA	4:D:371:MET:HG2	1.90	0.53
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.53
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.53
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.53
7:G:617:ARG:NH1	16:W:128:GLY:C	2.66	0.53
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.53
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
9:I:80:GLU:OE2	22:r:26:LEU:HD13	2.08	0.53
10:P:58:VAL:O	10:P:83:PRO:HD2	2.09	0.53
3:C:100:ARG:HH12	15:V:86:LYS:NZ	2.06	0.53
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.73	0.53
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.53
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.53
12:R:98:GLU:HA	12:R:113:GLN:CD	2.34	0.53
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.90	0.53
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.53
10:P:142:GLU:HA	10:P:146:VAL:HG12	1.90	0.53
10:P:353:LEU:HA	10:P:356:HIS:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.53
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.53
17:X:133:THR:HG23	20:b:58:ARG:NH1	2.23	0.53
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.53
4:D:210:MET:O	4:D:211:PHE:C	2.51	0.53
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.53
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.90	0.53
6:F:235:VAL:HG12	6:F:240:THR:OG1	2.08	0.53
6:F:339:PHE:HA	6:F:349:LEU:HB2	1.90	0.53
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.53
2:B:122:ARG:HH21	4:D:89:PRO:HB3	1.74	0.53
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.39	0.53
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.89	0.53
5:E:77:ALA:C	5:E:80:PRO:HD2	2.33	0.53
5:E:139:CYS:C	5:E:144:SER:HB3	2.33	0.53
6:F:85:LEU:HD13	6:F:262:PHE:CE2	2.44	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.44	0.53
14:T:118:ILE:HG23	14:T:122:MET:CE	2.37	0.53
20:b:59:ASP:HA	20:b:63:MET:HE2	1.89	0.53
21:q:73:THR:HA	21:q:76:ASP:OD1	2.09	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53
6:F:235:VAL:HG22	6:F:236:PHE:HD2	1.68	0.53
7:G:364:ASP:C	7:G:364:ASP:OD1	2.52	0.53
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.53
10:P:370:LYS:HG3	10:P:370:LYS:O	2.08	0.53
13:S:30:SER:O	13:S:31:GLN:C	2.49	0.53
14:T:100:VAL:O	14:T:141:PRO:HD2	2.09	0.53
21:q:55:PHE:CG	22:r:26:LEU:HD22	2.43	0.53
2:B:125:PRO:HB3	2:B:148:VAL:HG13	1.89	0.53
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.53
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.73	0.53
4:D:338:ARG:HH12	18:Z:23:ARG:HA	1.74	0.53
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.53
6:F:80:MET:HE2	6:F:95:THR:HG21	1.89	0.53
6:F:294:VAL:HG12	6:F:337:MET:HB2	1.90	0.53
6:F:329:LYS:HA	6:F:332:CYS:SG	2.49	0.53
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.53
8:H:292:ASN:O	20:b:18:VAL:HG11	2.09	0.53
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.53
14:T:87:LEU:HD23	14:T:122:MET:HE1	1.91	0.53
19:a:42:GLN:O	19:a:43:TYR:C	2.50	0.53
21:q:29:ARG:HD3	21:q:74:PHE:CE1	2.44	0.53
2:B:136:THR:HG21	4:D:118:ARG:HG2	1.90	0.53
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.53
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.27	0.53
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.24	0.53
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.53
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.73	0.53
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.39	0.53
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.91	0.53
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.53
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.91	0.53
1:A:112:GLU:C	1:A:113:TRP:CG	2.86	0.53
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.53
6:F:411:SER:HA	6:F:414:GLU:CD	2.34	0.53
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.53
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.91	0.53
8:H:142:TYR:CA	8:H:289:LEU:CD1	2.74	0.53
9:I:54:THR:HG22	20:b:13:TRP:HE1	1.74	0.53
9:I:80:GLU:HB3	22:r:26:LEU:HD11	1.90	0.53
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.53
10:P:336:GLU:CG	10:P:342:PRO:HD3	2.38	0.53
12:R:69:VAL:HG12	12:R:112:LYS:N	2.24	0.53
18:Z:65:LEU:HB3	20:b:50:PRO:O	2.09	0.53
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
8:H:249:ILE:HG21	17:X:99:HIS:CE1	2.45	0.52
4:D:189:THR:HG21	27:D:501:UQ1:HM22	1.92	0.52
5:E:65:ILE:HA	5:E:68:ASN:ND2	2.24	0.52
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.75	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52
7:G:372:PHE:H	7:G:532:PRO:HB2	1.74	0.52
8:H:23:VAL:HG11	19:a:9:LEU:CD2	2.39	0.52
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.52
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.52
10:P:265:PHE:HD1	10:P:334:GLY:HA3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:305:PHE:CG	10:P:314:THR:HG22	2.45	0.52
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.52
21:q:9:ARG:HA	21:q:12:GLN:CG	2.37	0.52
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.64	0.52
3:C:170:TRP:CZ2	16:W:91:MET:HE1	2.44	0.52
5:E:39:VAL:HG21	7:G:163:LYS:NZ	2.25	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.52
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.52
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.42	0.52
1:A:21:ALA:HB2	8:H:218:GLY:HA3	1.90	0.52
2:B:92:PRO:HD3	2:B:119:VAL:HG13	1.91	0.52
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.74	0.52
7:G:541:PRO:HB2	7:G:561:PRO:HD3	1.91	0.52
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.52
20:b:66:VAL:HG11	20:b:70:PRO:HA	1.92	0.52
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.07	0.52
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.23	0.52
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.85	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52
14:T:130:ILE:CG2	14:T:131:PRO:HD2	2.40	0.52
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.52
17:X:77:HIS:HD2	17:X:115:LEU:HD21	1.75	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52
1:A:113:TRP:CH2	8:H:287:HIS:CD2	2.98	0.52
3:C:104:ASN:O	22:r:97:PRO:HD3	2.10	0.52
7:G:617:ARG:HH12	16:W:129:HIS:N	2.07	0.52
10:P:283:MET:HE2	10:P:366:ILE:HG22	1.92	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
1:A:8:PHE:O	1:A:12:LEU:HG	2.10	0.52
5:E:177:GLY:O	28:E:301:FES:S1	2.68	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.44	0.52
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:O	1:A:20:VAL:C	2.50	0.52
1:A:102:LEU:HD11	1:A:111:LEU:HD11	1.91	0.52
2:B:81:LEU:HD22	26:B:302:PC1:H262	1.92	0.52
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.43	0.52
4:D:381:HIS:HE1	9:I:161:ALA:O	1.93	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.52
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
7:G:399:VAL:HG21	7:G:462:PHE:CZ	2.44	0.52
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.52
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.52
9:I:155:CYS:SG	25:I:302:SF4:S2	3.08	0.52
14:T:103:HIS:HD1	14:T:140:CYS:HG	1.52	0.52
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.35	0.52
16:W:94:GLN:HA	16:W:97:ILE:HG22	1.92	0.52
21:q:29:ARG:HD3	21:q:74:PHE:CD1	2.44	0.52
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.52
14:T:79:ILE:CG2	14:T:145:VAL:HG13	2.40	0.52
20:b:48:ALA:O	20:b:49:THR:C	2.53	0.52
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.52
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.91	0.52
2:B:126:ARG:NH1	8:H:61:MET:SD	2.82	0.52
6:F:126:LYS:HG3	6:F:275:LEU:CB	2.39	0.52
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.45	0.52
10:P:236:VAL:HG11	10:P:270:ARG:HH21	1.75	0.52
19:a:2:TRP:O	19:a:3:PHE:C	2.53	0.52
21:q:65:THR:CG2	21:q:66:THR:N	2.72	0.52
4:D:101:LEU:HG	4:D:106:VAL:HA	1.91	0.51
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	2.98	0.51
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.51
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.92	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
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.51
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.92	0.51
18:Z:61:LEU:O	18:Z:64:ASP:OD1	2.29	0.51
21:q:125:VAL:HG23	21:q:125:VAL:O	2.08	0.51
1:A:113:TRP:CH2	8:H:287:HIS:HD2	2.27	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.91	0.51
5:E:196:THR:O	5:E:197:PRO:C	2.54	0.51
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.51
21:q:56:PHE:HD1	21:q:59:HIS:NE2	2.06	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.92	0.51
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.51
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	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:99:ASN:OD1	19:a:40:ARG:HG3	2.11	0.51
8:H:222:LEU:O	8:H:223:PHE:C	2.50	0.51
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.51
10:P:192:ARG:NH1	10:P:198:ALA:HB3	2.25	0.51
6:F:331:VAL:O	6:F:335:VAL:HG23	2.10	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.51
9:I:71:GLY:O	22:r:15:ALA:HB1	2.11	0.51
10:P:157:LYS:O	10:P:158:GLU:C	2.53	0.51
17:X:25:LEU:O	17:X:29:ALA:N	2.44	0.51
4:D:304:LYS:HE2	9:I:35:THR:N	2.24	0.51
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.24	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
16:W:65:LYS:HE3	16:W:69:MET:HE2	1.92	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.93	0.51
3:C:73:GLN:NE2	15:V:112:TRP:HE1	2.07	0.51
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.11	0.51
5:E:39:VAL:HG11	7:G:163:LYS:HZ3	1.75	0.51
6:F:259:GLY:O	6:F:263:ALA:N	2.40	0.51
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.51
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.51
8:H:292:ASN:HB3	24:H:402:3PE:H31	1.92	0.51
10:P:374:THR:HG23	10:P:374:THR:O	2.11	0.51
14:T:140:CYS:HB2	14:T:143:GLU:CG	2.40	0.51
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.51
1:A:105:GLU:HG3	1:A:111:LEU:HG	1.91	0.51
4:D:144:MET:HE2	4:D:214:TYR:CE2	2.46	0.51
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.25	0.51
4:D:299:GLN:HB3	22:r:104:TRP:CE3	2.45	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	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:305:PHE:HB2	10:P:314:THR:HG22	1.92	0.51
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.51
20:b:11:ASN:OD1	20:b:12:ALA:N	2.44	0.51
2:B:94:THR:OG1	27:D:501:UQ1:H103	2.10	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	2.36	0.51
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.51
6:F:225:LEU:HB2	11:Q:160:TYR:CZ	2.45	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.51
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.51
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.75	0.51
1:A:106:TRP:CD1	1:A:111:LEU:HD12	2.45	0.51
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.41	0.51
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.51
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
8:H:307:LEU:HD11	18:Z:47:TYR:CD1	2.46	0.51
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.51
14:T:87:LEU:HD23	14:T:122:MET:CE	2.41	0.51
15:V:44:TYR:CD1	15:V:48:THR:HG23	2.46	0.51
5:E:70:PRO:HB3	23:s:60:PRO:HG3	1.92	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.51
10:P:234:LYS:HG2	10:P:234:LYS:O	2.10	0.51
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.11	0.51
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.92	0.50
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.50
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.40	0.50
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.50
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.50
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.46	0.50
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.46	0.50
17:X:4:ILE:CG2	17:X:5:VAL:N	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:130:LYS:CE	20:b:67:PRO:HB3	2.42	0.50
1:A:11:ILE:CD1	24:A:401:3PE:H2D1	2.41	0.50
3:C:241:PHE:H	7:G:146:PHE:HE1	1.58	0.50
4:D:345:GLU:HB2	18:Z:19:ILE:HD12	1.93	0.50
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.50
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.50
2:B:99:CYS:C	2:B:101:ALA:H	2.19	0.50
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.45	0.50
4:D:359:ASP:O	7:G:150:ARG:NH2	2.44	0.50
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.50
6:F:217:GLU:CD	11:Q:166:TRP:HE1	2.18	0.50
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.50
7:G:651:PRO:HD2	13:S:56:ARG:HD2	1.93	0.50
10:P:108:TRP:CZ2	31:P:401:NDP:H2A	2.46	0.50
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.50
11:Q:167:ASN:C	11:Q:168:LYS:HG2	2.36	0.50
14:T:130:ILE:HG23	14:T:131:PRO:CD	2.40	0.50
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.93	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
2:B:171:TYR:HE1	4:D:120:THR:HG22	1.76	0.50
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.94	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.50
10:P:65:LEU:HD23	10:P:129:LEU:HD22	1.93	0.50
10:P:209:ARG:N	10:P:352:VAL:HG22	2.26	0.50
17:X:38:LYS:O	17:X:42:GLU:HG3	2.11	0.50
2:B:84:TRP:HA	2:B:87:ARG:HG2	1.93	0.50
6:F:49:HIS:O	6:F:50:ASP:C	2.54	0.50
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.50
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.50
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.50
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.91	0.50
12:R:55:VAL:HG22	12:R:56:ASN:H	1.77	0.50
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.50
14:T:105:MET:HB2	14:T:139:MET:SD	2.51	0.50
14:T:140:CYS:O	14:T:144:ILE:HG13	2.12	0.50
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.50
2:B:81:LEU:CG	8:H:53:MET:HE1	2.34	0.50
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.42	0.50
2:B:99:CYS:O	2:B:101:ALA:N	2.44	0.50
2:B:171:TYR:CE1	4:D:120:THR:HG22	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:LEU:HD11	12:R:89:PRO:CB	2.41	0.50
8:H:17:MET:CE	8:H:225:MET:HB3	2.41	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
2:B:94:THR:OG1	27:D:501:UQ1:H101	2.09	0.50
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.50
4:D:289:SER:N	4:D:293:LEU:HG	2.26	0.50
5:E:55:THR:O	5:E:56:PRO:C	2.54	0.50
5:E:245:GLN:HB3	6:F:256:ARG:O	2.11	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:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	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
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.50
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.50
16:W:97:ILE:C	16:W:99:VAL:H	2.18	0.50
4:D:97:LEU:HD23	4:D:111:PRO:HA	1.94	0.50
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	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
13:S:42:VAL:O	13:S:46:LYS:HG3	2.12	0.50
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.50
17:X:137:LEU:HG	17:X:138:PRO:HD2	1.92	0.50
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.50
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.50
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.50
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.94	0.50
10:P:70:VAL:HG12	10:P:97:MET:SD	2.52	0.50
10:P:135:GLU:CG	10:P:140:ASP:HA	2.41	0.50
10:P:367:GLU:HG2	10:P:368:GLU:N	2.26	0.50
13:S:24:CYS:N	13:S:58:CYS:SG	2.85	0.50
14:T:138:LEU:HD13	14:T:144:ILE:CD1	2.42	0.50
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.50
19:a:4:GLU:O	19:a:7:PRO:HD2	2.11	0.50
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.50
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.41	0.49
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.49
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:185:ASN:HA	6:F:189:SER:O	2.11	0.49
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.49
18:Z:66:GLU:HA	18:Z:69:ILE:HG12	1.93	0.49
1:A:54:LYS:O	1:A:58:VAL:HG23	2.12	0.49
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
4:D:185:MET:CE	4:D:207:ARG:NH2	2.52	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
6:F:383:THR:O	6:F:384:PRO:C	2.55	0.49
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.49
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.49
7:G:272:ARG:HH11	7:G:274:LEU:HD23	1.77	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
19:a:3:PHE:O	19:a:6:LEU:HG	2.11	0.49
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.95	0.49
3:C:73:GLN:HE21	15:V:112:TRP:HE1	1.60	0.49
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.49
4:D:148:GLU:O	4:D:149:GLN:C	2.55	0.49
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.49
4:D:460:GLU:O	4:D:463:ARG:HG2	2.11	0.49
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.49
11:Q:160:TYR:CD2	11:Q:164:PHE:CE2	2.91	0.49
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.49
18:Z:129:THR:HG22	18:Z:131:GLU:H	1.77	0.49
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.49
3:C:224:GLU:OE2	10:P:45:LYS:HB3	2.13	0.49
4:D:142:VAL:CG1	4:D:182:ASN:HD22	2.25	0.49
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.49
6:F:427:LEU:HB2	29:F:501:FMN:C7M	2.43	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
10:P:172:ALA:H	10:P:202:ARG:HH21	1.59	0.49
10:P:192:ARG:CZ	10:P:200:ILE:HD11	2.42	0.49
10:P:315:THR:H	10:P:318:LYS:HB3	1.76	0.49
12:R:67:GLN:HG2	12:R:109:LEU:HD21	1.95	0.49
17:X:49:GLU:HB3	17:X:138:PRO:HG3	1.93	0.49
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.31	0.49
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.93	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.47	0.49
6:F:342:LEU:HD12	6:F:349:LEU:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:162:ASP:O	7:G:163:LYS:HD3	2.12	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
8:H:155:LEU:O	8:H:315:PRO:HG3	2.12	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
10:P:238:GLN:HB2	10:P:270:ARG:HG2	1.94	0.49
17:X:33:GLY:CA	18:Z:70:ALA:HB1	2.43	0.49
18:Z:69:ILE:HG23	20:b:54:PRO:CD	2.41	0.49
18:Z:140:PHE:O	18:Z:141:THR:C	2.56	0.49
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.49
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.49
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.49
10:P:235:THR:O	10:P:236:VAL:C	2.56	0.49
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.49
16:W:42:TRP:CE2	16:W:93:LEU:HD12	2.47	0.49
17:X:73:GLN:OE1	17:X:117:TRP:HZ2	1.96	0.49
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.93	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
8:H:12:PRO:O	19:a:15:CYS:HB3	2.13	0.49
8:H:303:TRP:CZ3	20:b:28:LEU:HG	2.48	0.49
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.49
9:I:106:TYR:O	9:I:107:PRO:C	2.55	0.49
10:P:64:PHE:CZ	10:P:211:ASP:HB3	2.48	0.49
10:P:197:GLU:HB3	10:P:259:VAL:HG23	1.93	0.49
14:T:88:LYS:NZ	14:T:96:GLU:H	2.11	0.49
1:A:18:ILE:O	1:A:21:ALA:HB3	2.13	0.49
24:A:401:3PE:O14	24:A:401:3PE:N	2.38	0.49
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.49
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.49
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.42	0.49
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
7:G:179:CYS:HG	25:G:802:SF4:FE3	1.28	0.49
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.49
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.49
15:V:56:LEU:HA	15:V:59:VAL:HB	1.94	0.49
1:A:72:LEU:HB3	8:H:151:LEU:HD21	1.95	0.48
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.26	0.48
4:D:279:THR:HG23	15:V:13:GLY:CA	2.23	0.48
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.48
6:F:379:CYS:SG	25:F:502:SF4:S1	3.11	0.48
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.48
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	0.48
9:I:49:ASP:O	9:I:50:MET:C	2.55	0.48
9:I:114:ILE:HD13	12:R:106:TYR:CD1	2.48	0.48
26:I:301:PC1:H133	18:Z:30:LEU:O	2.13	0.48
1:A:109:LYS:HD2	1:A:112:GLU:OE2	2.14	0.48
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.48
4:D:145:MET:HG3	4:D:214:TYR:CE2	2.48	0.48
4:D:202:TRP:CH2	9:I:72:MET:HG2	2.48	0.48
4:D:279:THR:HA	15:V:12:VAL:CG1	2.43	0.48
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.48
5:E:39:VAL:HG21	7:G:163:LYS:HZ2	1.78	0.48
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.48
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.95	0.48
6:F:126:LYS:HG3	6:F:275:LEU:HB3	1.94	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.48	0.48
8:H:66:THR:HA	8:H:124:ASN:OD1	2.13	0.48
8:H:93:HIS:CE1	19:a:24:ALA:CA	2.94	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.48
8:H:296:LEU:CD2	24:H:402:3PE:H351	2.43	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
17:X:53:PRO:HD2	18:Z:116:TRP:HD1	1.75	0.48
3:C:176:PHE:CE1	16:W:87:ILE:HG21	2.48	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
12:R:32:THR:CG2	12:R:36:GLN:H	2.18	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
17:X:115:LEU:HD13	17:X:117:TRP:CZ3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.48
6:F:343:VAL:O	6:F:344:GLN:C	2.54	0.48
7:G:34:VAL:HG11	7:G:96:VAL:HG22	1.94	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.48
13:S:36:PHE:CZ	13:S:44:LEU:HD11	2.36	0.48
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.48
17:X:112:LEU:HD13	17:X:118:VAL:HG22	1.95	0.48
1:A:11:ILE:HD11	24:A:401:3PE:H2D1	1.95	0.48
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.49	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.48
5:E:45:GLU:CD	5:E:45:GLU:H	2.21	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
20:b:23:PHE:CD2	24:b:201:3PE:H281	2.40	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
3:C:234:LEU:O	4:D:387:GLU:HG3	2.13	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.73	0.48
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.48
8:H:20:LEU:HA	19:a:12:MET:SD	2.53	0.48
9:I:171:PRO:HB3	21:q:93:MET:CE	2.38	0.48
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.14	0.48
14:T:90:TYR:HE2	14:T:92:LYS:HB3	1.78	0.48
14:T:119:ILE:HG13	14:T:135:ALA:HB1	1.95	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.95	0.48
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.48
5:E:143:ASP:O	5:E:144:SER:C	2.55	0.48
5:E:221:ARG:HH21	5:E:227:ALA:HB2	1.79	0.48
5:E:222:PHE:O	5:E:223:CYS:C	2.56	0.48
7:G:33:GLU:OE2	7:G:40:SER:HA	2.14	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
8:H:93:HIS:HE1	19:a:24:ALA:HA	1.74	0.48
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.48
17:X:17:GLU:HB3	17:X:19:LYS:HG3	1.96	0.48
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.48
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ASP:O	2:B:116:ARG:C	2.55	0.48
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.48
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.49	0.48
6:F:270:ASN:ND2	6:F:338:ASP:HB3	2.29	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.48
9:I:54:THR:HG21	18:Z:33:TYR:CE2	2.49	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
11:Q:64:LEU:HD12	16:W:85:LEU:HD21	1.95	0.48
18:Z:85:GLN:O	18:Z:89:GLU:HG3	2.14	0.48
1:A:102:LEU:HG	1:A:106:TRP:HE1	1.79	0.48
2:B:174:SER:HB2	4:D:123:LEU:HD21	1.96	0.48
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.49	0.48
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.48
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.48
10:P:191:VAL:CG1	10:P:192:ARG:HH21	2.26	0.48
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.43	0.48
12:R:89:PRO:HG2	12:R:106:TYR:CE2	2.49	0.48
14:T:104:PHE:CZ	14:T:118:ILE:HG21	2.48	0.48
4:D:137:ASP:OD1	4:D:148:GLU:HG2	2.13	0.48
4:D:142:VAL:CG2	4:D:185:MET:SD	3.02	0.48
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.48	0.48
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.95	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.48
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.96	0.48
10:P:294:PRO:HB3	10:P:296:PHE:HD1	1.79	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
3:C:151:PRO:HG2	16:W:23:ILE:HG23	1.96	0.47
4:D:189:THR:HG22	27:D:501:UQ1:HM33	1.96	0.47
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.24	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.95	0.47
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.47
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.47
17:X:122:LEU:HD21	20:b:81:LEU:HD23	1.95	0.47
20:b:68:SER:O	20:b:69:HIS:C	2.56	0.47
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
6:F:299:LEU:HD11	6:F:300:ILE:HG23	1.95	0.47
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	0.47
8:H:272:TRP:HH2	26:I:301:PC1:H381	1.79	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
13:S:50:ASN:O	13:S:51:LEU:C	2.57	0.47
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.47
24:b:201:3PE:H281	24:b:201:3PE:H252	1.62	0.47
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.49	0.47
2:B:224:ARG:HG3	10:P:85:ARG:HH22	1.79	0.47
5:E:142:ARG:O	5:E:143:ASP:HB2	2.13	0.47
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.49	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
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.47
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.14	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.79	0.47
10:P:170:LEU:HG	10:P:171:ASN:N	2.28	0.47
10:P:311:GLU:O	10:P:312:PRO:C	2.57	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	2.14	0.47
16:W:120:ASP:OD1	16:W:121:PHE:N	2.46	0.47
17:X:123:GLY:HA2	18:Z:66:GLU:OE2	2.14	0.47
2:B:126:ARG:NH1	8:H:61:MET:HB3	2.28	0.47
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.47
6:F:110:PRO:O	6:F:238:CYS:HB3	2.15	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
3:C:209:LEU:HD21	16:W:108:ARG:NH1	2.29	0.47
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.48	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
7:G:688:GLN:HA	7:G:693:ASP:CB	2.44	0.47
8:H:180:PRO:CD	18:Z:43:LEU:HD21	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:116:ILE:O	15:V:116:ILE:CG2	2.61	0.47
17:X:39:THR:CG2	17:X:40:ASN:N	2.77	0.47
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.47
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.29	0.47
5:E:145:ASP:O	5:E:146:SER:C	2.56	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
10:P:304:LEU:O	10:P:307:LEU:HB3	2.14	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
2:B:99:CYS:O	2:B:100:CYS:C	2.57	0.47
2:B:117:PHE:HA	8:H:39:ILE:HG21	1.95	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
6:F:425:CYS:SG	25:F:502:SF4:S4	3.13	0.47
7:G:82:ILE:HG21	7:G:100:TRP:HB3	1.96	0.47
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.47
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.47
7:G:541:PRO:HB2	7:G:561:PRO:CG	2.44	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
8:H:224:PHE:CZ	30:H:401:UQ9:C13	2.94	0.47
8:H:310:PHE:HB3	20:b:33:PRO:HA	1.96	0.47
9:I:209:TYR:CG	12:R:86:LEU:HD21	2.50	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
16:W:32:LYS:O	16:W:36:ARG:HG3	2.15	0.47
16:W:32:LYS:CE	33:W:201:EHZ:C19	2.90	0.47
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.40	0.47
18:Z:87:LEU:HD21	18:Z:119:PRO:HG3	1.97	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
3:C:70:LYS:HB2	15:V:99:PRO:O	2.14	0.47
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.45	0.47
6:F:44:ASN:ND2	6:F:133:HIS:O	2.48	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.47
6:F:281:HIS:HB3	6:F:358:ASP:CG	2.40	0.47
9:I:49:ASP:O	9:I:53:ALA:N	2.41	0.47
9:I:188:GLU:OE1	12:R:56:ASN:CB	2.63	0.47
10:P:76:MET:HE1	10:P:254:LYS:CE	2.45	0.47
10:P:212:ARG:O	10:P:213:PHE:C	2.55	0.47
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.97	0.47
10:P:287:THR:HG23	10:P:289:ILE:HD11	1.97	0.47
13:S:58:CYS:HB2	13:S:61:VAL:CG1	2.43	0.47
17:X:80:GLU:O	17:X:81:PRO:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:8:LYS:HG2	21:q:12:GLN:HE21	1.79	0.47
1:A:87:MET:HE3	1:A:87:MET:HB3	1.84	0.47
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.47
4:D:280:ALA:CB	15:V:11:LEU:CG	2.90	0.47
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.97	0.47
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
17:X:7:LEU:CD1	18:Z:87:LEU:HB3	2.45	0.47
17:X:139:GLU:O	17:X:140:ASN:C	2.57	0.47
19:a:49:GLU:CD	19:a:52:ARG:HH11	2.22	0.47
22:r:109:ASP:O	22:r:110:GLN:OE1	2.32	0.47
23:s:55:PHE:O	23:s:56:ARG:C	2.57	0.47
1:A:108:GLN:C	1:A:110:GLY:N	2.72	0.47
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.47	0.47
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.47
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.97	0.47
6:F:251:SER:N	6:F:252:PRO:HD2	2.30	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
8:H:224:PHE:CZ	30:H:401:UQ9:H11	2.48	0.47
10:P:55:VAL:HG12	10:P:123:SER:HA	1.96	0.47
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.96	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
16:W:46:VAL:O	16:W:50:VAL:HG23	2.14	0.47
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.44	0.47
21:q:14:VAL:HA	21:q:23:LEU:HD13	1.97	0.47
4:D:142:VAL:CG1	4:D:185:MET:SD	3.03	0.46
4:D:299:GLN:OE1	22:r:104:TRP:HB2	2.14	0.46
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.46
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.96	0.46
7:G:496:MET:O	7:G:500:ILE:HG13	2.14	0.46
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	0.46
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.81	0.46
9:I:64:THR:HG21	18:Z:35:MET:HE1	1.97	0.46
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.03	0.46
10:P:207:PHE:CD2	10:P:241:TYR:HD1	2.33	0.46
10:P:276:LEU:O	10:P:280:ILE:HG13	2.15	0.46
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.46
12:R:88:HIS:HE1	12:R:91:VAL:HG22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:115:LEU:HD13	17:X:117:TRP:CZ2	2.51	0.46
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.49	0.46
3:C:134:LEU:H	3:C:134:LEU:HD12	1.80	0.46
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.46
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.46
6:F:213:ILE:CG2	6:F:224:ARG:HH21	2.27	0.46
8:H:1:MET:HE3	19:a:29:PHE:CE1	2.50	0.46
9:I:53:ALA:O	9:I:54:THR:C	2.56	0.46
10:P:245:VAL:HA	10:P:265:PHE:CD2	2.49	0.46
14:T:114:ASP:OD1	16:W:67:ARG:NH1	2.48	0.46
17:X:35:GLN:HG3	17:X:70:PHE:HE1	1.80	0.46
2:B:116:ARG:HA	8:H:37:PRO:HA	1.97	0.46
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.97	0.46
7:G:275:PRO:HB3	7:G:286:ILE:HG23	1.96	0.46
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.46
10:P:235:THR:HG22	10:P:323:HIS:O	2.15	0.46
13:S:19:ILE:HD12	13:S:94:VAL:CG1	2.44	0.46
17:X:20:VAL:CG2	17:X:24:VAL:HG21	2.40	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.58	0.46
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.96	0.46
2:B:140:LYS:O	2:B:143:PRO:HD2	2.14	0.46
6:F:39:ASP:CA	6:F:261:TRP:HZ2	2.28	0.46
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.46
10:P:209:ARG:O	10:P:210:GLU:HB2	2.15	0.46
12:R:33:HIS:HE1	12:R:56:ASN:HD22	1.64	0.46
15:V:22:GLU:O	15:V:26:ILE:HG12	2.16	0.46
16:W:50:VAL:HA	16:W:55:LEU:HD12	1.97	0.46
19:a:58:ASN:HB2	19:a:61:TYR:CE2	2.50	0.46
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.97	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
4:D:144:MET:HE3	4:D:222:MET:HA	1.97	0.46
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.39	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
6:F:358:ASP:C	6:F:360:SER:H	2.22	0.46
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.96	0.46
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:32:THR:HA	12:R:55:VAL:CG2	2.46	0.46
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.46
18:Z:62:ILE:CG1	20:b:49:THR:HG22	2.44	0.46
21:q:55:PHE:CD1	22:r:26:LEU:CD2	2.95	0.46
21:q:71:LYS:HB2	21:q:73:THR:HG23	1.97	0.46
2:B:94:THR:HB	2:B:104:MET:CE	2.45	0.46
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.81	0.46
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.50	0.46
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.97	0.46
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.46
9:I:90:LYS:HG2	21:q:90:LEU:HD21	1.97	0.46
12:R:38:TYR:CD1	12:R:44:ARG:HB2	2.51	0.46
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.46
14:T:117:GLU:HG2	16:W:43:TYR:CZ	2.51	0.46
14:T:119:ILE:CD1	14:T:138:LEU:HD11	2.43	0.46
15:V:72:LEU:CD1	15:V:72:LEU:C	2.89	0.46
21:q:48:TYR:OH	21:q:83:PRO:HD2	2.15	0.46
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.46
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
24:H:402:3PE:H361	9:I:61:LEU:O	2.16	0.46
9:I:123:CYS:SG	25:I:302:SF4:S4	3.13	0.46
12:R:39:ASP:CG	12:R:40:GLU:N	2.74	0.46
17:X:33:GLY:HA3	18:Z:70:ALA:HB1	1.98	0.46
23:s:52:LEU:HB3	23:s:56:ARG:HH11	1.81	0.46
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.46
5:E:143:ASP:O	5:E:146:SER:N	2.49	0.46
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.51	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
7:G:689:LEU:HD12	7:G:689:LEU:HA	1.79	0.46
10:P:66:GLY:O	10:P:69:VAL:N	2.48	0.46
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.46
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.50	0.46
16:W:97:ILE:C	16:W:99:VAL:N	2.73	0.46
17:X:54:ARG:HD3	18:Z:116:TRP:CE3	2.51	0.46
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.46
6:F:51:TRP:CB	6:F:133:HIS:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.46
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.46
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.46
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.46
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.46
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.97	0.46
10:P:261:LYS:HB2	10:P:263:PHE:CE1	2.51	0.46
20:b:28:LEU:O	20:b:32:MET:HG2	2.15	0.46
3:C:79:CYS:O	3:C:80:LEU:CB	2.60	0.46
4:D:198:THR:HA	8:H:32:GLN:HG2	1.98	0.46
4:D:368:ARG:NH2	9:I:165:ASP:HB2	2.31	0.46
6:F:35:LEU:HG	6:F:39:ASP:HB2	1.97	0.46
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.46
7:G:176:CYS:SG	25:G:802:SF4:S1	3.14	0.46
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.46
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.46
10:P:157:LYS:O	10:P:160:GLY:N	2.49	0.46
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.46
14:T:87:LEU:CD2	14:T:122:MET:HE1	2.46	0.46
17:X:5:VAL:CG1	17:X:7:LEU:HG	2.46	0.46
20:b:38:TYR:O	20:b:39:THR:C	2.59	0.46
2:B:99:CYS:O	2:B:102:VAL:N	2.45	0.45
2:B:126:ARG:HG3	8:H:213:VAL:O	2.16	0.45
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.45
6:F:51:TRP:HZ2	23:s:36:GLN:HG3	1.80	0.45
6:F:137:LYS:HG2	6:F:249:ALA:HB1	1.98	0.45
6:F:398:ARG:HH12	6:F:408:GLU:CD	2.25	0.45
7:G:82:ILE:HG23	7:G:100:TRP:HB3	1.96	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.45
10:P:220:TYR:HA	10:P:223:PHE:CD2	2.51	0.45
15:V:56:LEU:HD13	15:V:60:LYS:HE2	1.98	0.45
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.28	0.45
20:b:45:ILE:N	20:b:80:TRP:HH2	2.14	0.45
24:A:401:3PE:H352	24:A:401:3PE:H262	1.98	0.45
3:C:75:VAL:HG23	3:C:83:LEU:HD11	1.98	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.45
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.45
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.99	0.45
5:E:163:THR:O	5:E:166:LYS:HD3	2.16	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
9:I:92:PRO:HB3	21:q:92:CYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:131:GLY:HA3	31:P:401:NDP:O3D	2.15	0.45
11:Q:160:TYR:CE1	11:Q:164:PHE:HZ	2.25	0.45
13:S:42:VAL:HB	13:S:46:LYS:HE3	1.98	0.45
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.32	0.45
4:D:144:MET:O	4:D:148:GLU:HG3	2.16	0.45
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.45
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.74	0.45
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.45
6:F:249:ALA:O	6:F:252:PRO:HD2	2.16	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.30	0.45
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.45
8:H:90:PRO:O	8:H:91:MET:C	2.60	0.45
9:I:188:GLU:OE1	12:R:56:ASN:HB2	2.16	0.45
15:V:56:LEU:HD11	15:V:57:ASP:OD1	2.17	0.45
16:W:99:VAL:HG13	16:W:99:VAL:O	2.15	0.45
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.45
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.45
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.98	0.45
5:E:59:TYR:O	5:E:62:ILE:HB	2.17	0.45
6:F:299:LEU:CD1	6:F:300:ILE:N	2.67	0.45
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.45
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.45
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.45
8:H:140:ILE:HG13	8:H:141:SER:N	2.30	0.45
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.45
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
10:P:259:VAL:H	10:P:261:LYS:HG2	1.82	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
5:E:45:GLU:O	5:E:50:THR:HG21	2.15	0.45
5:E:162:THR:CG2	5:E:166:LYS:HA	2.46	0.45
6:F:227:PRO:HB2	6:F:228:PRO:HD3	1.99	0.45
7:G:97:MET:HB2	7:G:100:TRP:NE1	2.30	0.45
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.98	0.45
7:G:401:LEU:HD11	7:G:462:PHE:CE2	2.51	0.45
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.45
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:285:HIS:CE1	10:P:364:SER:HB3	2.51	0.45
14:T:87:LEU:CD2	14:T:104:PHE:CE1	2.94	0.45
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.16	0.45
2:B:136:THR:HG21	2:B:177:VAL:CG2	2.44	0.45
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.45
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.45
5:E:81:VAL:O	5:E:82:LEU:C	2.60	0.45
5:E:184:MET:HG3	5:E:192:TYR:O	2.16	0.45
6:F:224:ARG:HG2	11:Q:164:PHE:CZ	2.52	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.45
24:H:402:3PE:H241	24:H:402:3PE:H272	1.61	0.45
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.32	0.45
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.98	0.45
17:X:7:LEU:HD13	18:Z:87:LEU:HB3	1.98	0.45
21:q:21:ARG:O	21:q:25:ARG:HG3	2.17	0.45
1:A:109:LYS:HA	1:A:112:GLU:CD	2.42	0.45
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.97	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	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	1.99	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
7:G:355:LYS:NZ	7:G:528:LEU:O	2.47	0.45
10:P:315:THR:HB	10:P:318:LYS:HB2	1.98	0.45
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.45
14:T:133:ILE:O	14:T:136:GLU:N	2.46	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:53:PRO:HG2	18:Z:116:TRP:NE1	2.32	0.45
4:D:84:PHE:CE2	4:D:91:ALA:HB2	2.51	0.45
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.45
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.45
5:E:134:CYS:SG	5:E:139:CYS:SG	3.06	0.45
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.45
7:G:382:ARG:HD2	13:S:56:ARG:HD3	1.99	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
8:H:295:PRO:HB3	24:b:201:3PE:H382	1.98	0.45
10:P:170:LEU:HD12	10:P:171:ASN:H	1.81	0.45
10:P:218:ALA:HB2	10:P:280:ILE:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.45
3:C:73:GLN:NE2	15:V:107:PRO:HB3	2.31	0.45
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.32	0.45
3:C:243:ALA:C	7:G:105:ASN:ND2	2.75	0.45
4:D:78:THR:O	4:D:79:ASN:C	2.59	0.45
4:D:100:GLU:C	4:D:101:LEU:HD12	2.41	0.45
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.45
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.45
5:E:163:THR:HG23	5:E:168:PHE:O	2.17	0.45
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.45
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.45
8:H:16:ALA:HB2	19:a:15:CYS:HB2	1.99	0.45
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.45
9:I:93:LEU:O	21:q:93:MET:CG	2.65	0.45
10:P:209:ARG:CA	10:P:352:VAL:HG22	2.47	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
18:Z:66:GLU:HA	18:Z:69:ILE:CG1	2.46	0.45
18:Z:69:ILE:CG2	20:b:54:PRO:CD	2.94	0.45
18:Z:86:ILE:CG2	18:Z:128:ARG:HE	2.16	0.45
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.45
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.98	0.45
3:C:141:ARG:NH1	4:D:410:TYR:CE1	2.81	0.45
3:C:170:TRP:CE2	16:W:91:MET:HE1	2.52	0.45
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.52	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.45
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.77	0.45
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.45
10:P:192:ARG:HH12	10:P:198:ALA:HB3	1.80	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
14:T:82:ARG:NH2	14:T:126:PHE:HD1	2.15	0.45
14:T:130:ILE:CG2	14:T:131:PRO:CD	2.95	0.45
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.44
4:D:261:MET:HE3	4:D:261:MET:HB3	1.72	0.44
5:E:52:PHE:O	5:E:99:LYS:HG3	2.17	0.44
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.44	0.44
5:E:90:GLY:HA3	5:E:126:VAL:HG12	1.99	0.44
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.44
6:F:225:LEU:N	11:Q:160:TYR:OH	2.38	0.44
6:F:382:CYS:HA	7:G:74:ASN:O	2.18	0.44
7:G:341:ILE:HD12	7:G:555:ILE:CG1	2.47	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.44
9:I:50:MET:O	9:I:51:LYS:C	2.60	0.44
9:I:79:ARG:HG2	22:r:12:ARG:NH2	2.29	0.44
14:T:83:VAL:HG21	14:T:145:VAL:HG22	1.99	0.44
14:T:117:GLU:HA	14:T:120:MET:CE	2.41	0.44
14:T:133:ILE:HG23	14:T:134:ASP:N	2.32	0.44
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.44
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.52	0.44
24:A:401:3PE:H322	24:A:401:3PE:H32	1.85	0.44
2:B:82:ILE:CG1	8:H:57:MET:CE	2.82	0.44
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.44
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.44
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.44
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
12:R:39:ASP:H	12:R:42:ASP:CG	2.21	0.44
12:R:91:VAL:HG11	12:R:106:TYR:HE2	1.82	0.44
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	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
23:s:52:LEU:O	23:s:56:ARG:HG2	2.17	0.44
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.81	0.44
5:E:222:PHE:H	5:E:225:GLU:CD	2.25	0.44
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.44
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
7:G:607:LYS:HG2	11:Q:78:ARG:HH11	1.82	0.44
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.80	0.44
8:H:293:PHE:HE1	24:H:402:3PE:H32	1.82	0.44
10:P:122:HIS:HB3	12:R:46:VAL:HG12	1.98	0.44
10:P:245:VAL:HA	10:P:265:PHE:HD2	1.82	0.44
12:R:32:THR:HG21	21:q:129:THR:HG23	1.98	0.44
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.44
14:T:79:ILE:O	14:T:83:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:109:ASP:O	22:r:110:GLN:CG	2.64	0.44
2:B:80:ASP:O	2:B:81:LEU:C	2.59	0.44
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.98	0.44
3:C:98:PHE:HB2	15:V:94:MET:CE	2.47	0.44
3:C:136:PHE:O	3:C:137:ASN:C	2.60	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
6:F:126:LYS:O	6:F:129:GLU:HG2	2.18	0.44
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.98	0.44
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.44
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.48	0.44
8:H:25:ARG:NH1	30:H:401:UQ9:H10A	2.32	0.44
10:P:55:VAL:HA	10:P:79:GLN:O	2.18	0.44
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
13:S:51:LEU:HA	13:S:52:PRO:HD3	1.86	0.44
14:T:113:LEU:O	14:T:116:VAL:HB	2.17	0.44
15:V:56:LEU:C	15:V:56:LEU:CD1	2.85	0.44
6:F:119:GLU:HB3	6:F:124:THR:HG22	2.00	0.44
6:F:427:LEU:HB2	29:F:501:FMN:HM73	2.00	0.44
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.44
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.44
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.44
9:I:78:PHE:HB2	22:r:12:ARG:CG	2.48	0.44
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.44
10:P:305:PHE:CB	10:P:314:THR:HG22	2.47	0.44
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.44
12:R:47:ARG:HG3	12:R:48:PHE:N	2.32	0.44
16:W:71:MET:O	16:W:72:LYS:C	2.59	0.44
17:X:46:CYS:SG	17:X:135:ARG:NH1	2.90	0.44
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.44
1:A:112:GLU:O	1:A:113:TRP:C	2.58	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.18	0.44
4:D:258:VAL:O	4:D:259:GLU:C	2.60	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44
6:F:292:MET:O	6:F:293:SER:OG	2.33	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
9:I:90:LYS:HG3	21:q:90:LEU:CD2	2.48	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44
18:Z:72:MET:O	18:Z:73:PRO:C	2.59	0.44
2:B:93:MET:CE	2:B:95:PHE:CE2	3.00	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.48	0.44
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.44
10:P:156:SER:HB2	10:P:161:VAL:CG2	2.47	0.44
12:R:79:CYS:O	12:R:88:HIS:CE1	2.71	0.44
13:S:20:ARG:HG3	13:S:54:LEU:CB	2.43	0.44
2:B:71:ALA:O	2:B:75:VAL:N	2.47	0.44
2:B:90:LEU:O	2:B:119:VAL:HA	2.18	0.44
4:D:338:ARG:NH1	18:Z:23:ARG:CA	2.80	0.44
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.44
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.14	0.44
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.57	0.44
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.44
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.44
10:P:130:ILE:N	10:P:130:ILE:HD12	2.33	0.44
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.44
13:S:23:LEU:HB3	13:S:33:VAL:HG12	2.00	0.44
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.44
16:W:45:GLU:O	16:W:46:VAL:C	2.58	0.44
18:Z:129:THR:HG22	18:Z:131:GLU:N	2.33	0.44
19:a:37:ARG:HB2	19:a:48:MET:HE2	1.99	0.44
1:A:73:LEU:O	8:H:160:TYR:OH	2.25	0.44
2:B:96:GLY:CA	2:B:101:ALA:HB2	2.41	0.44
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.44
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.44
4:D:139:LEU:HD13	4:D:424:ILE:HG21	1.99	0.44
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:114:TYR:O	8:H:115:SER:C	2.60	0.44
9:I:42:LYS:HA	9:I:42:LYS:HD3	1.84	0.44
9:I:197:TRP:CZ3	21:q:84:PRO:HA	2.53	0.44
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.82	0.44
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.44
12:R:88:HIS:ND1	12:R:89:PRO:O	2.50	0.44
13:S:30:SER:O	13:S:33:VAL:N	2.51	0.44
1:A:63:LEU:O	1:A:64:LEU:C	2.60	0.43
2:B:146:ARG:NH2	3:C:211:TYR:CZ	2.86	0.43
3:C:70:LYS:O	15:V:103:LEU:HA	2.18	0.43
3:C:124:ARG:HD2	11:Q:140:LYS:HZ1	1.82	0.43
4:D:91:ALA:O	4:D:92:HIS:C	2.60	0.43
4:D:185:MET:HE2	4:D:207:ARG:HH22	1.74	0.43
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.43
4:D:271:ARG:CD	8:H:279:ARG:O	2.62	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
5:E:192:TYR:OH	5:E:213:PRO:HD2	2.18	0.43
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.46	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
7:G:362:ASP:HB2	13:S:71:PHE:CD1	2.52	0.43
8:H:63:PRO:HD2	8:H:66:THR:HG21	2.00	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.96	0.43
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.43
10:P:168:SER:O	10:P:202:ARG:HA	2.17	0.43
21:q:14:VAL:HG13	21:q:23:LEU:CD2	2.43	0.43
1:A:18:ILE:HG12	8:H:222:LEU:CD2	2.48	0.43
2:B:70:ARG:HG3	2:B:70:ARG:O	2.18	0.43
3:C:100:ARG:HH12	15:V:86:LYS:HZ1	1.66	0.43
3:C:221:GLU:OE1	16:W:114:GLU:HB2	2.18	0.43
4:D:259:GLU:O	4:D:263:THR:HG22	2.18	0.43
5:E:124:LYS:HB3	5:E:125:PRO:HD2	2.00	0.43
5:E:195:LEU:HD21	5:E:218:ARG:HG2	1.99	0.43
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.43
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.43
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.43
8:H:43:TYR:CE2	21:q:27:PHE:CZ	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.18	0.43
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.43
13:S:24:CYS:SG	13:S:61:VAL:HG12	2.58	0.43
16:W:20:VAL:HG21	16:W:80:ARG:CZ	2.48	0.43
16:W:71:MET:O	16:W:74:ALA:N	2.39	0.43
18:Z:28:ARG:O	18:Z:28:ARG:CG	2.64	0.43
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.52	0.43
21:q:3:LEU:O	21:q:6:VAL:CG2	2.66	0.43
4:D:99:LEU:HB3	4:D:101:LEU:HD11	2.00	0.43
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.43
6:F:413:TRP:CH2	6:F:436:GLN:HG2	2.53	0.43
7:G:31:LEU:HA	7:G:31:LEU:HD23	1.79	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:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.43
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
5:E:60:LYS:O	5:E:61:ARG:C	2.62	0.43
5:E:183:PRO:HB2	5:E:195:LEU:N	2.33	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	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:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.43
7:G:466:LEU:O	7:G:467:LYS:C	2.61	0.43
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
9:I:78:PHE:HB2	22:r:12:ARG:HG2	2.00	0.43
10:P:170:LEU:O	10:P:171:ASN:CG	2.61	0.43
15:V:56:LEU:CD1	15:V:57:ASP:OD1	2.67	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
8:H:306:SER:OG	20:b:33:PRO:HG3	2.19	0.43
10:P:76:MET:HE1	10:P:254:LYS:HE2	2.01	0.43
10:P:197:GLU:HB3	10:P:259:VAL:HG22	1.99	0.43
16:W:120:ASP:HB3	16:W:123:SER:OG	2.19	0.43
20:b:23:PHE:CZ	24:b:201:3PE:H351	2.46	0.43
21:q:22:GLY:O	21:q:26:VAL:HG23	2.18	0.43
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.43
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:232:VAL:CG2	4:D:356:ILE:HB	2.48	0.43
6:F:38:GLU:HG3	6:F:39:ASP:N	2.34	0.43
6:F:166:ALA:HB1	23:s:45:PHE:HD2	1.84	0.43
6:F:416:SER:O	6:F:419:ILE:CG2	2.65	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.52	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:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	2.00	0.43
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.43
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.43
5:E:48:PRO:C	5:E:50:THR:N	2.74	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.43
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.83	0.43
7:G:466:LEU:HD13	7:G:500:ILE:HD13	2.00	0.43
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.43
17:X:29:ALA:CB	18:Z:71:LEU:HD11	2.43	0.43
17:X:40:ASN:O	17:X:41:LYS:C	2.58	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:25:PRO:HG3	8:H:60:PRO:CD	2.42	0.43
2:B:117:PHE:HA	8:H:39:ILE:CG2	2.49	0.43
3:C:139:ARG:NH2	4:D:406:GLU:OE2	2.48	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
5:E:140:MET:HE1	6:F:366:ALA:HA	2.01	0.43
6:F:340:ASP:O	6:F:343:VAL:HB	2.19	0.43
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.43
7:G:117:MET:SD	7:G:143:SER:HB2	2.58	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
10:P:310:PHE:O	10:P:311:GLU:C	2.60	0.43
14:T:118:ILE:HD13	14:T:118:ILE:HA	1.83	0.43
20:b:15:LYS:O	20:b:15:LYS:HG3	2.18	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
5:E:165:ASP:O	5:E:166:LYS:C	2.62	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
6:F:419:ILE:HG23	6:F:432:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.43
14:T:92:LYS:O	14:T:92:LYS:HG2	2.16	0.43
17:X:10:LEU:H	17:X:10:LEU:HD12	1.84	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
3:C:55:LYS:HE2	3:C:55:LYS:HB3	1.84	0.43
4:D:92:HIS:CE1	4:D:457:VAL:HA	2.53	0.43
4:D:198:THR:HG23	8:H:275:ALA:O	2.18	0.43
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.43
5:E:81:VAL:HB	5:E:104:LEU:HD11	2.00	0.43
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.43
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.34	0.43
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.43
6:F:126:LYS:HG3	6:F:275:LEU:HB2	2.01	0.43
6:F:294:VAL:CG1	6:F:337:MET:HG3	2.48	0.43
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.43
7:G:279:GLU:HG3	11:Q:154:LYS:HG3	2.00	0.43
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.43
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.43
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.43
8:H:123:SER:HB3	8:H:214:GLU:HG3	2.00	0.43
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.43
9:I:152:CYS:SG	25:I:302:SF4:S3	3.17	0.43
10:P:259:VAL:N	10:P:261:LYS:HG2	2.33	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
11:Q:160:TYR:CE1	11:Q:164:PHE:CZ	3.02	0.43
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.43
14:T:93:ILE:HD11	14:T:118:ILE:HD11	2.00	0.43
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.43
16:W:38:LEU:HG	16:W:70:PHE:HZ	1.84	0.43
19:a:55:SER:O	19:a:56:GLY:C	2.61	0.43
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	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:50:ASP:O	6:F:55:GLY:HA3	2.19	0.42
6:F:224:ARG:HD3	11:Q:164:PHE:CD1	2.55	0.42
7:G:496:MET:HG2	7:G:500:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
7:G:617:ARG:NH1	16:W:129:HIS:N	2.67	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.52	0.42
8:H:33:LEU:HD21	22:r:25:GLN:HG2	2.01	0.42
8:H:179:TRP:CD1	18:Z:43:LEU:HD21	2.54	0.42
10:P:64:PHE:CE1	10:P:209:ARG:O	2.69	0.42
10:P:237:LYS:HE3	10:P:322:ILE:O	2.19	0.42
12:R:45:ARG:HA	12:R:48:PHE:HE1	1.83	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.62	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
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.42
1:A:73:LEU:N	1:A:74:PRO:HD2	2.35	0.42
5:E:94:ILE:HD13	7:G:209:TYR:CE2	2.53	0.42
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.42
6:F:333:GLU:HG2	6:F:334:THR:N	2.34	0.42
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.42
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.42
8:H:93:HIS:CD2	19:a:27:HIS:ND1	2.87	0.42
8:H:257:THR:O	8:H:260:MET:HB3	2.19	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
10:P:376:ASN:O	10:P:377:TYR:C	2.61	0.42
12:R:48:PHE:CD2	21:q:125:VAL:HG21	2.54	0.42
14:T:109:GLY:O	14:T:110:LEU:C	2.61	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.54	0.42
16:W:78:ASP:HA	16:W:79:PRO:HD3	1.94	0.42
16:W:83:ASP:O	16:W:86:VAL:CG2	2.66	0.42
17:X:75:LYS:O	17:X:79:ALA:HB2	2.19	0.42
18:Z:86:ILE:HA	18:Z:128:ARG:NH2	2.33	0.42
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.42
1:A:52:SER:O	1:A:53:MET:C	2.61	0.42
2:B:111:ARG:CZ	4:D:208:GLU:HG2	2.50	0.42
5:E:221:ARG:HB2	5:E:225:GLU:HG2	2.01	0.42
6:F:398:ARG:NH1	6:F:408:GLU:CD	2.78	0.42
8:H:174:LEU:HD23	8:H:174:LEU:HA	1.81	0.42
24:H:402:3PE:H331	9:I:63:TRP:CZ2	2.55	0.42
9:I:78:PHE:HD1	19:a:2:TRP:CD1	2.37	0.42
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.00	0.42
16:W:120:ASP:OD1	16:W:120:ASP:C	2.61	0.42
18:Z:74:LEU:O	18:Z:78:GLU:HG3	2.20	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:82:LYS:HB3	20:b:82:LYS:HE2	1.81	0.42
22:r:113:LEU:HD12	22:r:113:LEU:HA	1.76	0.42
1:A:73:LEU:O	1:A:76:PRO:HD2	2.18	0.42
3:C:64:VAL:HG11	3:C:85:ILE:HD13	2.02	0.42
4:D:92:HIS:O	4:D:458:PHE:CE2	2.72	0.42
4:D:140:ASP:HB2	4:D:460:GLU:HB3	2.02	0.42
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.42
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.42
6:F:291:GLU:OE2	6:F:292:MET:N	2.53	0.42
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.42
7:G:664:TYR:OH	13:S:23:LEU:HD11	2.20	0.42
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.42
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
9:I:162:CYS:SG	25:I:303:SF4:S2	3.17	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
2:B:94:THR:OG1	2:B:104:MET:HE1	2.20	0.42
3:C:141:ARG:HE	3:C:141:ARG:HB2	1.41	0.42
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
6:F:47:GLY:N	6:F:133:HIS:ND1	2.68	0.42
6:F:47:GLY:C	6:F:49:HIS:H	2.27	0.42
7:G:36:VAL:O	7:G:39:GLN:HG2	2.19	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
8:H:17:MET:HE1	8:H:225:MET:HE3	2.01	0.42
10:P:220:TYR:CG	10:P:226:VAL:HG13	2.55	0.42
11:Q:104:ARG:HA	11:Q:104:ARG:HD3	1.88	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
17:X:52:ASP:O	17:X:53:PRO:C	2.61	0.42
18:Z:102:PRO:O	18:Z:103:ASN:C	2.62	0.42
22:r:12:ARG:HB3	22:r:20:LEU:CD2	2.49	0.42
2:B:91:TRP:CE3	30:H:401:UQ9:H1M	2.54	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.19	0.42
4:D:83:ASN:C	4:D:85:GLY:N	2.74	0.42
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.49	0.42
6:F:261:TRP:CE2	6:F:265:PHE:CZ	3.08	0.42
8:H:68:MET:HG3	8:H:68:MET:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	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
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.42
10:P:300:TRP:NE1	10:P:304:LEU:HD21	2.35	0.42
18:Z:120:LEU:HD12	18:Z:121:ILE:H	1.85	0.42
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
23:s:35:LEU:HA	23:s:37:HIS:CE1	2.55	0.42
2:B:94:THR:CB	2:B:104:MET:CE	2.97	0.42
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:235:VAL:O	6:F:236:PHE:C	2.62	0.42
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.42
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.42
10:P:207:PHE:O	10:P:241:TYR:HA	2.19	0.42
13:S:16:LEU:HD13	13:S:19:ILE:HD11	2.02	0.42
13:S:19:ILE:O	13:S:53:ILE:HD12	2.20	0.42
22:r:10:LYS:O	22:r:11:LEU:C	2.62	0.42
23:s:53:SER:HA	23:s:56:ARG:HG2	2.02	0.42
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.83	0.42
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.46	0.42
4:D:89:PRO:HA	27:D:501:UQ1:HM53	2.01	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
7:G:163:LYS:HE2	12:R:97:LYS:HZ2	1.85	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
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	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
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.42
21:q:5:GLU:HG3	21:q:9:ARG:HE	1.84	0.42
1:A:8:PHE:CE1	24:A:401:3PE:H2C1	2.48	0.42
1:A:20:VAL:O	1:A:21:ALA:C	2.63	0.42
24:A:401:3PE:H362	8:H:104:PHE:CE2	2.55	0.42
3:C:101:ASP:OD1	15:V:86:LYS:HE3	2.19	0.42
3:C:243:ALA:C	7:G:105:ASN:HD21	2.28	0.42
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.42
8:H:19:PHE:CB	19:a:12:MET:HG3	2.49	0.42
9:I:35:THR:HG22	22:r:107:SER:HA	1.97	0.42
9:I:68:ARG:HH22	18:Z:26:PRO:HD2	1.83	0.42
10:P:228:LEU:HD11	10:P:288:PHE:CZ	2.54	0.42
12:R:31:ILE:HG22	12:R:55:VAL:HG21	2.02	0.42
14:T:87:LEU:CD2	14:T:122:MET:CE	2.98	0.42
14:T:90:TYR:CD2	14:T:92:LYS:HB3	2.54	0.42
16:W:28:LEU:O	16:W:32:LYS:HG3	2.20	0.42
16:W:93:LEU:HD23	16:W:93:LEU:C	2.45	0.42
17:X:41:LYS:O	17:X:42:GLU:C	2.59	0.42
18:Z:108:GLU:O	18:Z:109:SER: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
26:B:302:PC1:H372	8:H:53:MET:SD	2.60	0.42
3:C:48:PRO:HD3	4:D:162:GLN:OE1	2.20	0.42
3:C:241:PHE:O	3:C:242:PRO:C	2.62	0.42
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.42
30:H:401:UQ9:H15B	30:H:401:UQ9:H17	1.80	0.42
9:I:89:GLU:CG	21:q:61:TRP:HB3	2.50	0.42
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.42
11:Q:85:ASN:C	11:Q:87:MET:N	2.76	0.42
14:T:80:LYS:O	14:T:84:LEU:HG	2.20	0.42
14:T:123:GLU:HG2	14:T:130:ILE:HD12	2.02	0.42
19:a:49:GLU:O	19:a:50:ARG:C	2.62	0.42
20:b:11:ASN:O	20:b:15:LYS:HG2	2.20	0.42
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.41
5:E:136:THR:HB	28:E:301:FES:S2	2.60	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:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.41
6:F:410:ASP:OD1	6:F:411:SER:N	2.53	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.55	0.41
9:I:152:CYS:SG	25:I:302:SF4:S1	3.17	0.41
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.41
10:P:331:ASP:CG	10:P:332:LEU:H	2.28	0.41
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.41
20:b:69:HIS:HD2	20:b:70:PRO:CD	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:18:GLN:OE1	22:r:18:GLN:N	2.53	0.41
1:A:81:THR:O	20:b:46:ASN:ND2	2.53	0.41
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.41
5:E:62:ILE:HG21	5:E:103:VAL:HG11	2.02	0.41
5:E:134:CYS:SG	5:E:175:CYS:HA	2.60	0.41
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.41
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:160:VAL:CG1	7:G:161:GLU:N	2.83	0.41
8:H:25:ARG:HD2	30:H:401:UQ9:C10	2.48	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
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.41
13:S:20:ARG:HD2	13:S:22:HIS:NE2	2.35	0.41
19:a:49:GLU:OE2	19:a:49:GLU:HA	2.20	0.41
20:b:31:ILE:O	20:b:32:MET:C	2.63	0.41
21:q:64:TYR:CD1	21:q:77:VAL:HG11	2.54	0.41
1:A:24:LEU:HD13	1:A:24:LEU:O	2.20	0.41
2:B:146:ARG:NH2	3:C:211:TYR:CE2	2.89	0.41
3:C:102:HIS:CE1	15:V:48:THR:CG2	2.89	0.41
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.41
4:D:198:THR:N	4:D:199:PRO:CD	2.84	0.41
4:D:266:ARG:CA	9:I:65:GLU:OE2	2.68	0.41
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.41
5:E:69:TYR:HB3	5:E:70:PRO:CD	2.50	0.41
5:E:203:ILE:HG12	5:E:218:ARG:NH1	2.35	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.41
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.41
7:G:272:ARG:HH11	7:G:274:LEU:CD2	2.33	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.89	0.41
8:H:42:PRO:HD2	8:H:45:ILE:HD11	2.02	0.41
10:P:230:SER:O	10:P:231:LEU:C	2.63	0.41
10:P:231:LEU:HD11	10:P:290:PRO:HB2	2.02	0.41
10:P:243:ALA:O	10:P:244:ASP:C	2.62	0.41
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.41
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:81:GLY:HA3	12:R:88:HIS:CD2	2.55	0.41
1:A:112:GLU:O	1:A:113:TRP:CD1	2.73	0.41
2:B:91:TRP:CZ2	30:H:401:UQ9:C1M	3.03	0.41
2:B:95:PHE:HE2	2:B:131:MET:CE	2.33	0.41
3:C:72:VAL:HG23	3:C:72:VAL:O	2.20	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.02	0.41
4:D:134:PRO:O	4:D:138:ARG:NH1	2.49	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
4:D:199:PRO:HG3	4:D:262:LEU:HD11	2.02	0.41
5:E:225:GLU:O	5:E:226:PRO:C	2.60	0.41
6:F:126:LYS:HE2	6:F:274:LYS:HZ3	1.85	0.41
6:F:257:ARG:CG	6:F:261:TRP:CD2	2.93	0.41
6:F:300:ILE:CD1	6:F:307:VAL:HG23	2.49	0.41
7:G:32:ILE:CG2	7:G:98:LYS:HA	2.50	0.41
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.85	0.41
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.28	0.41
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.41
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41
20:b:25:VAL:O	20:b:26:TRP:C	2.64	0.41
4:D:144:MET:N	4:D:144:MET:SD	2.94	0.41
4:D:202:TRP:HZ2	9:I:73:THR:HG22	1.86	0.41
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
5:E:48:PRO:HD3	5:E:94:ILE:CG2	2.51	0.41
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.41
6:F:119:GLU:CD	29:F:501:FMN:HN3	2.28	0.41
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	0.41
6:F:337:MET:HE2	6:F:337:MET:HA	2.02	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.51	0.41
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
10:P:316:LYS:C	10:P:316:LYS:HD3	2.46	0.41
16:W:76:VAL:HG13	16:W:82:VAL:HG22	2.02	0.41
19:a:12:MET:HE2	19:a:12:MET:HB3	1.90	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:70:LYS:HD3	3:C:71:TYR:CZ	2.56	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.36	0.41
4:D:197:MET:HG3	8:H:32:GLN:NE2	2.36	0.41
4:D:201:PHE:HB2	8:H:32:GLN:HB3	2.03	0.41
4:D:240:LEU:O	4:D:241:LEU:C	2.62	0.41
4:D:265:ASN:C	4:D:267:ILE:H	2.29	0.41
4:D:376:GLU:HG2	7:G:121:LEU:CD1	2.51	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41
6:F:280:GLY:O	6:F:356:VAL:HB	2.20	0.41
6:F:311:TRP:CH2	6:F:333:GLU:HB3	2.55	0.41
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.41
8:H:311:THR:O	18:Z:51:MET:CG	2.66	0.41
12:R:60:ALA:O	12:R:61:ILE:C	2.63	0.41
13:S:16:LEU:CB	13:S:69:TYR:CD1	2.97	0.41
17:X:70:PHE:CE1	17:X:117:TRP:CZ3	3.08	0.41
17:X:70:PHE:O	17:X:74:ILE:HG13	2.20	0.41
2:B:137:LEU:HD11	2:B:142:ALA:HA	2.03	0.41
2:B:163:SER:HB2	9:I:150:THR:O	2.20	0.41
5:E:142:ARG:HB3	5:E:182:ALA:HB3	2.02	0.41
5:E:167:LEU:HD23	5:E:168:PHE:HE1	1.86	0.41
5:E:192:TYR:CD2	5:E:203:ILE:HD13	2.56	0.41
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:541:PRO:HB2	7:G:561:PRO:CD	2.50	0.41
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.41
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.41
8:H:198:PHE:HB3	8:H:285:LEU:HD11	2.03	0.41
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.41
14:T:120:MET:O	14:T:121:ALA:C	2.63	0.41
15:V:98:LYS:HG2	15:V:100:TRP:CZ2	2.55	0.41
20:b:61:GLY:O	20:b:63:MET:HG3	2.21	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
4:D:339:GLN:HE21	9:I:37:LYS:HZ2	1.68	0.41
5:E:61:ARG:O	5:E:65:ILE:HG13	2.21	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:19:ILE:HG22	18:Z:20:ASP:N	2.36	0.41
18:Z:90:ASN:O	18:Z:94:GLU:HB2	2.21	0.41
20:b:16:GLU:N	20:b:17:PRO:HD3	2.35	0.41
2:B:145:LEU:O	2:B:146:ARG:C	2.64	0.41
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.84	0.41
3:C:101:ASP:O	15:V:90:LEU:HD13	2.21	0.41
4:D:79:ASN:HB2	4:D:100:GLU:HB3	2.03	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.03	0.41
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.41
5:E:39:VAL:HG11	7:G:163:LYS:HZ2	1.81	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
5:E:138:PRO:CG	6:F:122:PRO:HB3	2.47	0.41
5:E:238:LYS:HB3	5:E:242:PHE:CG	2.56	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.41
6:F:257:ARG:HG2	6:F:261:TRP:CE3	2.55	0.41
6:F:337:MET:O	6:F:338:ASP:OD1	2.38	0.41
7:G:32:ILE:HG22	7:G:33:GLU:N	2.36	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.41
7:G:314:LEU:HD23	7:G:583:ILE:HG13	2.02	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:82:ALA:HA	8:H:85:LEU:HD12	2.02	0.41
8:H:197:PRO:HG2	8:H:198:PHE:HD2	1.86	0.41
8:H:224:PHE:CD2	30:H:401:UQ9:H13	2.50	0.41
8:H:277:TYR:CE2	24:H:402:3PE:H271	2.56	0.41
8:H:306:SER:CB	8:H:310:PHE:HE2	2.34	0.41
10:P:135:GLU:HG3	10:P:140:ASP:HA	2.03	0.41
10:P:191:VAL:HG13	10:P:192:ARG:CZ	2.51	0.41
10:P:293:LEU:HD12	10:P:294:PRO:HD2	2.01	0.41
11:Q:55:VAL:HG21	16:W:80:ARG:HH11	1.85	0.41
12:R:55:VAL:HG22	12:R:56:ASN:N	2.35	0.41
14:T:107:ASP:OD1	14:T:108:LEU:N	2.54	0.41
18:Z:140:PHE:C	18:Z:142:TRP:N	2.77	0.41
21:q:50:GLU:HA	21:q:59:HIS:O	2.20	0.41
21:q:64:TYR:CE2	21:q:81:MET:HB2	2.56	0.41
21:q:129:THR:O	21:q:129:THR:CG2	2.67	0.41
22:r:24:LEU:HD23	22:r:24:LEU:HA	1.85	0.41
1:A:102:LEU:O	1:A:106:TRP:HD1	2.04	0.41
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.41
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.41
3:C:139:ARG:NH1	4:D:306:GLN:OE1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
4:D:310:VAL:C	4:D:312:ASP:H	2.29	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
4:D:339:GLN:HE21	9:I:37:LYS:NZ	2.17	0.41
4:D:357:LYS:HE2	4:D:357:LYS:HB3	1.83	0.41
6:F:300:ILE:HD13	6:F:307:VAL:N	2.21	0.41
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.54	0.41
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.41
7:G:217:GLU:C	7:G:219:SER:N	2.79	0.41
7:G:312:GLY:O	21:q:143:PRO:HA	2.21	0.41
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.41
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.41
8:H:172:MET:HE1	18:Z:46:GLY:HA3	2.01	0.41
8:H:251:LEU:HD11	8:H:254:LEU:HB2	2.03	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
21:q:68:MET:HE1	21:q:81:MET:O	2.21	0.41
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.54	0.40
6:F:117:ALA:HB3	6:F:158:ILE:CA	2.45	0.40
6:F:196:PHE:HD1	23:s:56:ARG:HH21	1.70	0.40
6:F:210:THR:CB	6:F:224:ARG:H	2.34	0.40
8:H:87:VAL:HB	8:H:88:PRO:HD3	2.04	0.40
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.40
9:I:162:CYS:HB3	9:I:165:ASP:HA	2.02	0.40
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.40
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.40
10:P:288:PHE:CZ	10:P:290:PRO:HB3	2.56	0.40
10:P:315:THR:HB	10:P:318:LYS:H	1.85	0.40
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.85	0.40
17:X:37:ASP:OD1	17:X:37:ASP:C	2.62	0.40
18:Z:58:ARG:CZ	20:b:49:THR:HG21	2.51	0.40
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.40
21:q:85:GLU:HG2	21:q:98:PRO:HB3	2.01	0.40
1:A:102:LEU:HG	1:A:106:TRP:NE1	2.36	0.40
2:B:111:ARG:NE	4:D:208:GLU:HG2	2.35	0.40
3:C:47:ARG:HG3	4:D:160:ASN:HA	2.03	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
6:F:205:ILE:O	6:F:206:CYS:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.40
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.40
6:F:329:LYS:O	6:F:330:SER:C	2.65	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:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.40
8:H:114:TYR:O	8:H:117:LEU:N	2.55	0.40
8:H:300:LEU:HD23	20:b:25:VAL:HG11	2.02	0.40
10:P:140:ASP:O	10:P:141:PHE:C	2.65	0.40
11:Q:64:LEU:HD11	16:W:85:LEU:HG	2.03	0.40
13:S:22:HIS:CD2	13:S:66:TRP:HD1	2.38	0.40
13:S:23:LEU:HB3	13:S:33:VAL:CG1	2.51	0.40
14:T:99:SER:HB2	14:T:102:SER:HB2	2.03	0.40
15:V:96:LYS:HE2	15:V:96:LYS:HB2	1.95	0.40
17:X:119:ARG:HA	17:X:120:PRO:HD3	1.94	0.40
21:q:7:LEU:O	21:q:11:VAL:HG23	2.21	0.40
21:q:39:VAL:CG1	21:q:97:PRO:HB3	2.52	0.40
24:A:401:3PE:H2H2	24:A:401:3PE:H2E1	1.83	0.40
2:B:138:THR:HG21	4:D:116:LEU:HA	2.02	0.40
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.85	0.40
5:E:138:PRO:HG3	6:F:355:ILE:HD13	2.03	0.40
6:F:85:LEU:HD13	6:F:262:PHE:HE2	1.86	0.40
6:F:306:GLY:O	6:F:307:VAL:C	2.64	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.09	0.40
8:H:63:PRO:O	8:H:66:THR:HG22	2.21	0.40
8:H:153:VAL:HG11	8:H:241:ILE:HG23	2.03	0.40
9:I:107:PRO:O	9:I:108:SER:C	2.64	0.40
16:W:117:ARG:HA	16:W:118:PRO:HD3	1.94	0.40
17:X:53:PRO:HG2	18:Z:116:TRP:HE1	1.87	0.40
18:Z:62:ILE:HG13	20:b:49:THR:HG22	2.02	0.40
21:q:66:THR:HG22	21:q:74:PHE:CB	2.28	0.40
22:r:20:LEU:C	22:r:20:LEU:CD1	2.89	0.40
1:A:16:THR:O	1:A:20:VAL:HG23	2.22	0.40
2:B:147:LYS:HD2	2:B:147:LYS:HA	1.74	0.40
3:C:98:PHE:HE1	15:V:44:TYR:CE1	2.39	0.40
3:C:224:GLU:OE1	10:P:50:SER:OG	2.40	0.40
4:D:235:ASP:OD2	18:Z:8:GLN:NE2	2.45	0.40
4:D:263:THR:HG23	4:D:264:ASN:CG	2.47	0.40
6:F:114:VAL:CG1	6:F:212:LEU:HD23	2.52	0.40
6:F:228:PRO:CG	11:Q:160:TYR:HD2	2.30	0.40
7:G:277:MET:HE1	11:Q:153:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.40
9:I:50:MET:HB3	18:Z:33:TYR:OH	2.21	0.40
9:I:90:LYS:CG	21:q:90:LEU:CD2	3.00	0.40
10:P:56:ALA:HA	10:P:125:VAL:O	2.20	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:146:VAL:HG13	10:P:147:ASN:OD1	2.21	0.40
10:P:302:GLY:HA2	10:P:314:THR:CG2	2.50	0.40
17:X:117:TRP:CD1	17:X:117:TRP:N	2.87	0.40
20:b:49:THR:HA	20:b:50:PRO:HD3	1.89	0.40
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.40
4:D:181:LEU:HD21	4:D:210:MET:CB	2.51	0.40
5:E:113:GLU:HG2	7:G:197:THR:O	2.21	0.40
7:G:355:LYS:HB2	7:G:366:LEU:CD2	2.52	0.40
9:I:50:MET:O	9:I:54:THR:N	2.37	0.40
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.55	0.40
13:S:59:SER:O	13:S:60:GLU:C	2.63	0.40
14:T:140:CYS:HB2	14:T:143:GLU:HB2	2.02	0.40
17:X:16:GLU:CD	17:X:68:LEU:HD13	2.46	0.40
17:X:23:ALA:HB2	17:X:95:GLN:HE22	1.81	0.40
19:a:9:LEU:O	19:a:10:ALA:C	2.64	0.40
20:b:11:ASN:CG	20:b:15:LYS:HE3	2.45	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%)	144 (94%)	9 (6%)	1 (1%)	21	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	196/263 (74%)	187 (95%)	9 (5%)	0	100	100
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%)	405 (96%)	19 (4%)	0	100	100
7	G	685/727 (94%)	630 (92%)	55 (8%)	0	100	100
8	H	306/318 (96%)	289 (94%)	16 (5%)	1 (0%)	36	65
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	P	338/377 (90%)	312 (92%)	26 (8%)	0	100	100
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	76 (94%)	5 (6%)	0	100	100
13	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
14	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
15	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
16	W	112/131 (86%)	110 (98%)	2 (2%)	0	100	100
17	X	140/172 (81%)	130 (93%)	10 (7%)	0	100	100
18	Z	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
19	a	64/70 (91%)	60 (94%)	4 (6%)	0	100	100
20	b	77/84 (92%)	71 (92%)	6 (8%)	0	100	100
21	q	116/145 (80%)	113 (97%)	3 (3%)	0	100	100
22	r	46/113 (41%)	44 (96%)	2 (4%)	0	100	100
23	s	24/104 (23%)	24 (100%)	0	0	100	100
All	All	4131/5036 (82%)	3896 (94%)	233 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/104 (82%)	85 (100%)	0	100	100
2	B	132/185 (71%)	132 (100%)	0	100	100
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	333/395 (84%)	333 (100%)	0	100	100
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	83
6	F	341/370 (92%)	340 (100%)	1 (0%)	86	86
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	88
8	H	274/280 (98%)	274 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	P	297/325 (91%)	295 (99%)	2 (1%)	76	80
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68	76
12	R	70/96 (73%)	69 (99%)	1 (1%)	59	73
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	73
14	T	69/135 (51%)	68 (99%)	1 (1%)	59	73
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	79
19	a	56/60 (93%)	56 (100%)	0	100	100
20	b	70/73 (96%)	70 (100%)	0	100	100
21	q	108/131 (82%)	108 (100%)	0	100	100
22	r	44/96 (46%)	44 (100%)	0	100	100
23	s	26/95 (27%)	26 (100%)	0	100	100
All	All	3630/4292 (85%)	3620 (100%)	10 (0%)	84	86

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

Mol	Chain	Res	Type
5	E	244	VAL
6	F	337	MET
7	G	271	MET
10	P	192	ARG

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

Mol	Chain	Res	Type
1	A	10	ASN
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	54	HIS
3	C	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	92	HIS
4	D	117	HIS
4	D	131	GLN
4	D	182	ASN
4	D	234	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	68	ASN
5	E	132	GLN
5	E	152	GLN
5	E	245	GLN
6	F	44	ASN
6	F	49	HIS
6	F	168	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN

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Mol	Chain	Res	Type
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	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
8	H	292	ASN
10	P	71	ASN
10	P	79	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	50	GLN
16	W	54	GLN
17	X	30	HIS

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Mol	Chain	Res	Type
17	X	77	HIS
18	Z	135	ASN
19	a	31	ASN
20	b	69	HIS
20	b	83	ASN
21	q	12	GLN
21	q	31	ASN
21	q	52	ASN
21	q	54	GLN
21	q	87	HIS
21	q	91	HIS
22	r	9	GLN
22	r	21	GLN
22	r	110	GLN
23	s	59	GLN

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PC1	B	302	-	34,34,53	1.14	2 (5%)	40,42,61	1.13	2 (5%)
25	SF4	B	301	2	0,12,12	-	-	-	-	-
26	PC1	I	301	-	46,46,53	0.99	2 (4%)	52,54,61	1.03	3 (5%)
24	3PE	b	201	-	45,45,50	1.11	5 (11%)	48,50,55	1.24	3 (6%)
25	SF4	G	801	7	0,12,12	-	-	-	-	-
31	NDP	P	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.66	11 (16%)
24	3PE	A	401	-	45,45,50	1.11	5 (11%)	48,50,55	1.19	3 (6%)
25	SF4	I	303	9	0,12,12	-	-	-	-	-
29	FMN	F	501	-	33,33,33	1.39	4 (12%)	48,50,50	1.21	6 (12%)
25	SF4	F	502	6	0,12,12	-	-	-	-	-
25	SF4	I	302	9	0,12,12	-	-	-	-	-
28	FES	G	803	7	0,4,4	-	-	-	-	-
27	UQ1	D	501	-	18,18,18	1.94	2 (11%)	22,25,25	1.35	3 (13%)
24	3PE	H	402	-	45,45,50	0.95	2 (4%)	48,50,55	1.09	3 (6%)
30	UQ9	H	401	-	35,35,58	0.83	2 (5%)	42,45,73	0.52	0
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%)
28	FES	E	301	5	0,4,4	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PC1	B	302	-	-	8/38/38/57	-
26	PC1	I	301	-	-	10/50/50/57	-
25	SF4	B	301	2	-	-	0/6/5/5
24	3PE	b	201	-	-	19/49/49/54	-
25	SF4	G	801	7	-	-	0/6/5/5
31	NDP	P	401	-	-	3/34/77/77	0/5/5/5
24	3PE	A	401	-	-	18/49/49/54	-
29	FMN	F	501	-	-	3/18/18/18	0/3/3/3
25	SF4	I	303	9	-	-	0/6/5/5
25	SF4	F	502	6	-	-	0/6/5/5
25	SF4	I	302	9	-	-	0/6/5/5
28	FES	G	803	7	-	-	0/1/1/1
27	UQ1	D	501	-	-	0/9/33/33	0/1/1/1
24	3PE	H	402	-	-	12/49/49/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	UQ9	H	401	-	-	14/30/54/81	0/1/1/1
25	SF4	G	802	7	-	-	0/6/5/5
33	EHZ	W	201	-	-	21/39/39/45	-
28	FES	E	301	5	-	-	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	501	UQ1	C6-C5	7.32	1.48	1.35
33	W	201	EHZ	C15-N2	5.39	1.45	1.33
33	W	201	EHZ	C12-N1	5.17	1.45	1.33
29	F	501	FMN	C9A-C5A	4.83	1.49	1.41
31	P	401	NDP	C5A-C4A	4.24	1.46	1.39
26	B	302	PC1	O31-C31	4.16	1.45	1.33
26	I	301	PC1	O31-C31	4.16	1.45	1.33
24	H	402	3PE	O31-C31	4.12	1.45	1.33
26	B	302	PC1	O21-C21	4.08	1.45	1.34
24	H	402	3PE	O21-C21	4.03	1.45	1.34
26	I	301	PC1	O21-C21	4.02	1.45	1.34
31	P	401	NDP	C6N-C5N	3.32	1.39	1.33
24	b	201	3PE	O21-C21	3.13	1.43	1.34
24	A	401	3PE	O21-C21	3.13	1.43	1.34
29	F	501	FMN	C8-C7	3.09	1.48	1.40
24	b	201	3PE	O31-C31	3.06	1.42	1.33
27	D	501	UQ1	C3-C2	3.04	1.48	1.36
24	A	401	3PE	O31-C31	3.01	1.42	1.33
30	H	401	UQ9	C3-C2	-2.80	1.40	1.48
29	F	501	FMN	C4-N3	-2.67	1.33	1.38
33	W	201	EHZ	P1-O7	2.55	1.64	1.54
33	W	201	EHZ	O4-C15	-2.50	1.18	1.23
30	H	401	UQ9	C4-C5	-2.49	1.41	1.48
31	P	401	NDP	C5A-C6A	2.48	1.48	1.41
33	W	201	EHZ	C9-S1	2.43	1.82	1.76
31	P	401	NDP	C5A-N7A	-2.41	1.34	1.39
33	W	201	EHZ	O3-C12	-2.38	1.18	1.23
31	P	401	NDP	C8A-N7A	2.37	1.36	1.31
29	F	501	FMN	C5A-N5	-2.32	1.35	1.39
33	W	201	EHZ	P1-OP3	-2.25	1.46	1.54
24	b	201	3PE	O21-C2	-2.23	1.41	1.46
24	A	401	3PE	O21-C2	-2.18	1.41	1.46
24	A	401	3PE	O31-C3	-2.17	1.40	1.45
24	b	201	3PE	O31-C3	-2.15	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	401	3PE	P-O12	-2.12	1.45	1.55
24	b	201	3PE	P-O12	-2.08	1.45	1.55

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	W	201	EHZ	C8-C9-S1	6.33	121.46	113.63
31	P	401	NDP	C5A-C4A-N3A	-6.09	118.80	126.75
31	P	401	NDP	N3A-C4A-N9A	4.77	134.94	127.08
24	A	401	3PE	O21-C21-C22	4.25	120.66	111.50
26	B	302	PC1	O21-C21-C22	4.10	120.34	111.50
24	b	201	3PE	O21-C21-C22	4.07	120.27	111.50
26	I	301	PC1	O21-C21-C22	3.98	120.07	111.50
31	P	401	NDP	C2A-N3A-C4A	3.89	120.95	111.75
24	H	402	3PE	O21-C21-C22	3.74	119.56	111.50
31	P	401	NDP	PN-O3-PA	-3.65	120.30	132.83
31	P	401	NDP	N3A-C2A-N1A	-3.23	123.54	128.60
31	P	401	NDP	C4A-C5A-N7A	-3.22	106.70	110.62
33	W	201	EHZ	C13-C12-N1	3.07	121.60	116.42
33	W	201	EHZ	C14-C13-C12	-3.03	107.32	112.36
26	B	302	PC1	O31-C31-C32	2.93	121.09	111.91
33	W	201	EHZ	OP3-P1-O9	-2.89	99.36	110.68
33	W	201	EHZ	C7-C8-C9	-2.86	107.37	113.89
24	H	402	3PE	O31-C31-C32	2.80	120.70	111.91
27	D	501	UQ1	CM5-C5-C6	-2.79	119.86	124.40
31	P	401	NDP	C5A-N7A-C8A	2.77	107.44	103.51
31	P	401	NDP	C4A-N9A-C8A	2.73	108.69	105.73
26	I	301	PC1	C2-O21-C21	-2.67	111.21	117.79
27	D	501	UQ1	C11-C9-C10	2.67	120.50	114.60
29	F	501	FMN	C4A-C10-N1	-2.56	118.78	124.73
24	A	401	3PE	O31-C31-C32	2.50	119.77	111.91
24	b	201	3PE	O31-C31-C32	2.49	119.73	111.91
24	H	402	3PE	C2-O21-C21	-2.49	111.67	117.79
29	F	501	FMN	C4-C4A-N5	2.43	121.69	118.23
29	F	501	FMN	O4-C4-C4A	-2.41	120.20	126.60
26	I	301	PC1	O31-C31-C32	2.40	119.45	111.91
33	W	201	EHZ	C5-C6-C7	-2.38	108.01	114.85
27	D	501	UQ1	C7-C8-C9	-2.32	119.99	127.26
33	W	201	EHZ	C10-S1-C9	2.26	108.91	101.87
31	P	401	NDP	C6A-C5A-N7A	2.21	136.14	132.02
29	F	501	FMN	O2-C2-N1	-2.21	118.17	121.83
31	P	401	NDP	N9A-C8A-N7A	-2.20	110.91	113.91

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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
31	P	401	NDP	C3D-C2D-C1D	2.17	105.55	101.43
29	F	501	FMN	C4A-C10-N10	2.17	119.65	116.48
24	b	201	3PE	O12-P-O14	-2.16	101.54	112.24
33	W	201	EHZ	O2-C9-S1	-2.15	119.83	122.61
29	F	501	FMN	C10-N1-C2	2.14	121.18	116.90
33	W	201	EHZ	O3-C12-N1	-2.11	119.03	123.01
33	W	201	EHZ	O6-P1-O9	2.11	112.39	106.47
24	A	401	3PE	O12-P-O14	-2.06	102.07	112.24

There are no chirality outliers.

All (108) 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	H	402	3PE	C11-O13-P-O11
24	H	402	3PE	C11-O13-P-O12
24	H	402	3PE	C11-O13-P-O14
24	b	201	3PE	C1-O11-P-O12
24	b	201	3PE	C1-O11-P-O14
24	b	201	3PE	O22-C21-O21-C2
26	I	301	PC1	C11-O13-P-O14
29	F	501	FMN	C5'-O5'-P-O2P
29	F	501	FMN	C5'-O5'-P-O3P
30	H	401	UQ9	C19-C21-C22-C23
30	H	401	UQ9	C20-C19-C21-C22
30	H	401	UQ9	C18-C19-C21-C22
30	H	401	UQ9	C17-C18-C19-C21
30	H	401	UQ9	C17-C18-C19-C20
30	H	401	UQ9	C15-C14-C16-C17
30	H	401	UQ9	C12-C13-C14-C16
30	H	401	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

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Mol	Chain	Res	Type	Atoms
33	W	201	EHZ	C16-C17-C20-O6
33	W	201	EHZ	C20-O6-P1-O7
33	W	201	EHZ	C20-O6-P1-O9
33	W	201	EHZ	C20-O6-P1-OP3
26	I	301	PC1	O32-C31-O31-C3
26	I	301	PC1	C32-C31-O31-C3
24	b	201	3PE	C22-C21-O21-C2
30	H	401	UQ9	C24-C26-C27-C28
30	H	401	UQ9	C22-C23-C24-C25
30	H	401	UQ9	C22-C23-C24-C26
24	A	401	3PE	C22-C21-O21-C2
30	H	401	UQ9	C13-C14-C16-C17
30	H	401	UQ9	C9-C11-C12-C13
24	b	201	3PE	C2B-C2C-C2D-C2E
24	A	401	3PE	O22-C21-O21-C2
24	H	402	3PE	C32-C31-O31-C3
24	b	201	3PE	C32-C31-O31-C3
24	b	201	3PE	C39-C3A-C3B-C3C
24	b	201	3PE	O32-C31-O31-C3
30	H	401	UQ9	C14-C16-C17-C18
24	H	402	3PE	O32-C31-O31-C3
24	A	401	3PE	C11-O13-P-O11
24	H	402	3PE	C1-O11-P-O13
24	b	201	3PE	C1-O11-P-O13
26	B	302	PC1	C22-C21-O21-C2
24	b	201	3PE	C27-C28-C29-C2A
26	B	302	PC1	O22-C21-O21-C2
24	A	401	3PE	C37-C38-C39-C3A
24	H	402	3PE	C22-C21-O21-C2
24	b	201	3PE	C1-C2-C3-O31
24	A	401	3PE	C3-C2-O21-C21
29	F	501	FMN	C5'-O5'-P-O1P
24	b	201	3PE	O11-C1-C2-C3
24	H	402	3PE	C24-C25-C26-C27
33	W	201	EHZ	N2-C15-C16-C17
24	b	201	3PE	C24-C25-C26-C27
26	I	301	PC1	C11-O13-P-O11
33	W	201	EHZ	C3-C4-C5-C6
33	W	201	EHZ	C5-C6-C7-O1
26	B	302	PC1	C32-C31-O31-C3
24	H	402	3PE	O22-C21-O21-C2
33	W	201	EHZ	O2-C9-S1-C10

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Mol	Chain	Res	Type	Atoms
24	A	401	3PE	C2A-C2B-C2C-C2D
24	A	401	3PE	C2-C1-O11-P
24	b	201	3PE	O11-C1-C2-O21
26	B	302	PC1	O32-C31-O31-C3
24	b	201	3PE	C11-O13-P-O11
26	I	301	PC1	C1-O11-P-O13
24	H	402	3PE	C1-O11-P-O12
24	H	402	3PE	C1-O11-P-O14
24	b	201	3PE	C11-O13-P-O12
31	P	401	NDP	O4D-C1D-N1N-C6N
26	B	302	PC1	C11-C12-N-C15
26	I	301	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
26	I	301	PC1	C11-C12-N-C13
24	H	402	3PE	C33-C34-C35-C36
33	W	201	EHZ	C2-C3-C4-C5
31	P	401	NDP	PN-O3-PA-O2A
24	A	401	3PE	C2B-C2C-C2D-C2E
26	B	302	PC1	C11-C12-N-C14
24	A	401	3PE	C28-C29-C2A-C2B
26	B	302	PC1	C11-C12-N-C13
26	I	301	PC1	C11-C12-N-C14
24	A	401	3PE	O11-C1-C2-O21
24	A	401	3PE	C25-C26-C27-C28
26	I	301	PC1	C2C-C2D-C2E-C2F
33	W	201	EHZ	N2-C15-C16-O5
33	W	201	EHZ	C18-C17-C20-O6
26	I	301	PC1	C2E-C2F-C2G-C2H
24	b	201	3PE	C25-C26-C27-C28
24	A	401	3PE	C33-C34-C35-C36
33	W	201	EHZ	C15-C16-C17-C18
24	A	401	3PE	O11-C1-C2-C3
33	W	201	EHZ	O5-C16-C17-C18
33	W	201	EHZ	O4-C15-C16-C17
26	B	302	PC1	O21-C21-C22-C23

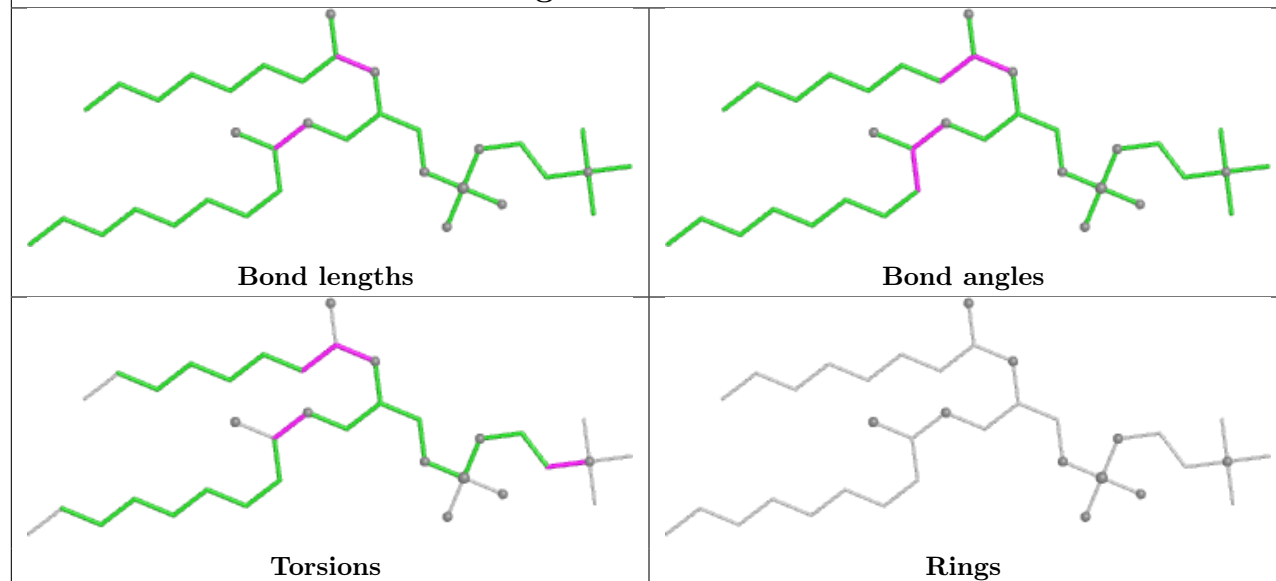
There are no ring outliers.

17 monomers are involved in 136 short contacts:

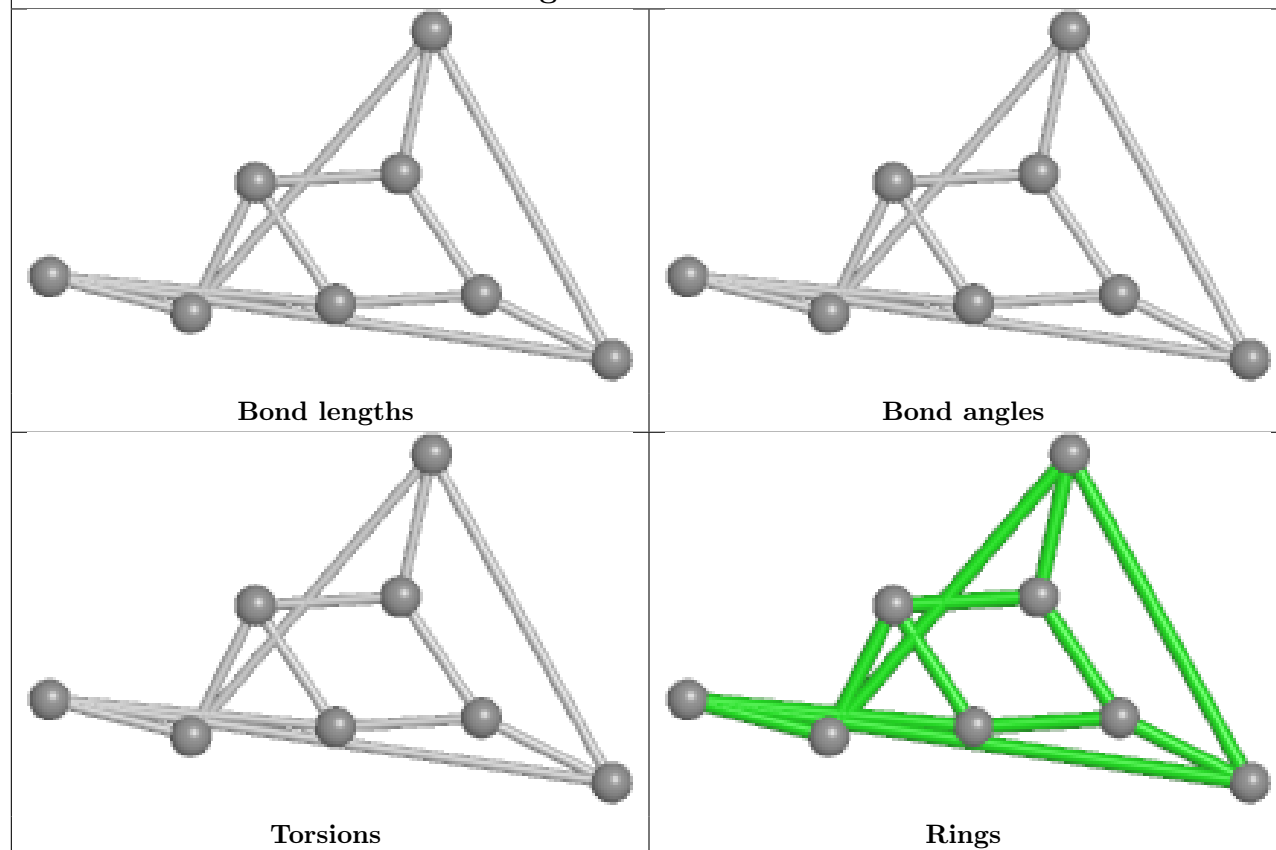
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	302	PC1	3	0
25	B	301	SF4	4	0
26	I	301	PC1	7	0
24	b	201	3PE	12	0
31	P	401	NDP	4	0
24	A	401	3PE	11	0
25	I	303	SF4	5	0
29	F	501	FMN	3	0
25	F	502	SF4	10	0
25	I	302	SF4	11	0
28	G	803	FES	4	0
27	D	501	UQ1	18	0
24	H	402	3PE	12	0
30	H	401	UQ9	16	0
25	G	802	SF4	5	0
33	W	201	EHZ	7	0
28	E	301	FES	4	0

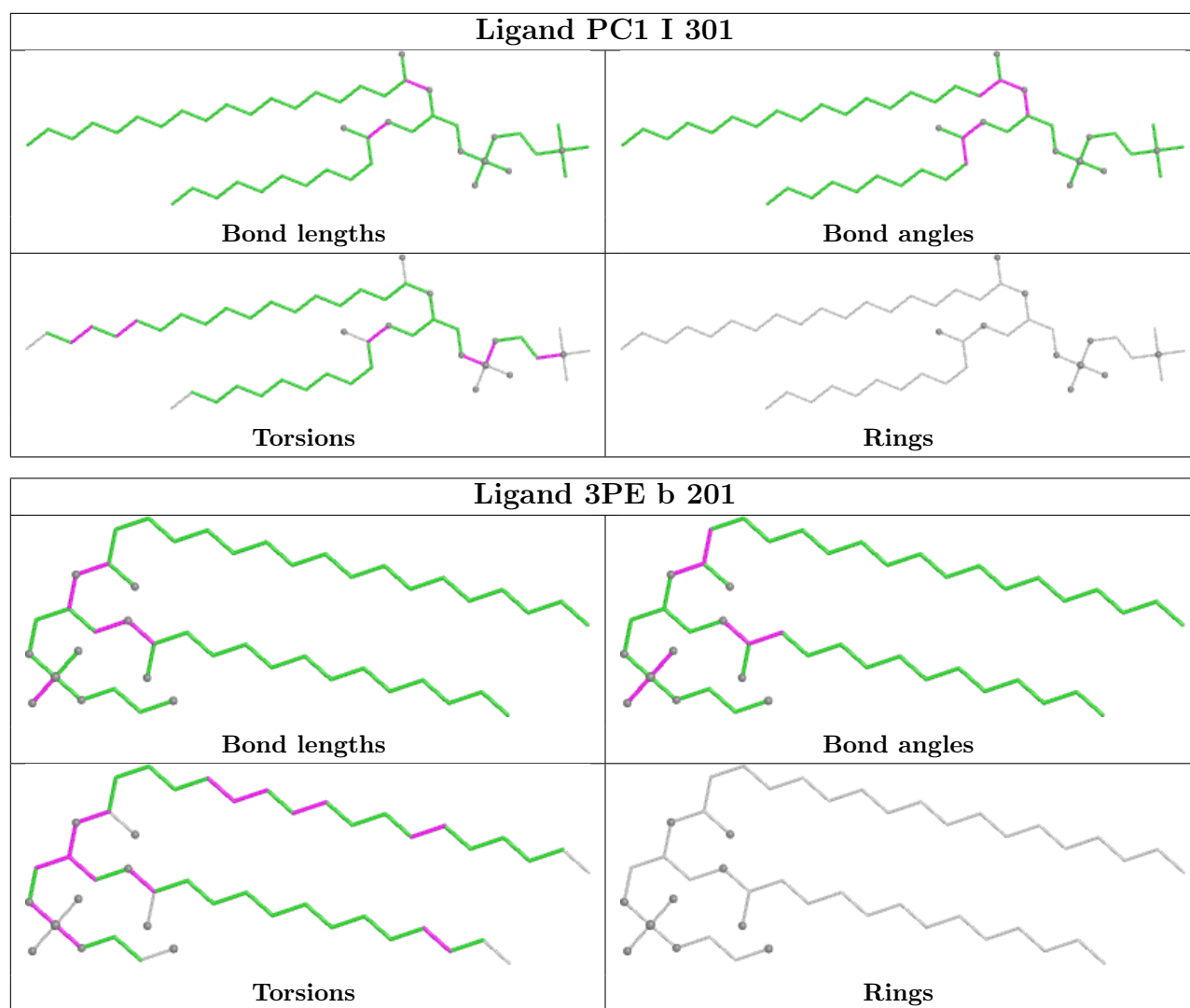
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

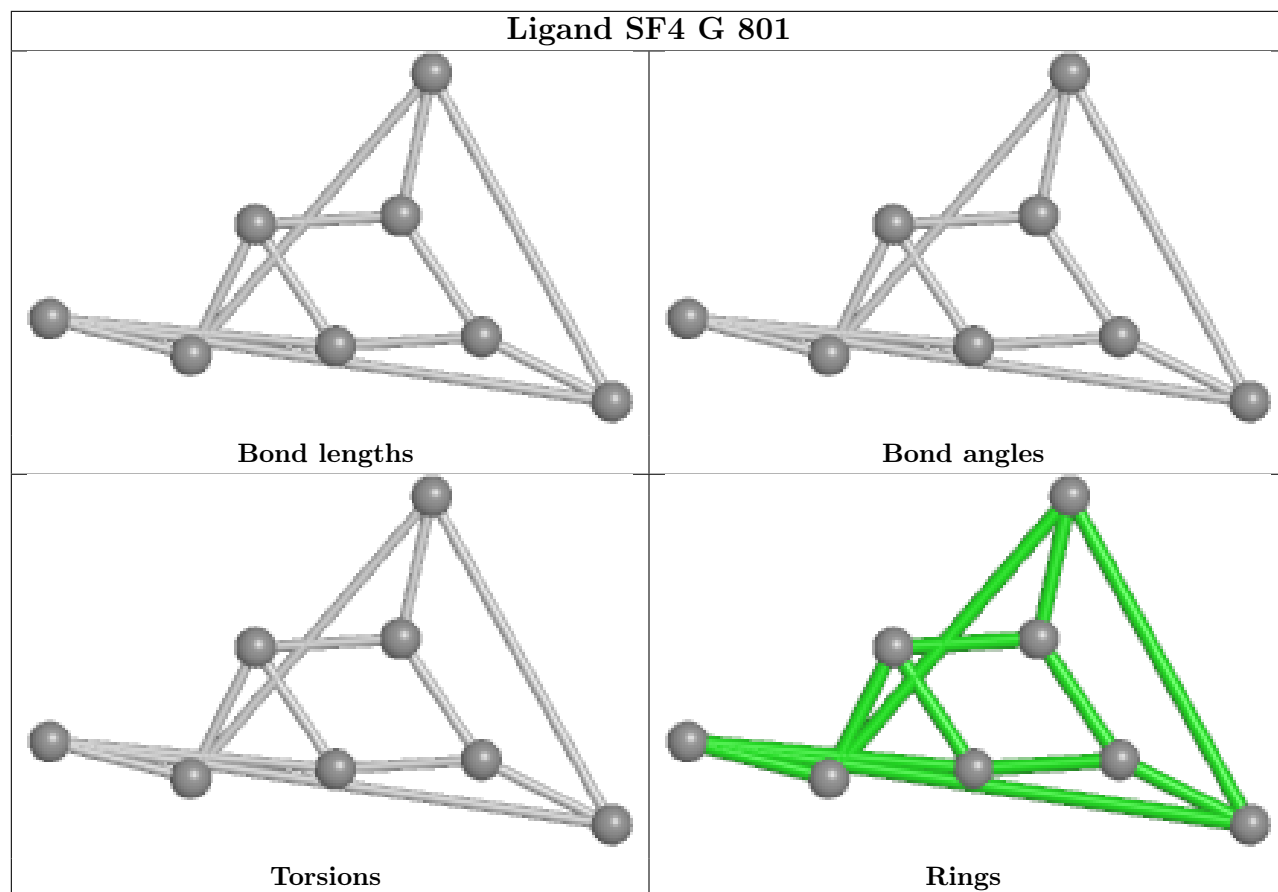
Ligand PC1 B 302

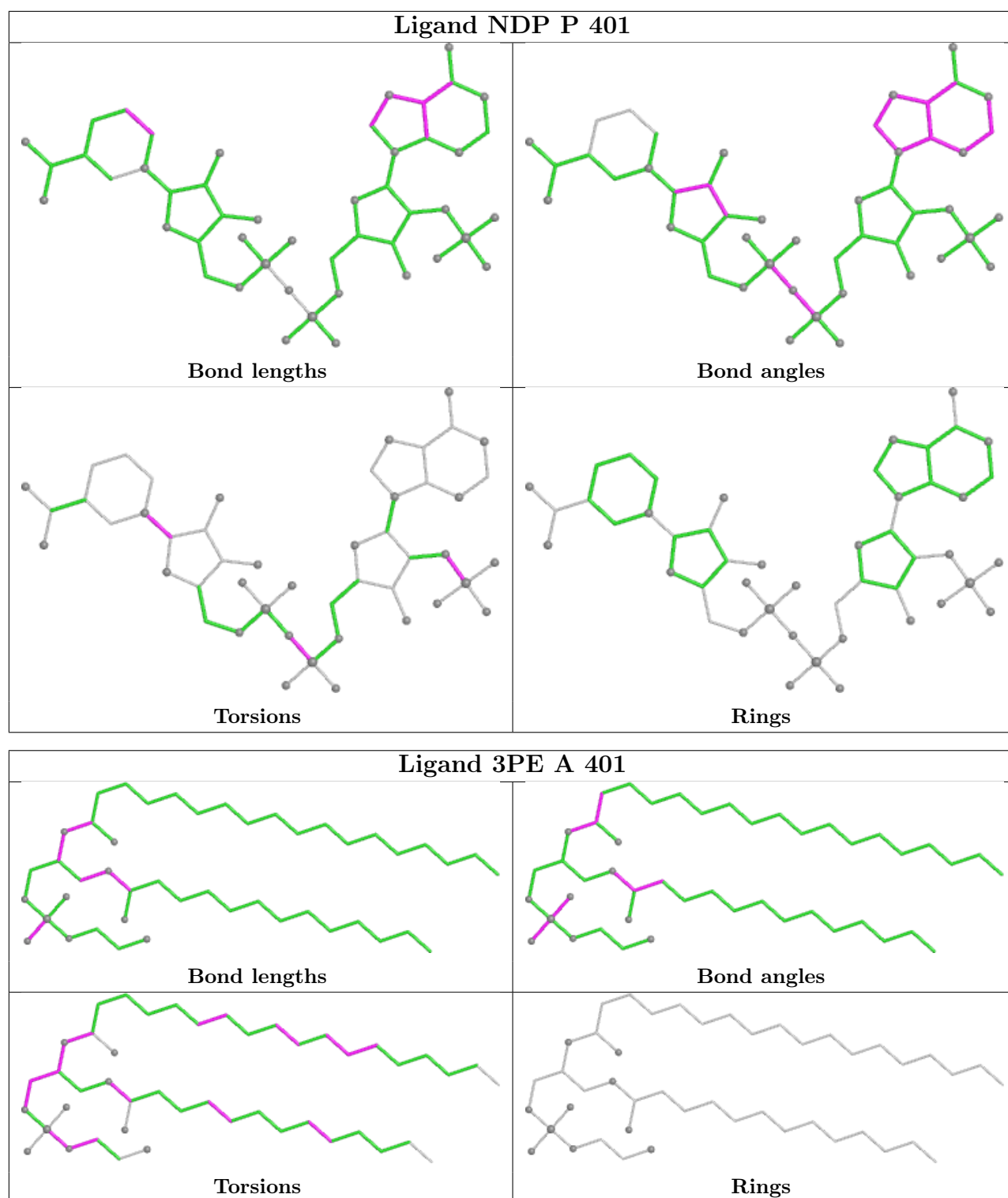


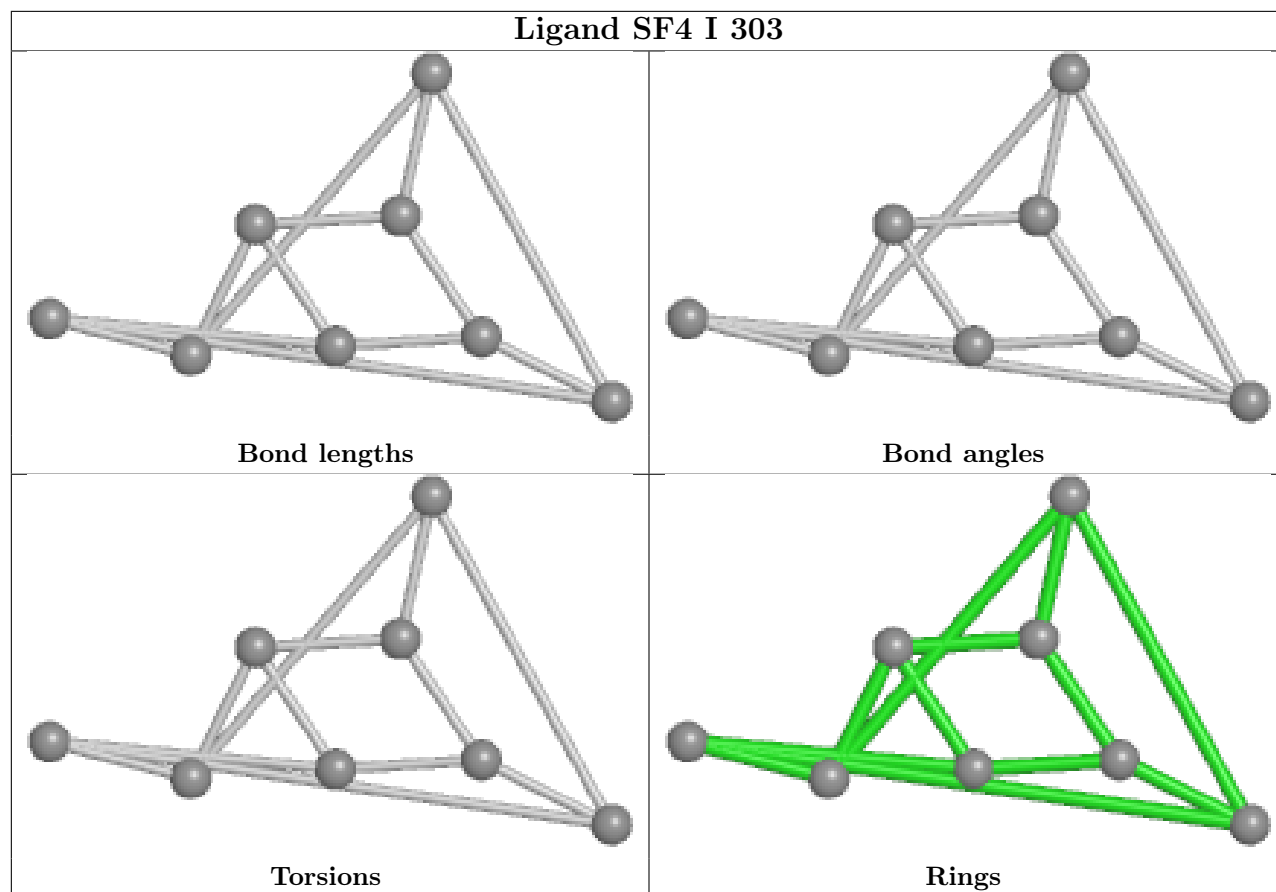
Ligand SF4 B 301

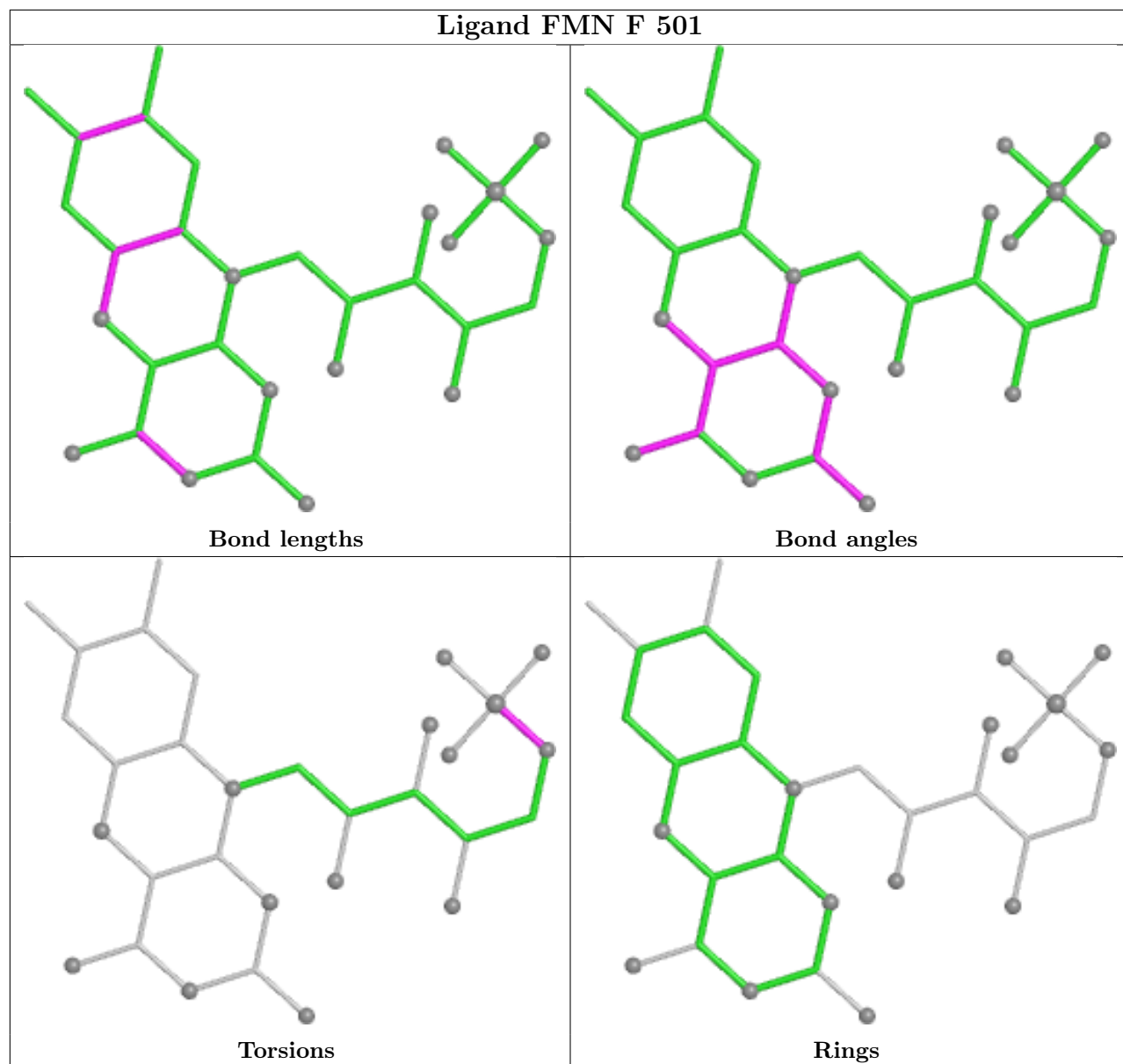




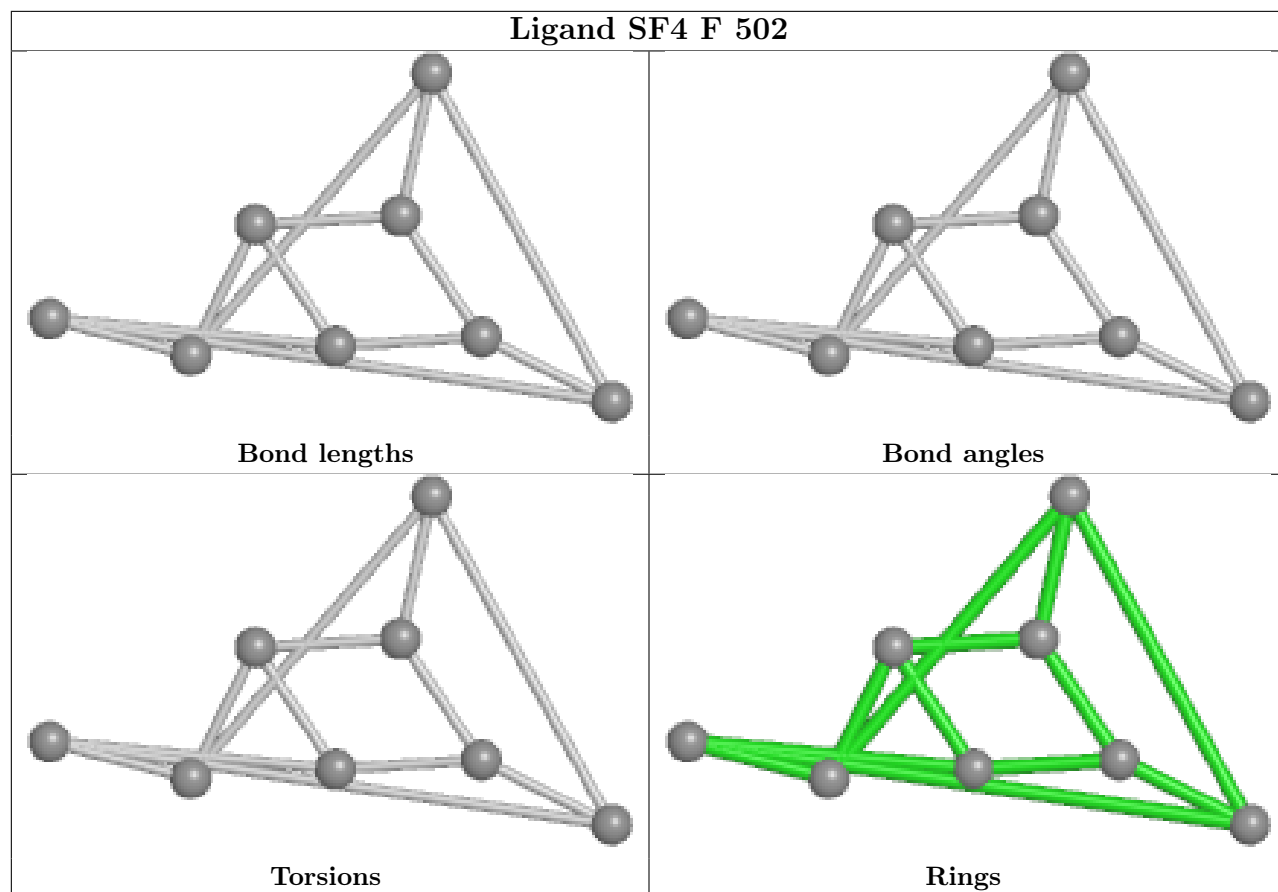




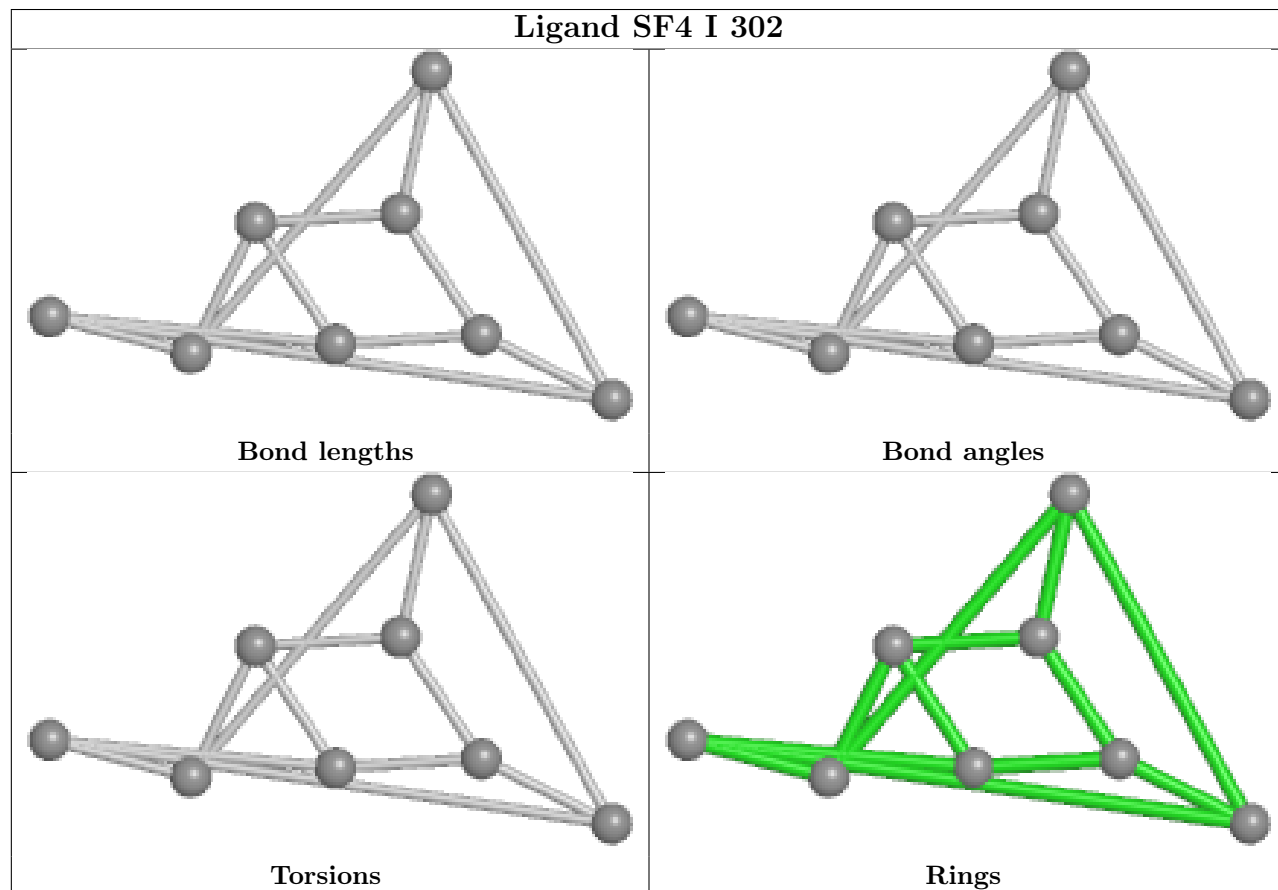


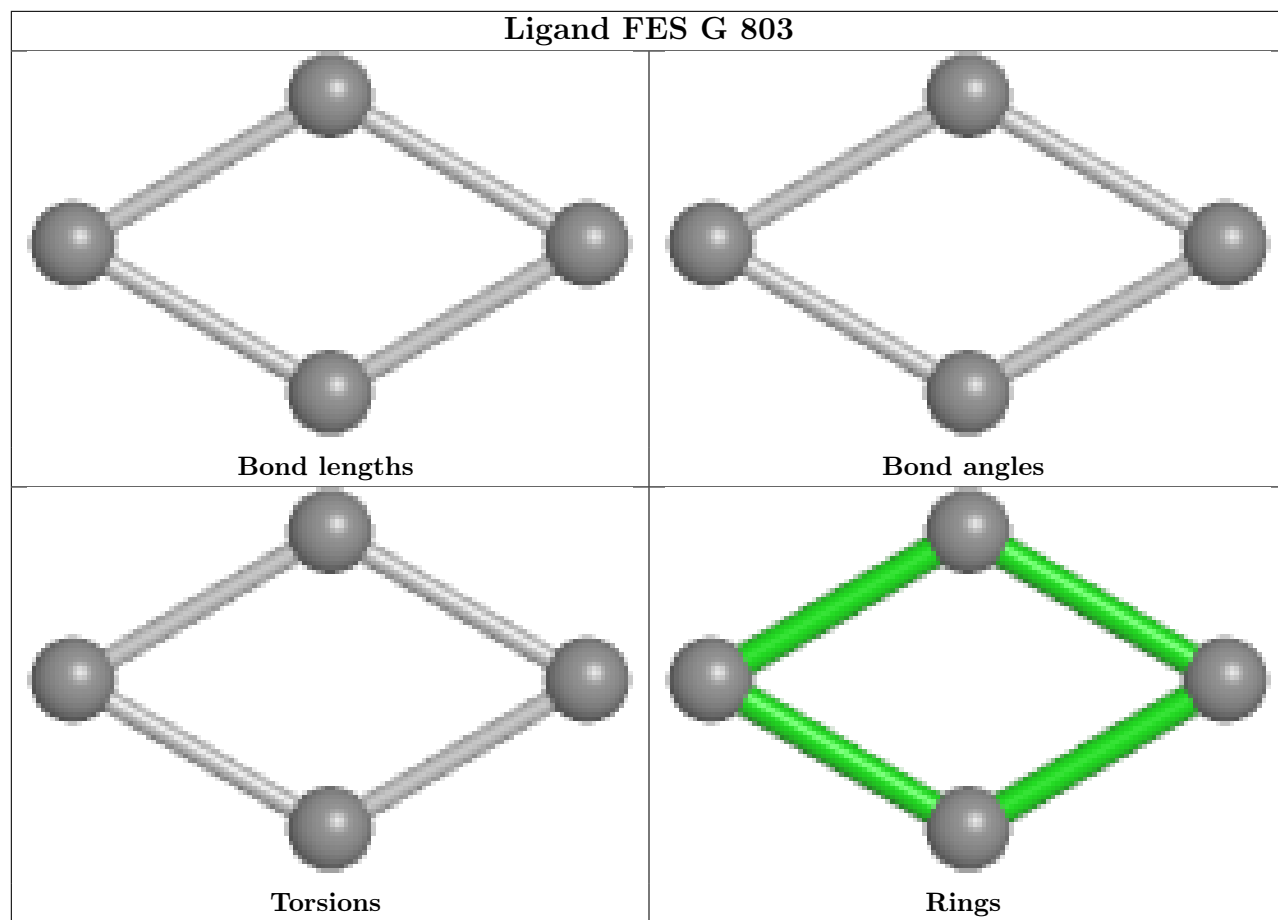


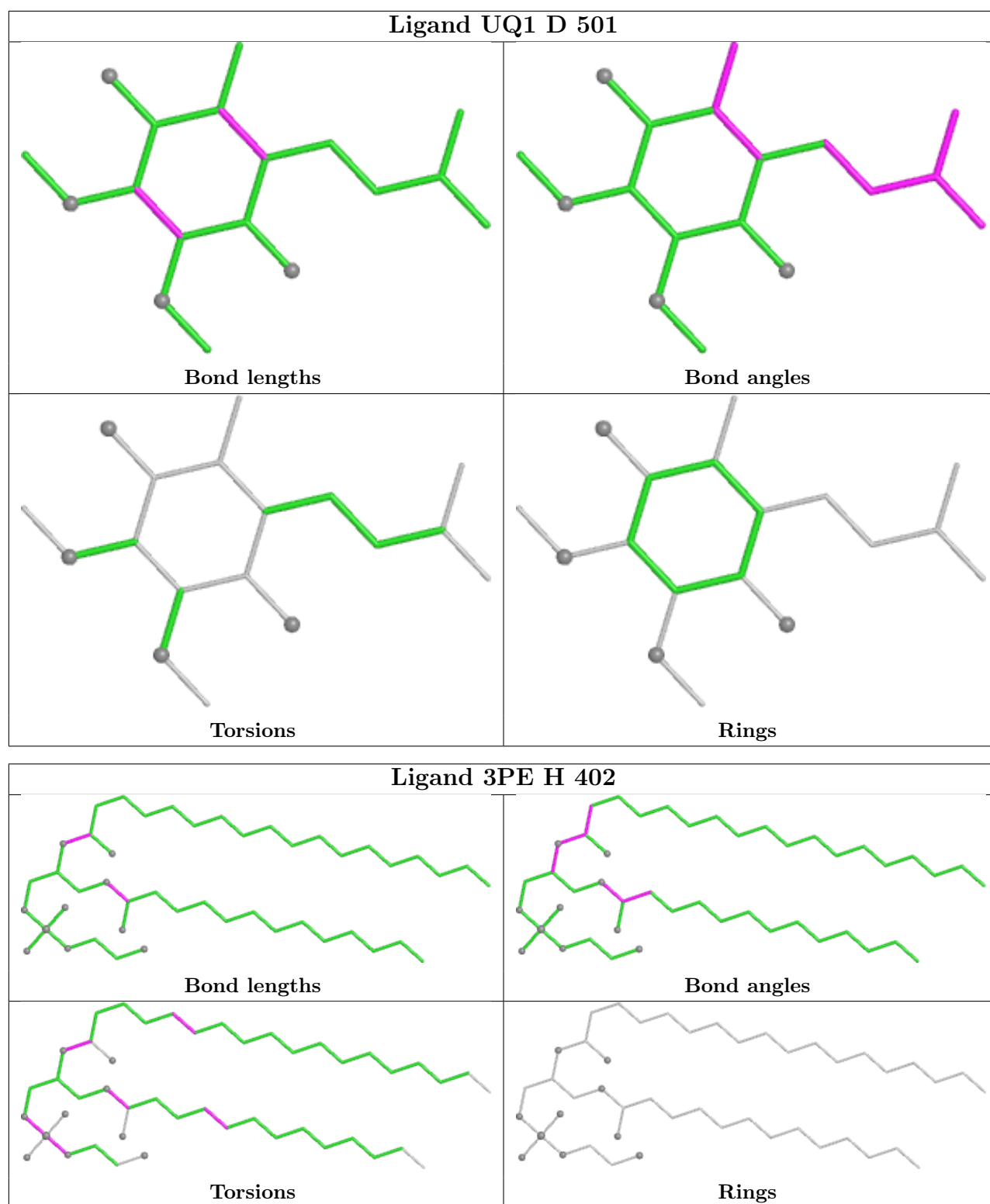
Ligand SF4 F 502

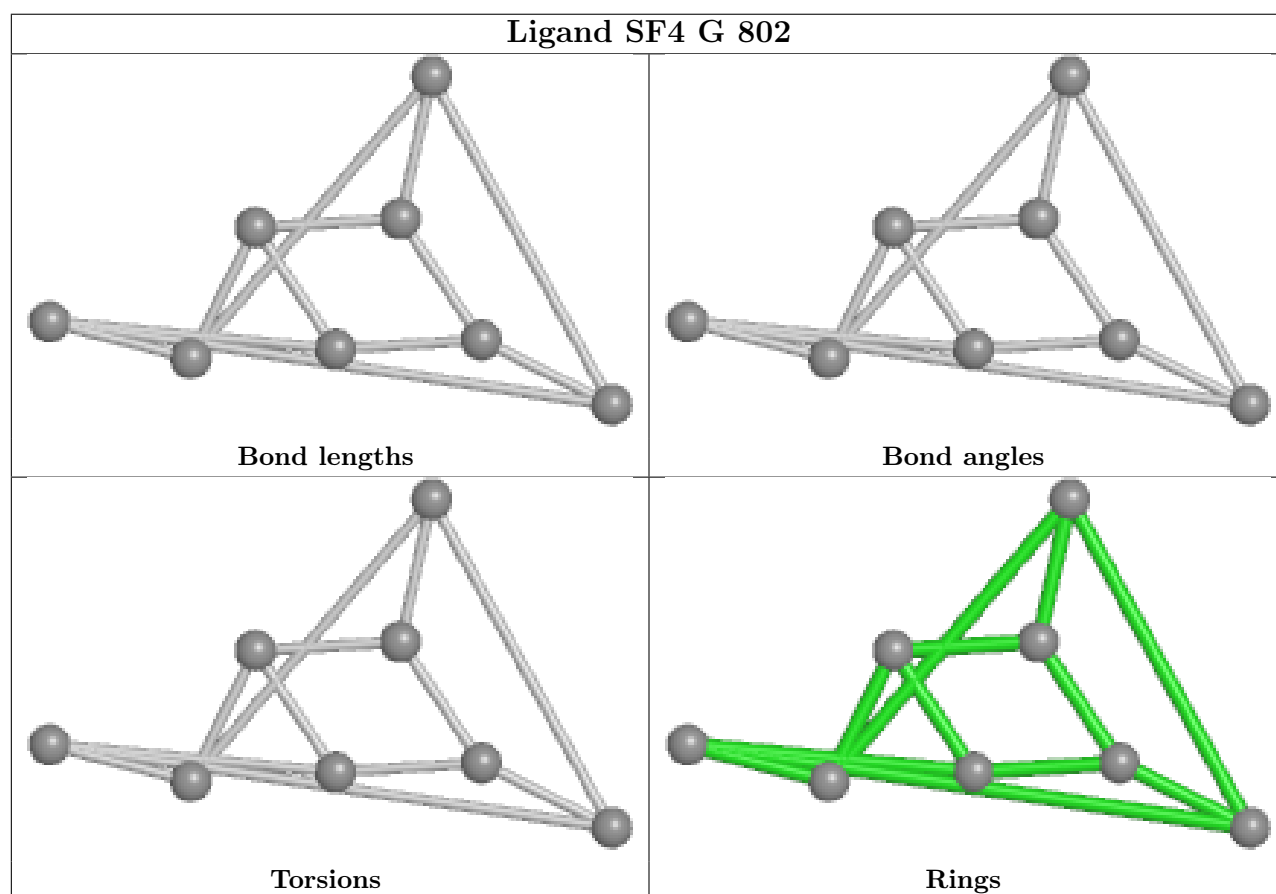
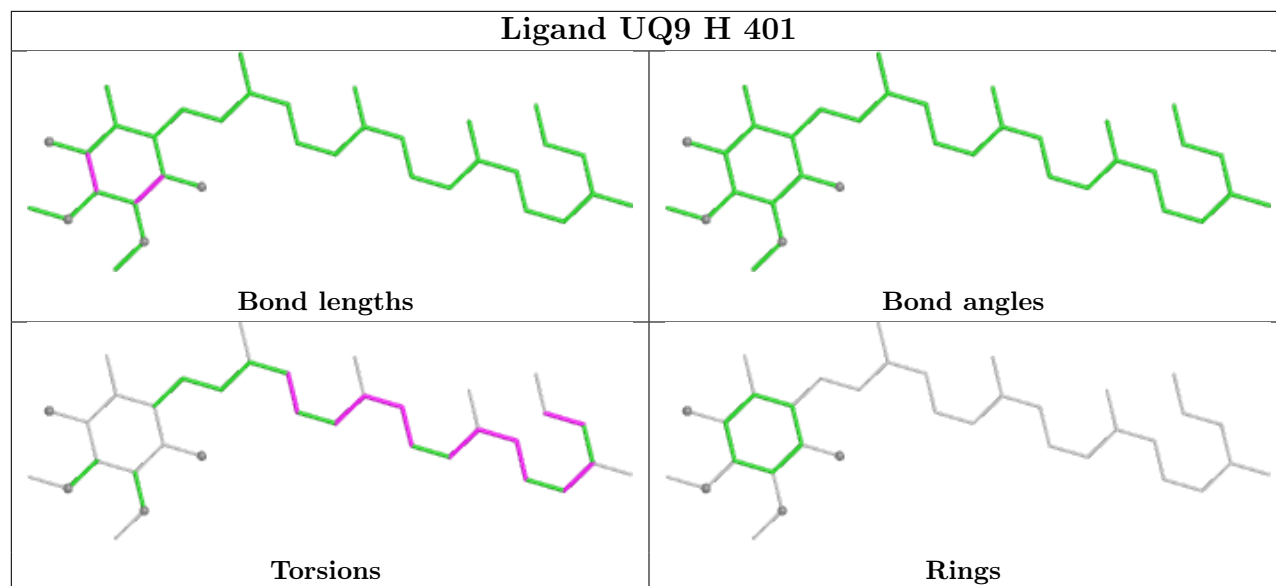


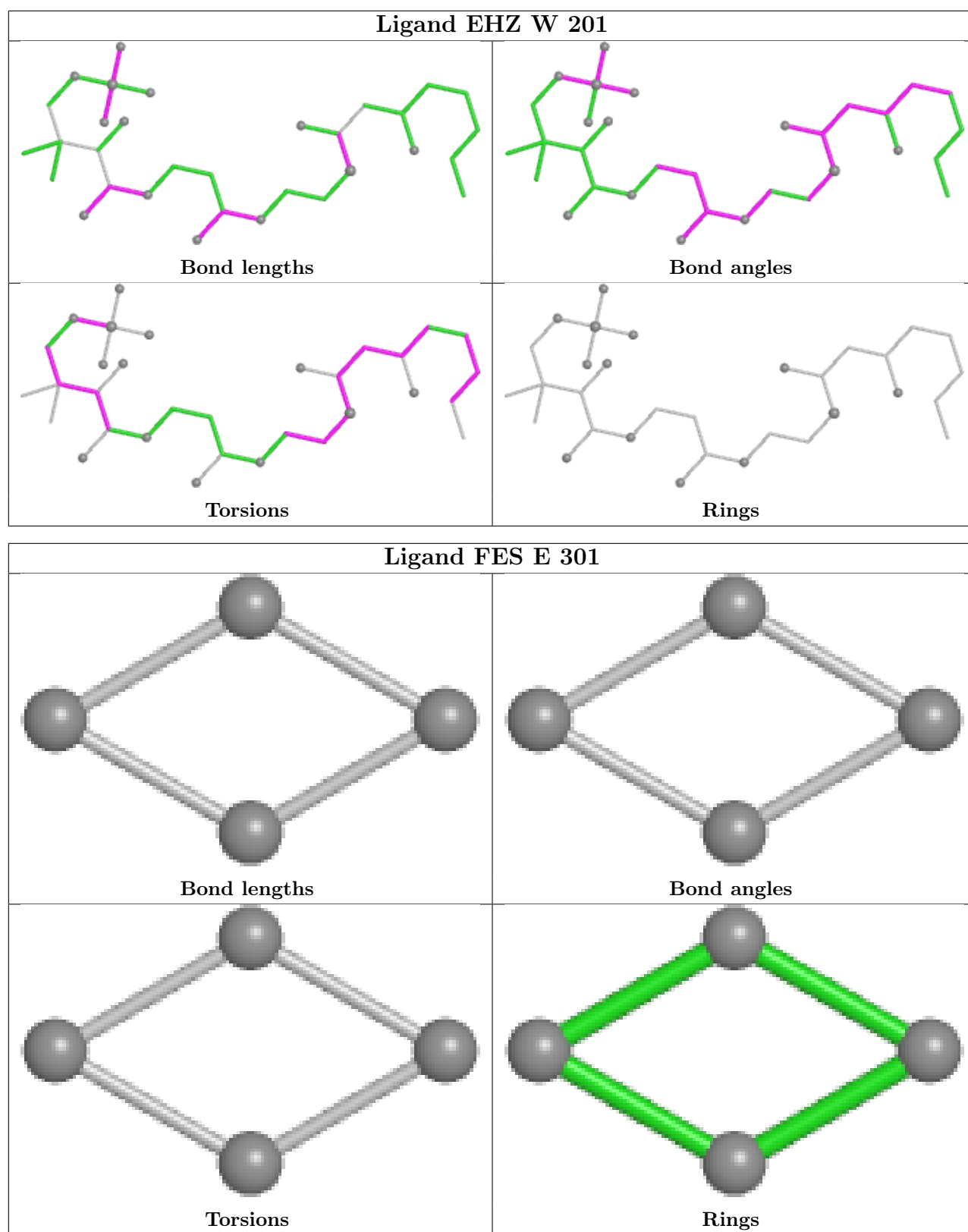
Ligand SF4 I 302











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

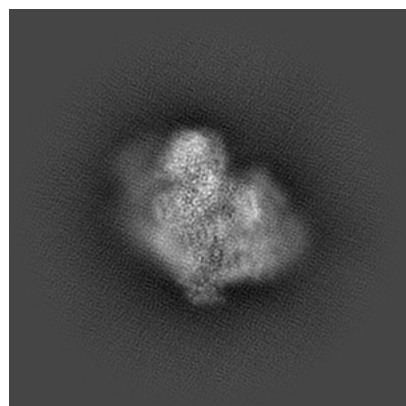
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38512. These allow visual inspection of the internal detail of the map and identification of artifacts.

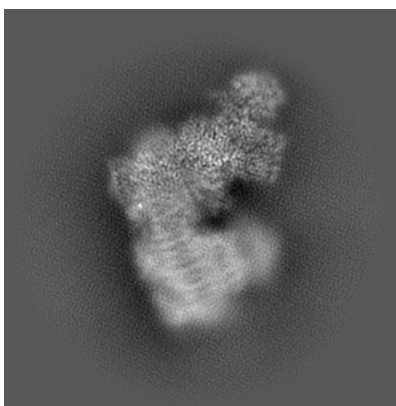
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

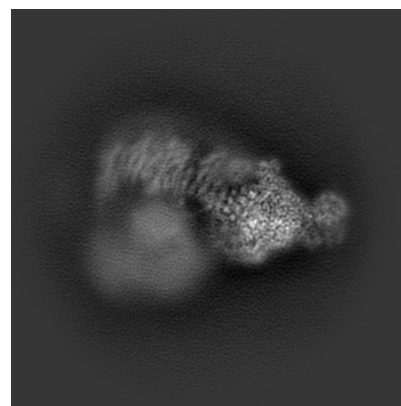
6.1.1 Primary map



X

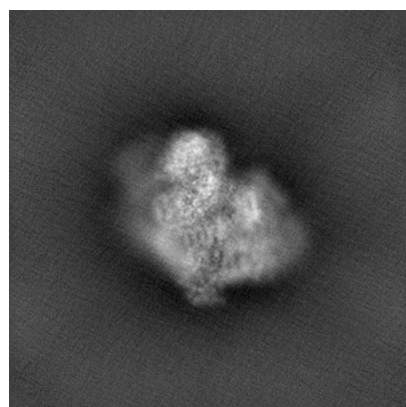


Y

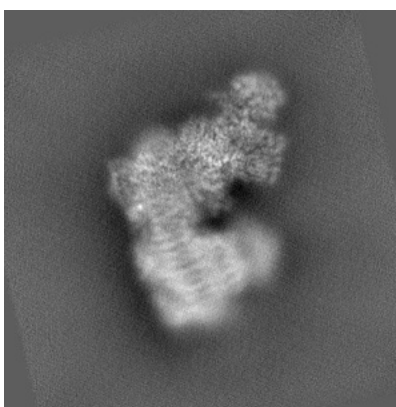


Z

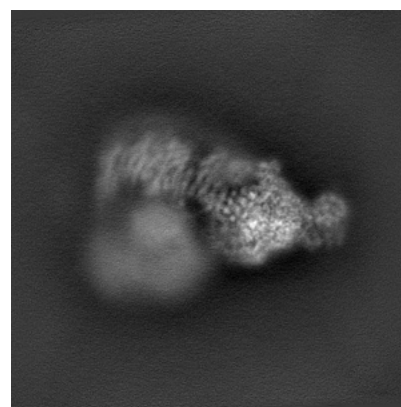
6.1.2 Raw map



X



Y

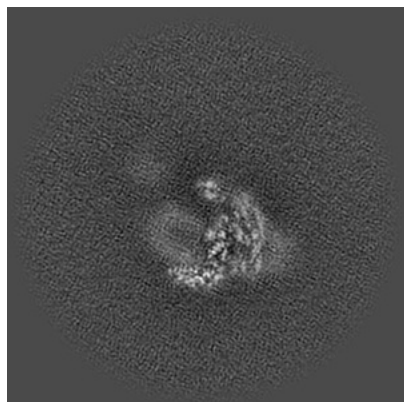


Z

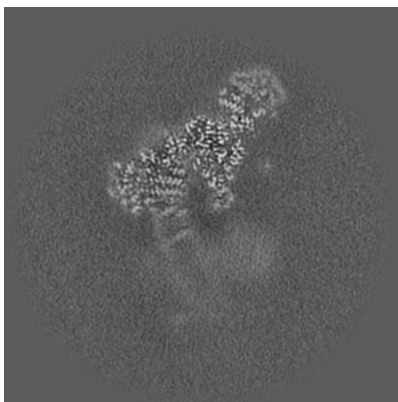
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

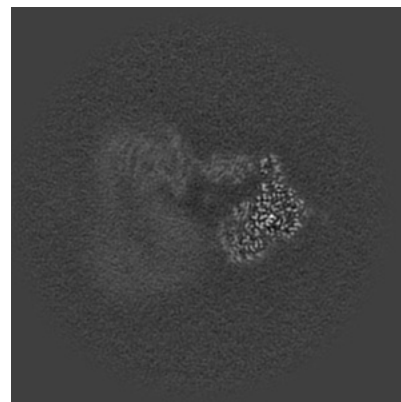
6.2.1 Primary map



X Index: 192

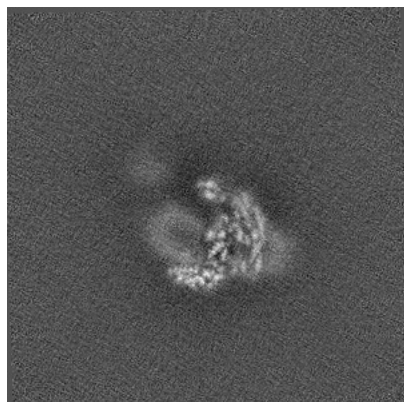


Y Index: 192

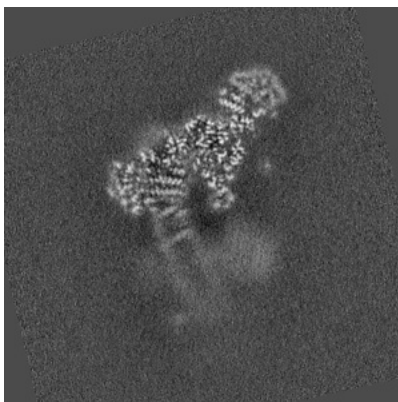


Z Index: 192

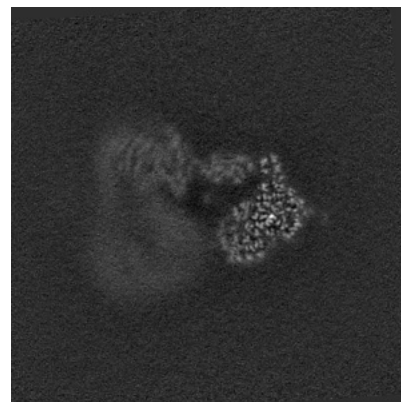
6.2.2 Raw map



X Index: 192



Y Index: 192

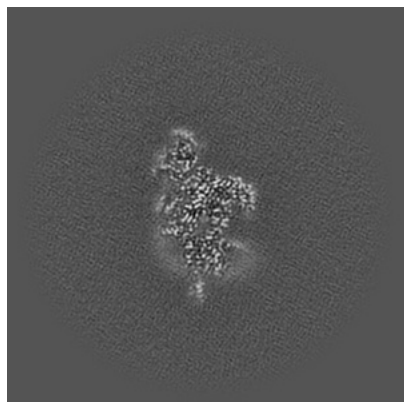


Z Index: 192

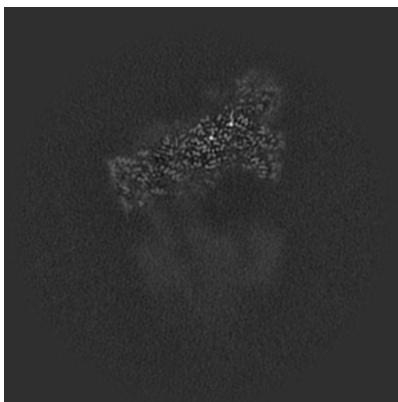
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

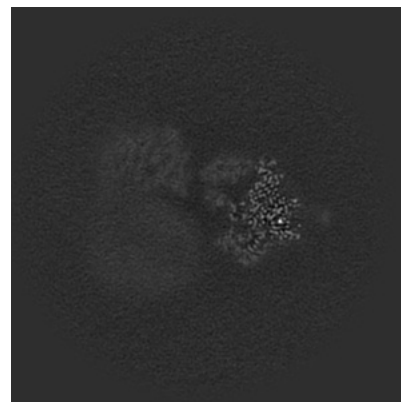
6.3.1 Primary map



X Index: 240

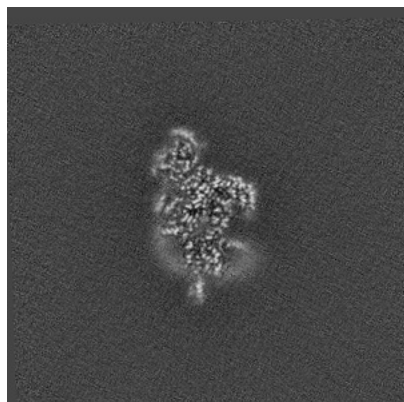


Y Index: 178

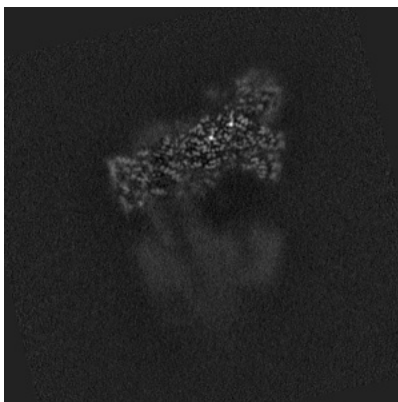


Z Index: 198

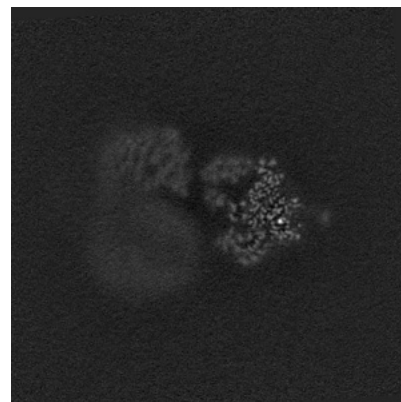
6.3.2 Raw map



X Index: 240



Y Index: 178

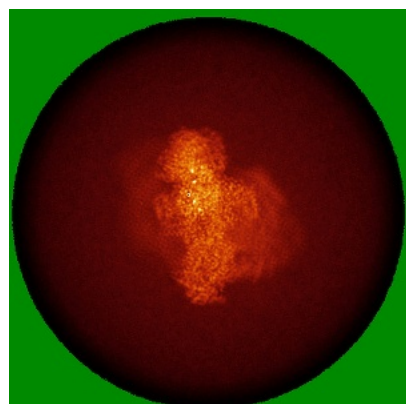


Z Index: 198

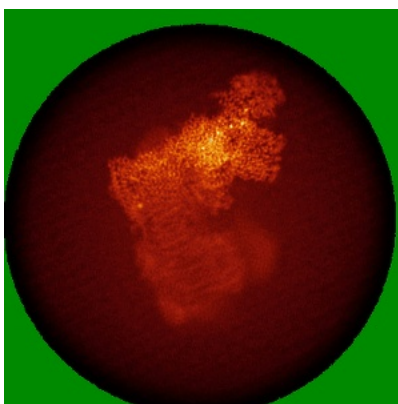
The images above show the largest variance slices of the map in three orthogonal directions.

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

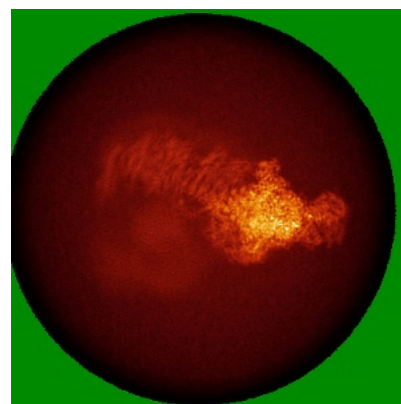
6.4.1 Primary map



X

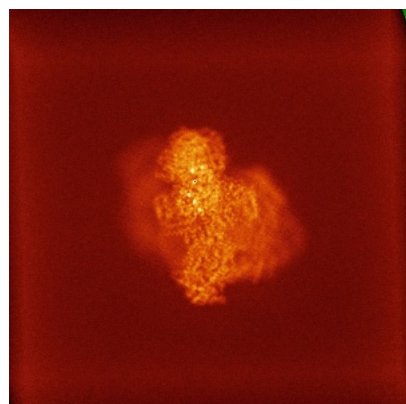


Y

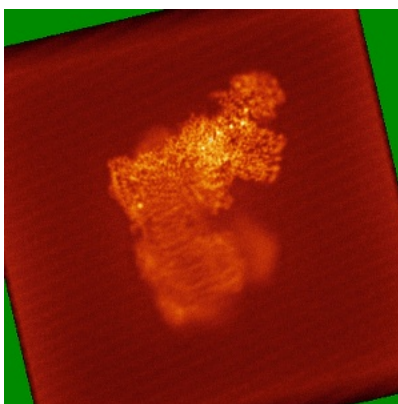


Z

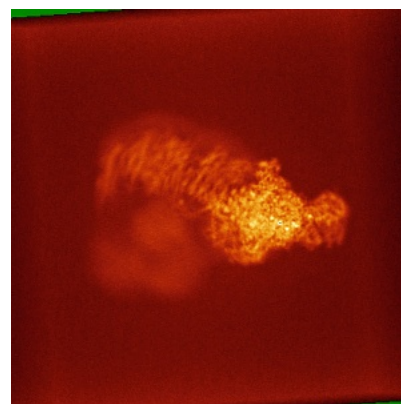
6.4.2 Raw map



X



Y



Z

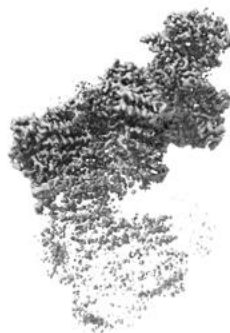
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

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

6.5.2 Raw map



X



Y



Z

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

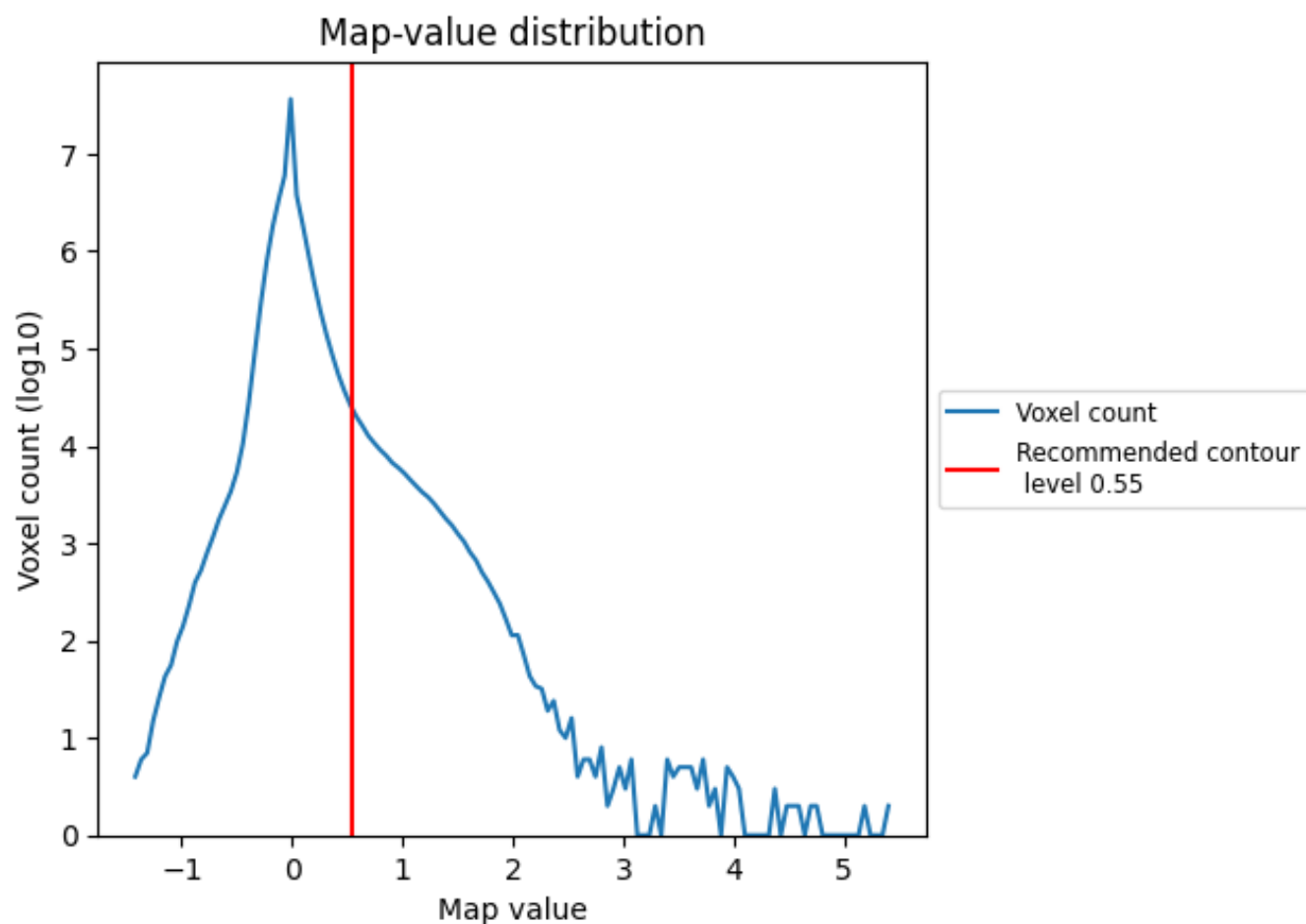
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

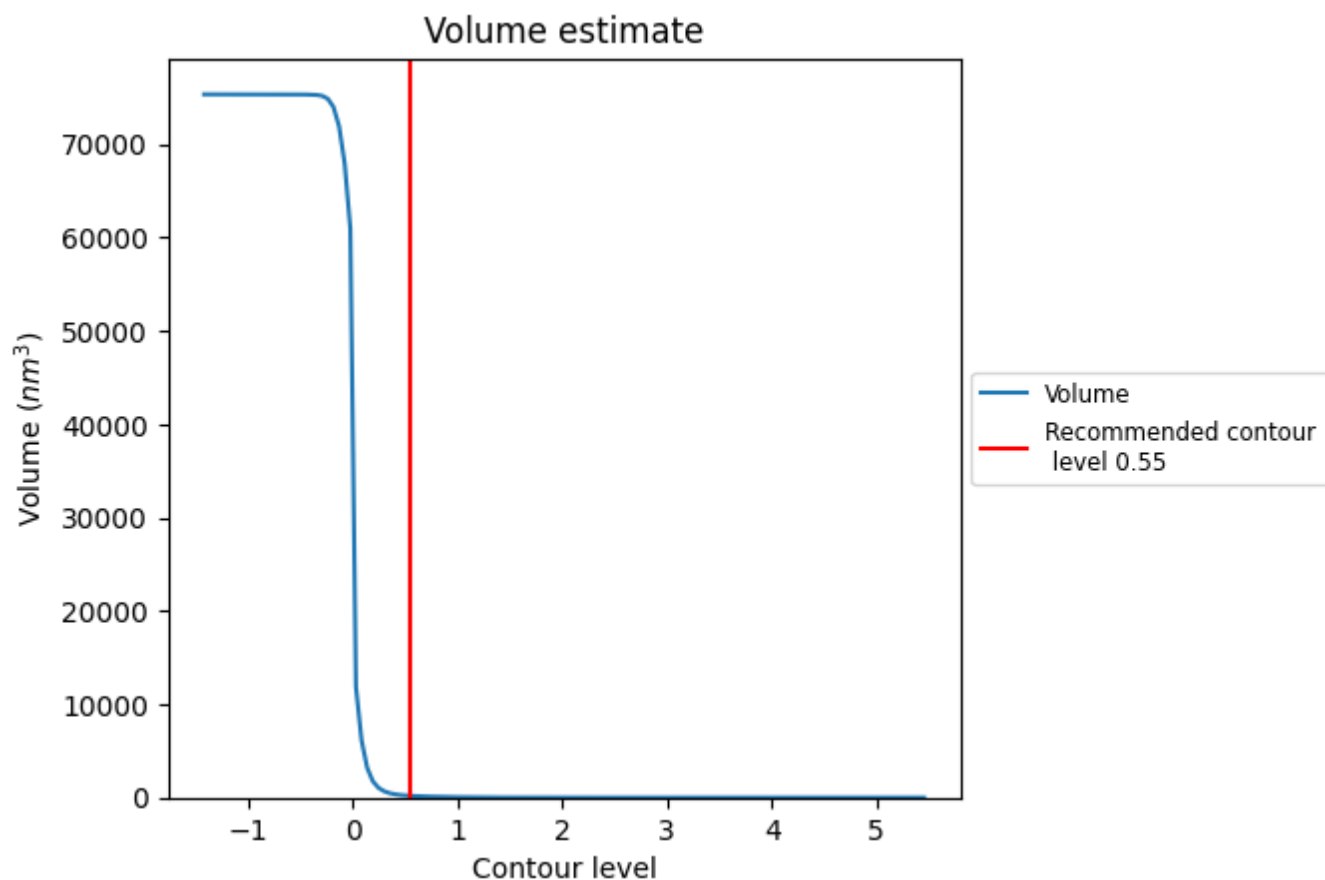
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

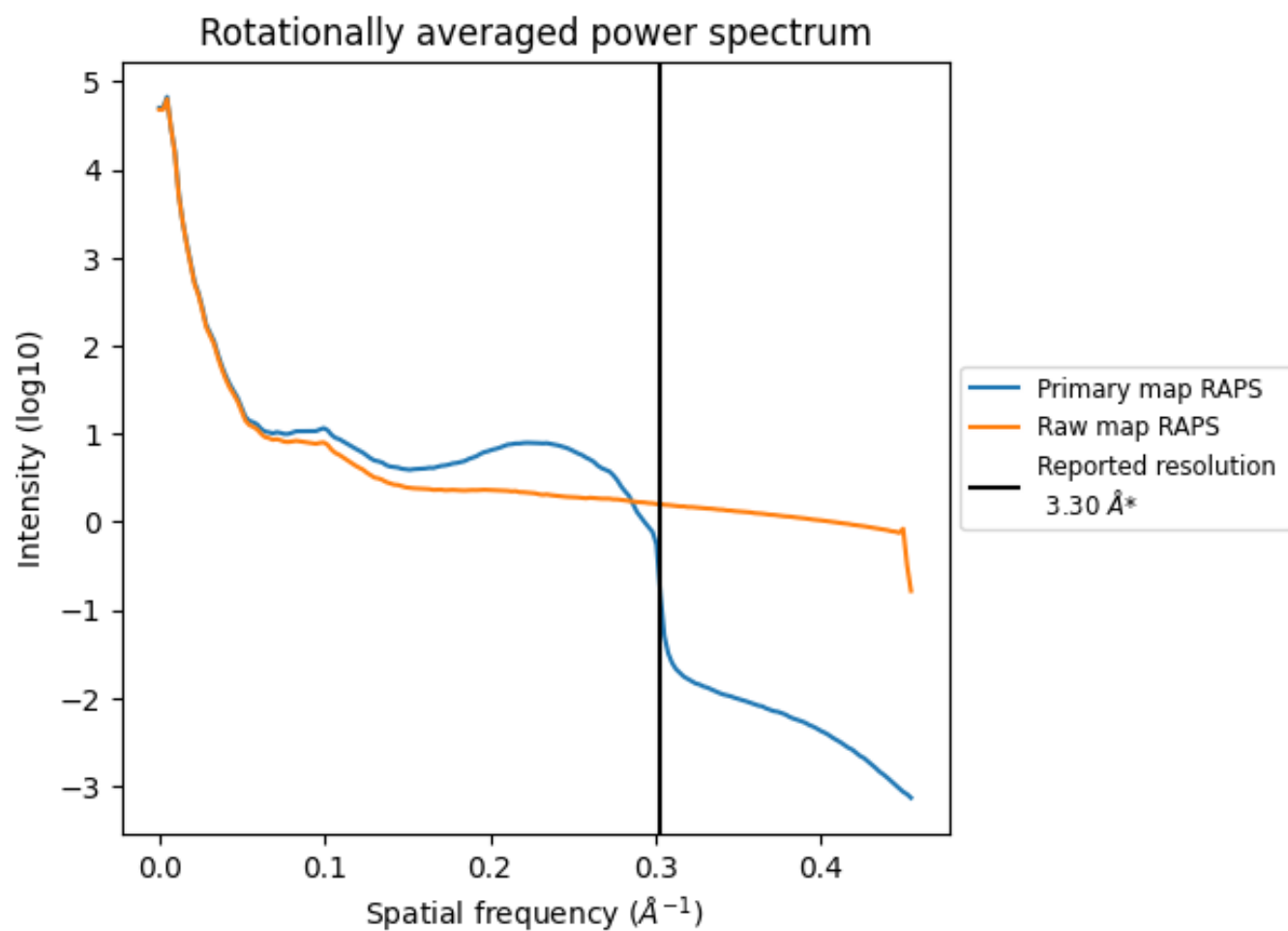
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm³; this corresponds to an approximate mass of 166 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

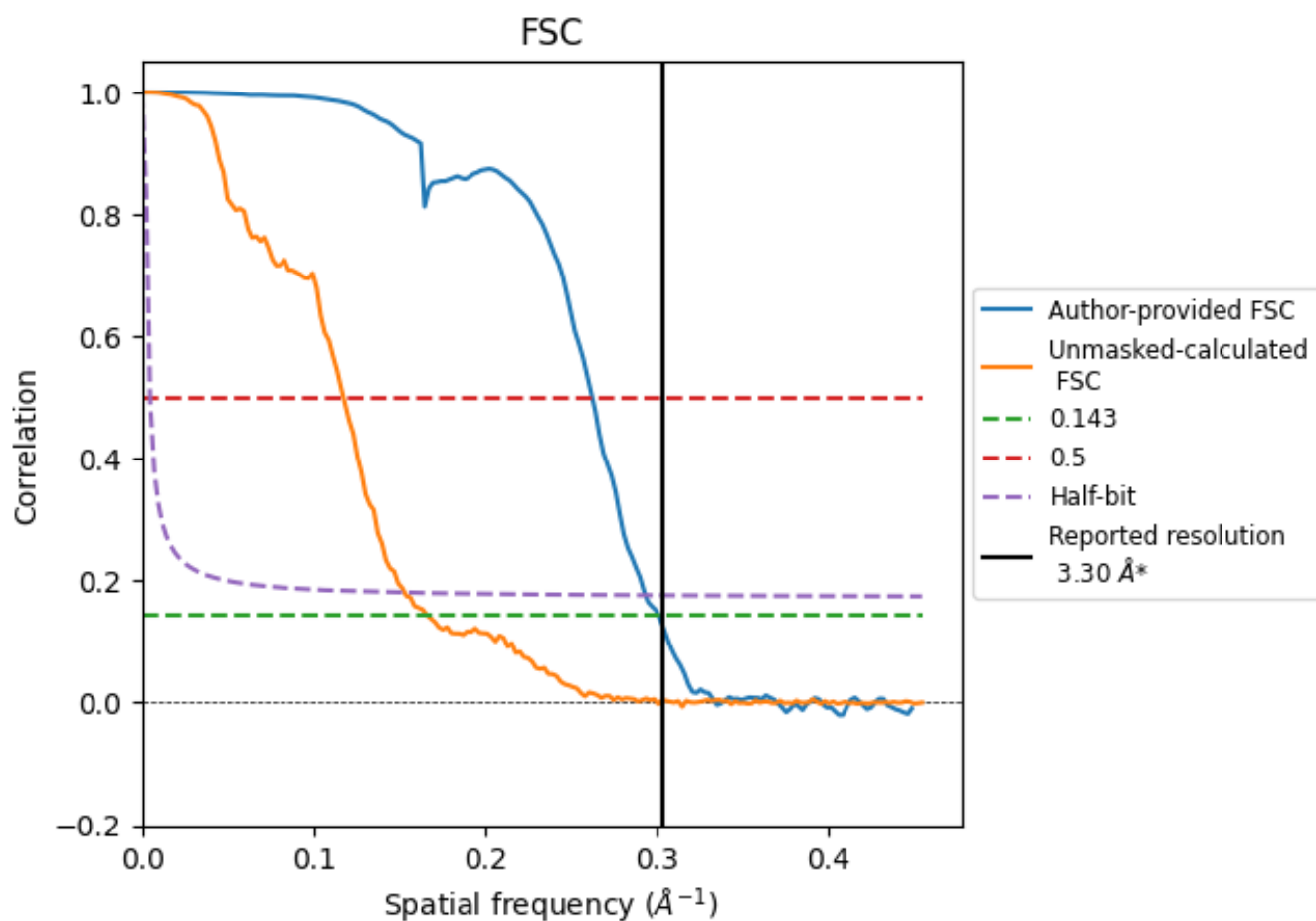


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

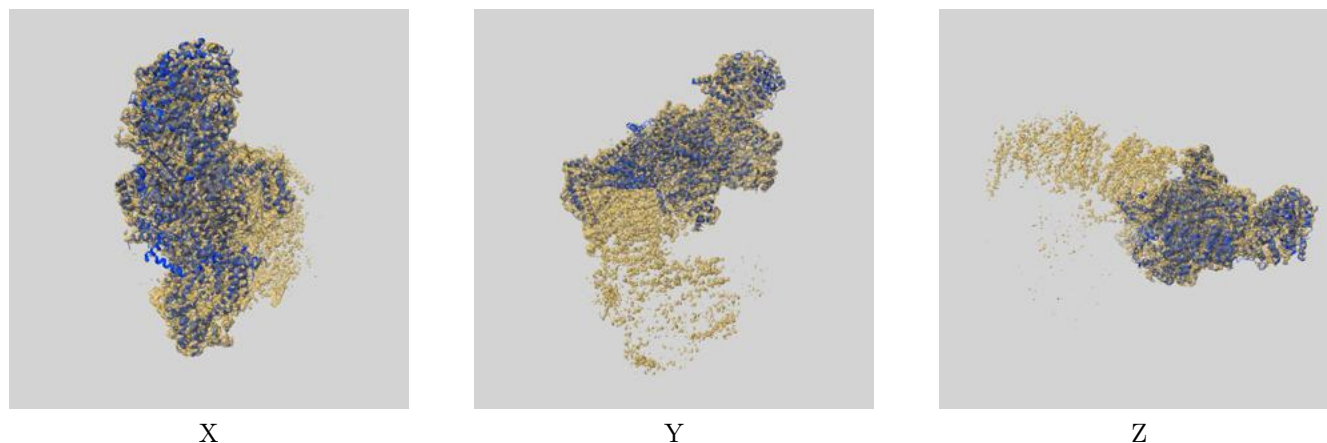
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.81	3.41
Unmasked-calculated*	6.02	8.53	6.54

*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 6.02 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

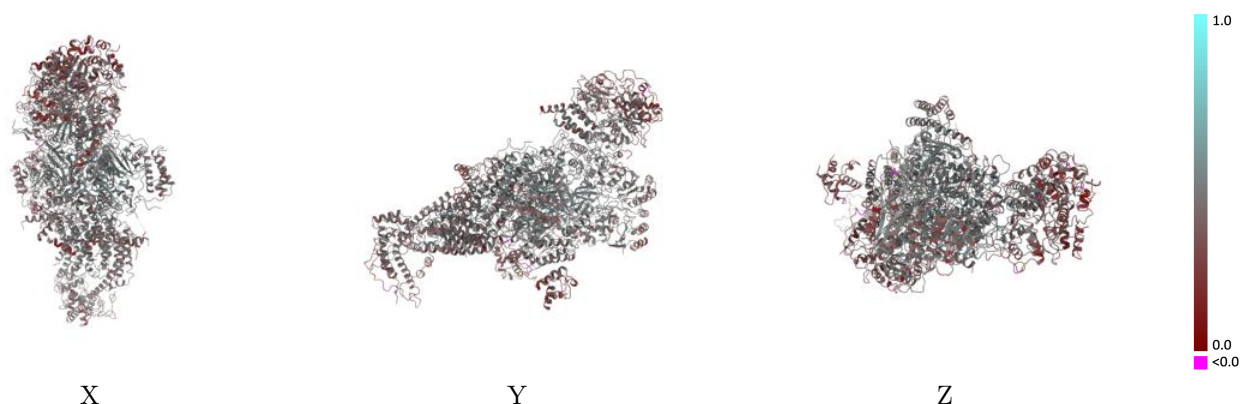
This section contains information regarding the fit between EMDB map EMD-38512 and PDB model 8XNR. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



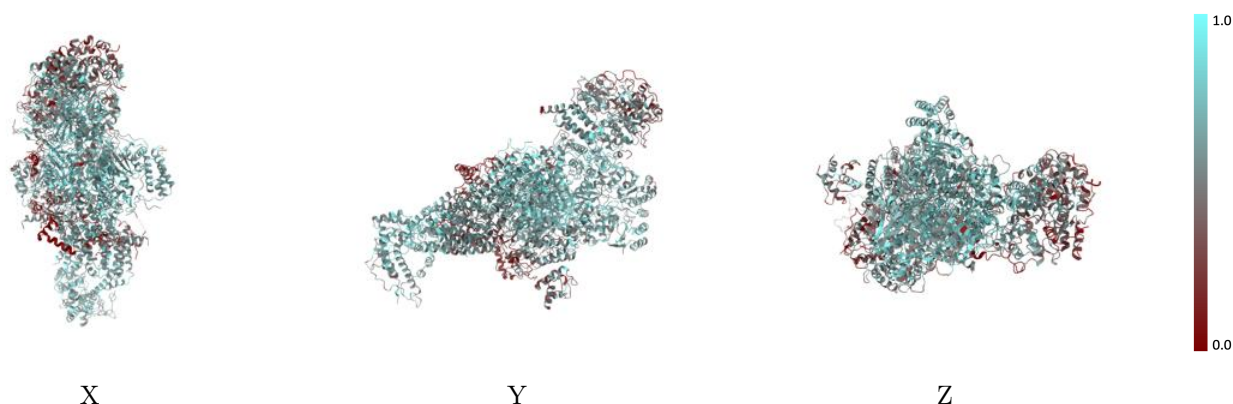
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



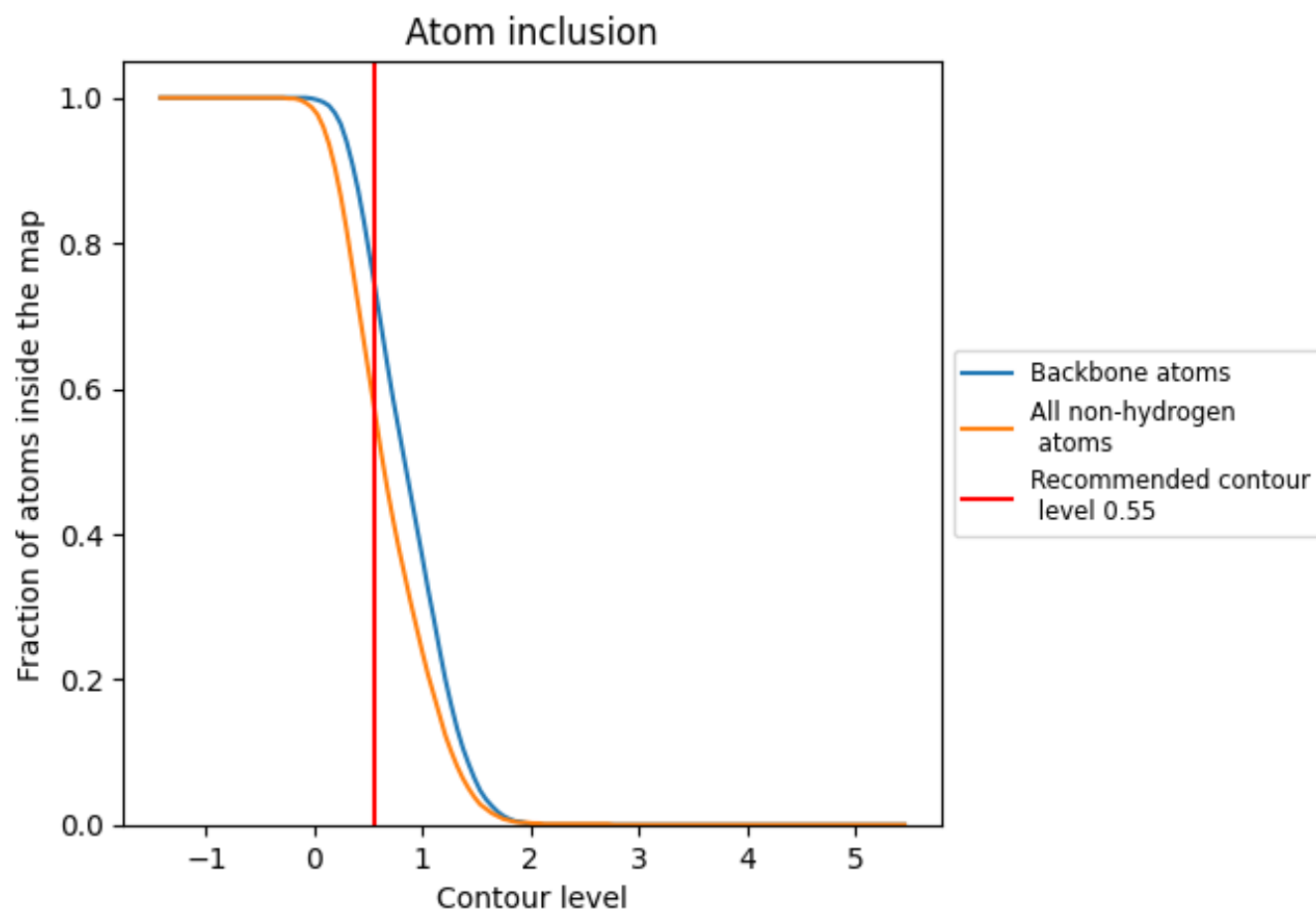
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 58% 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	 0.5760	 0.4220
A	 0.5080	 0.4130
B	 0.6970	 0.4830
C	 0.7210	 0.5040
D	 0.7000	 0.4900
E	 0.4210	 0.3380
F	 0.5060	 0.3740
G	 0.6660	 0.4450
H	 0.6150	 0.4590
I	 0.7150	 0.4740
P	 0.4250	 0.3640
Q	 0.5870	 0.4560
R	 0.2870	 0.3830
S	 0.6330	 0.4090
T	 0.4220	 0.2930
V	 0.6530	 0.4240
W	 0.5750	 0.4370
X	 0.6270	 0.3840
Z	 0.6120	 0.4000
a	 0.7160	 0.4430
b	 0.5550	 0.3800
q	 0.1990	 0.3650
r	 0.3040	 0.3640
s	 0.0950	 0.2890

