



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 10:34 PM JST

PDB ID : 8XNT / pdb_00008xnt
EMDB ID : EMD-38514
Title : Respiratory complex Peripheral Arm of CI, close form C, focus-refined map of type IB, Wild type mouse under Cold Acclimation
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-12-30
Resolution : 4.10 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

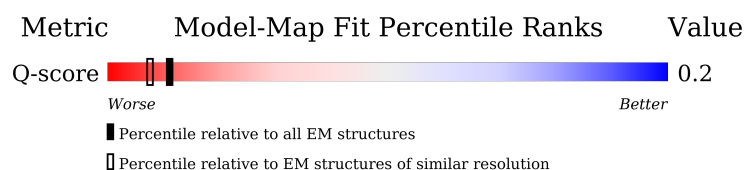
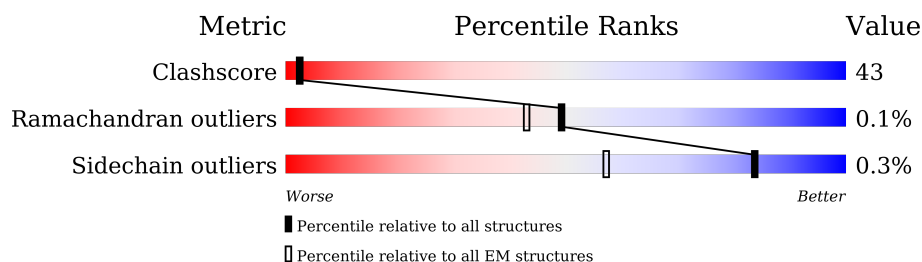
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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
24	SF4	B	301	-	-	X	-
24	SF4	F	502	-	-	X	-
24	SF4	G	802	-	-	X	-
24	SF4	I	301	-	-	X	-
24	SF4	I	302	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	FES	E	301	-	-	X	-
26	FES	G	803	-	-	X	-
31	3PE	b	201	-	-	X	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 32434 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	386	Total	C	N	O	S	0	0
			3095	1974	534	564	23		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	316	Total	C	N	O	S	0	0
			2525	1698	382	423	22		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	41	Total	C	N	O	S	0	0
			305	190	55	57	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	6	Total	C	N	O	S	0	0
			44	25	6	11	2		

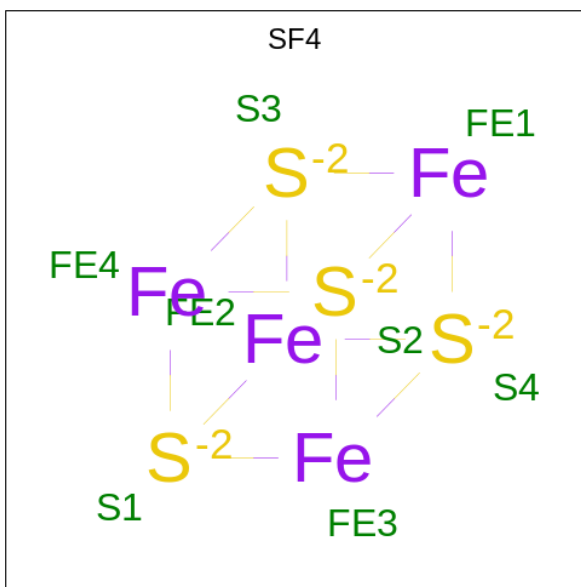
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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.

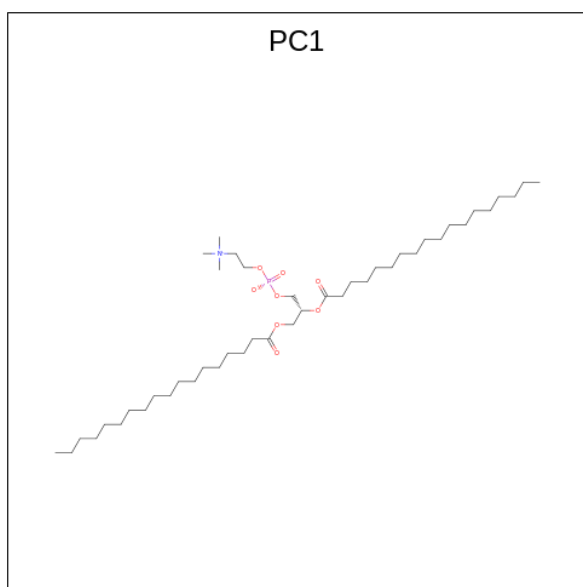
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	26	Total	C	N	O	0	0
			226	147	38	41		

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



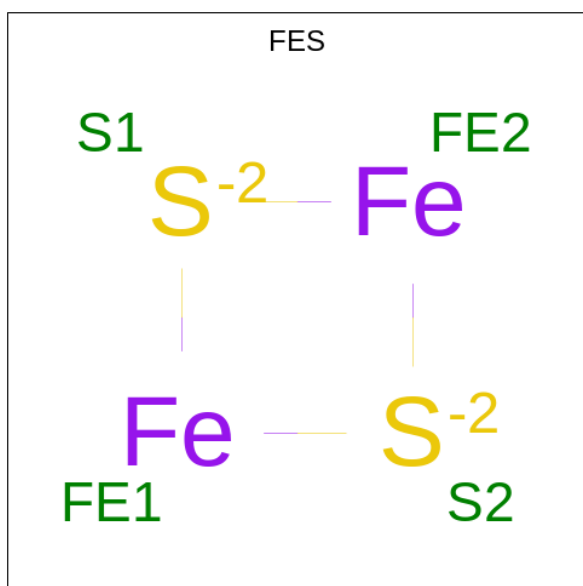
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	Fe	S	0
			8	4	4	
24	F	1	Total	Fe	S	
			8	4	4	
24	G	1	Total	Fe	S	
			8	4	4	
24	G	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	
			8	4	4	
24	I	1	Total	Fe	S	
			8	4	4	

- Molecule 25 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



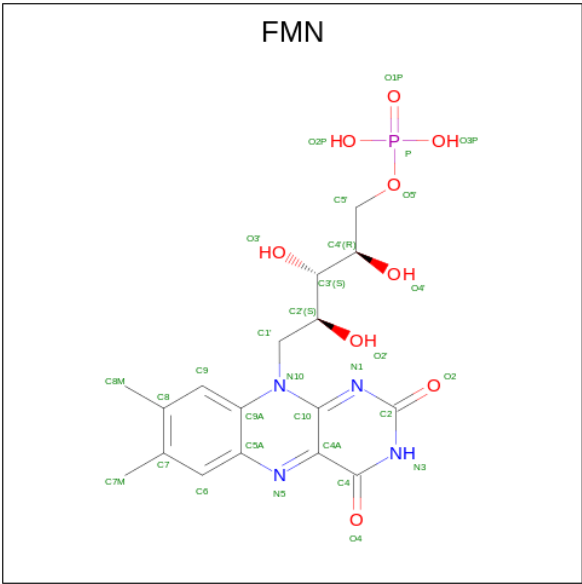
Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 26 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).

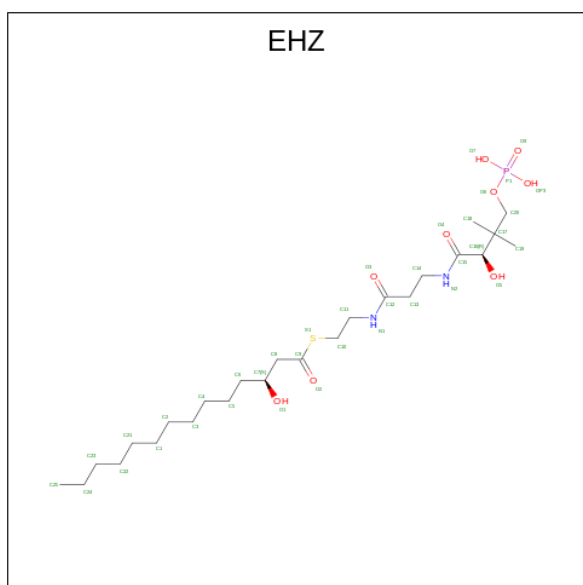


Mol	Chain	Residues	Atoms					AltConf
28	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

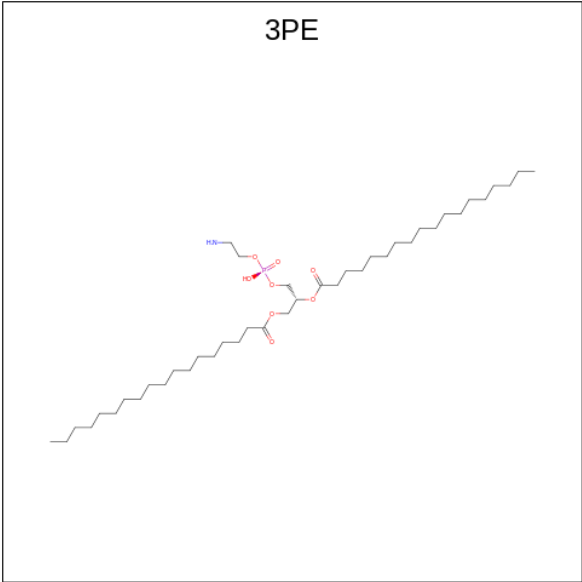
Mol	Chain	Residues	Atoms		AltConf
29	R	1	Total	Zn	0
			1	1	

- Molecule 30 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).

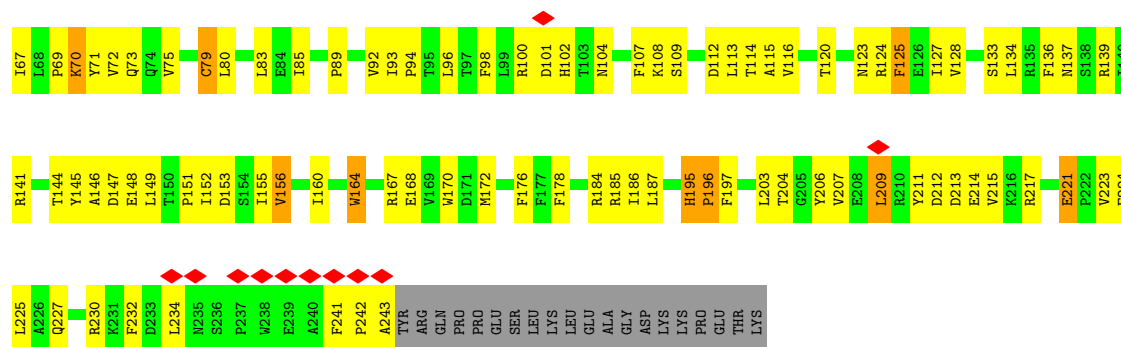


Mol	Chain	Residues	Atoms						AltConf
30	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

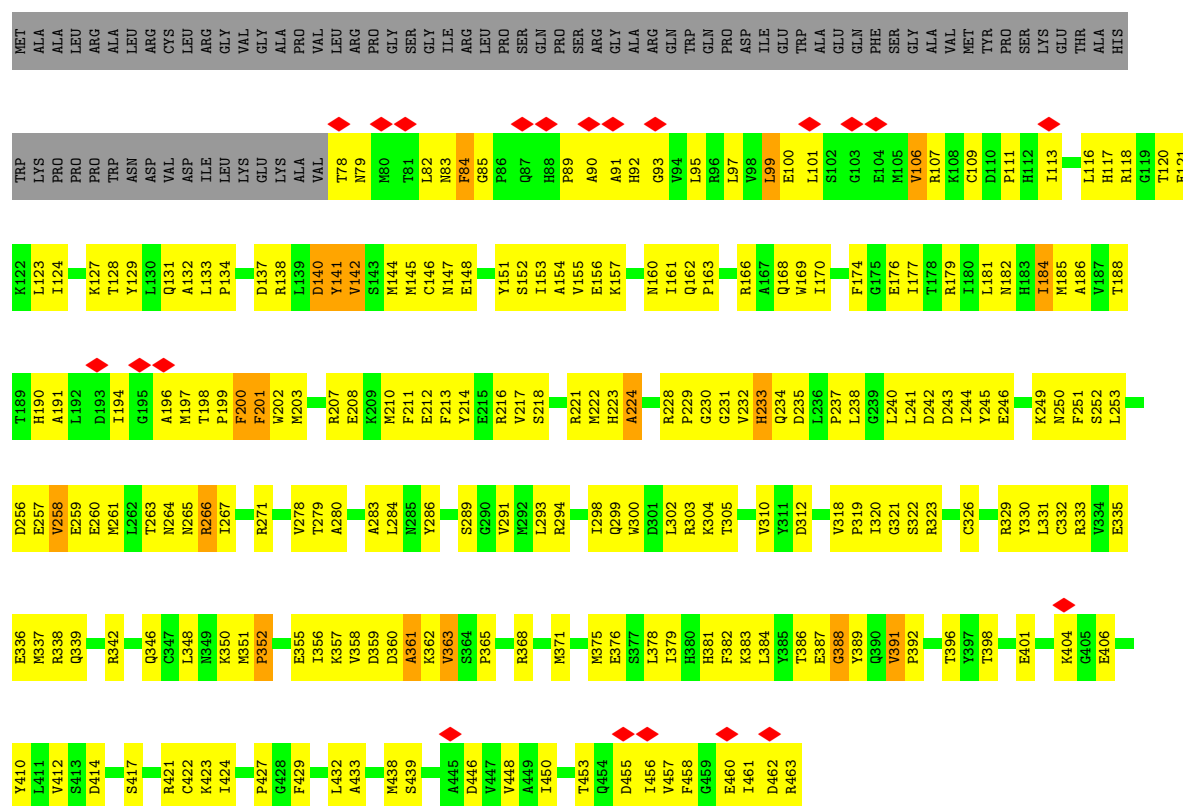
- Molecule 31 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



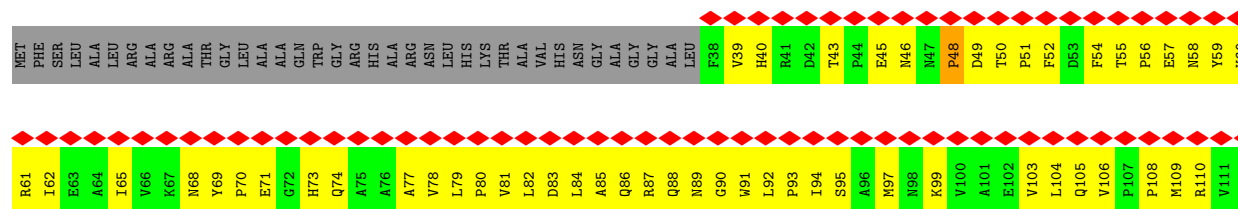
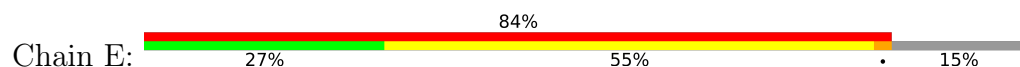
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
31	b	1	46	36	1	8	1	0

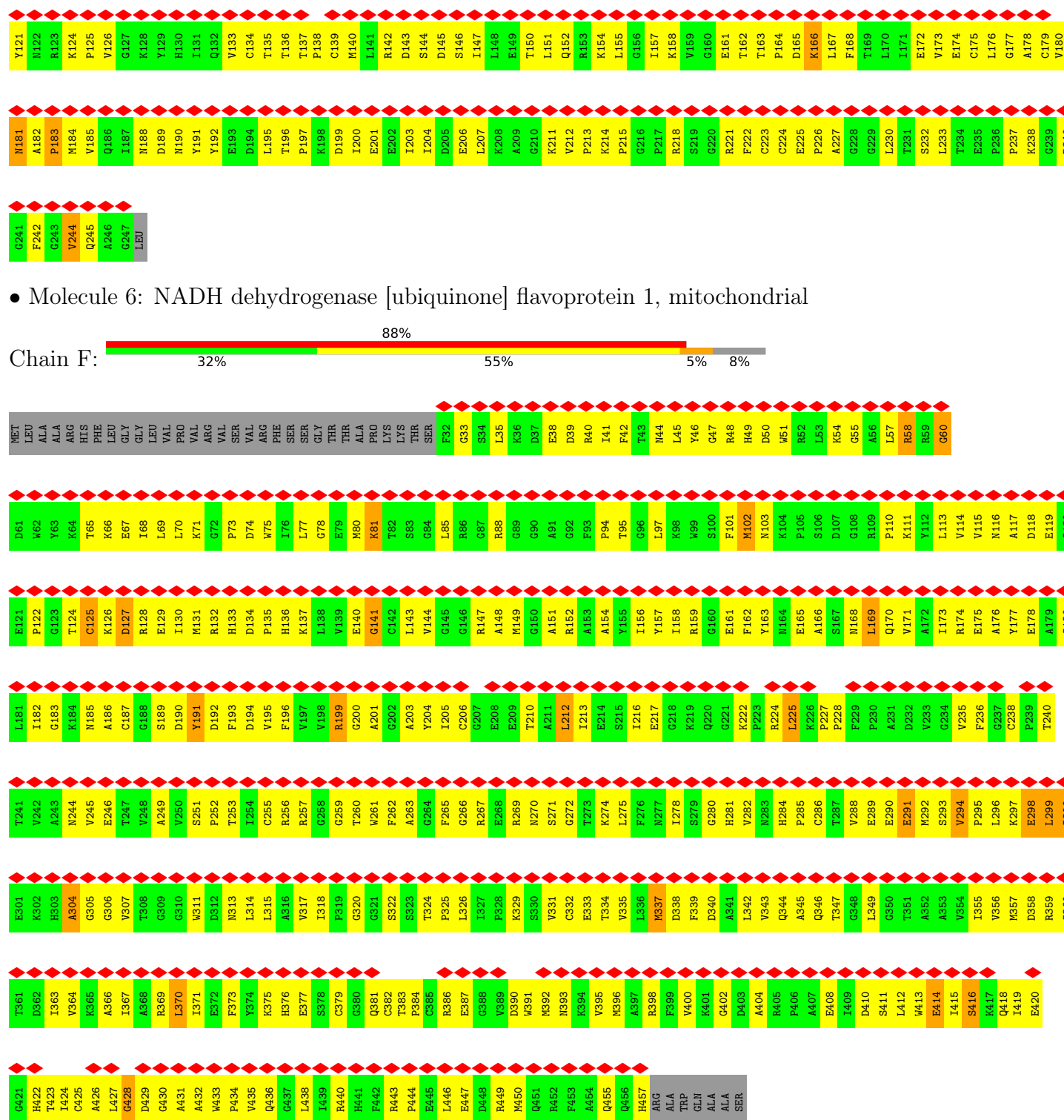


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

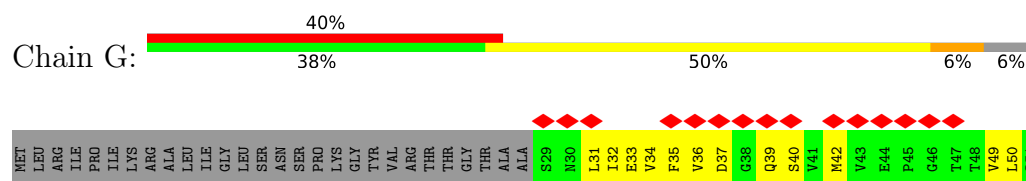


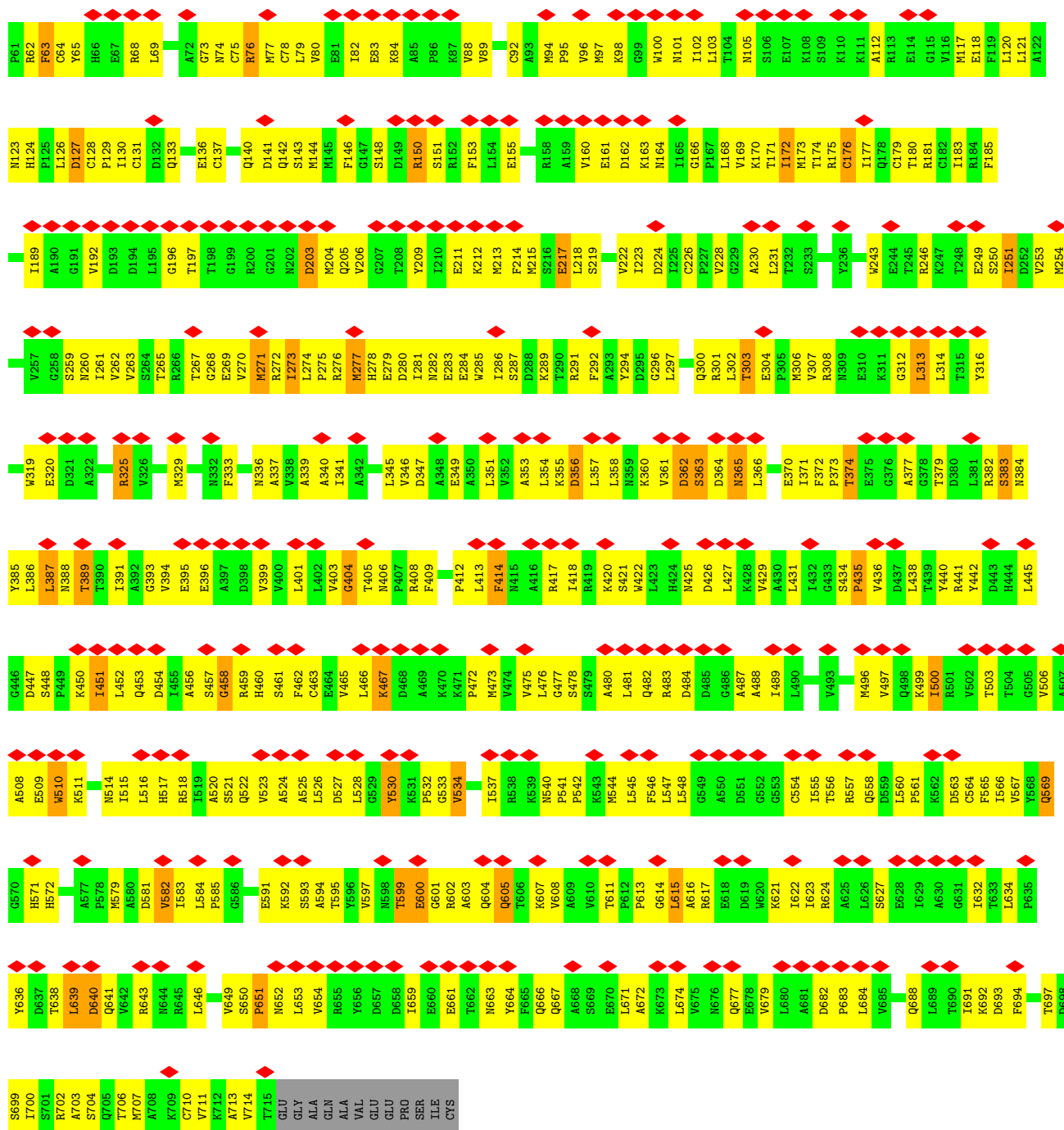
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



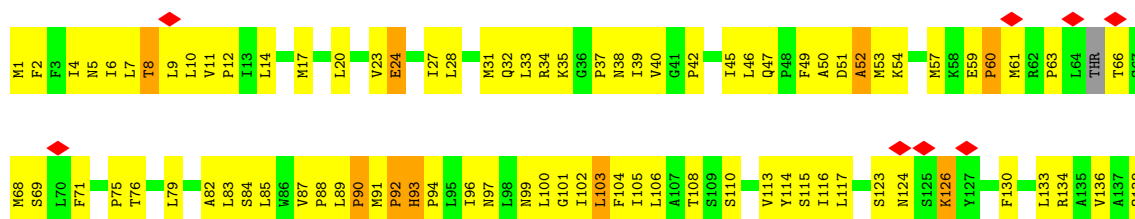


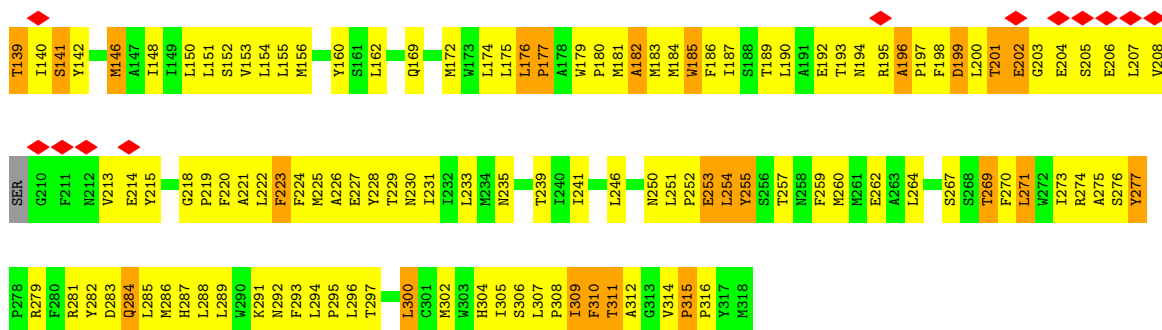
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



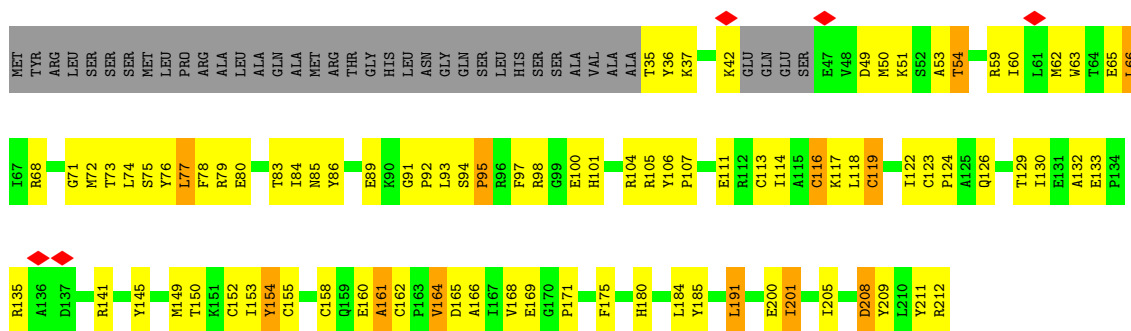


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

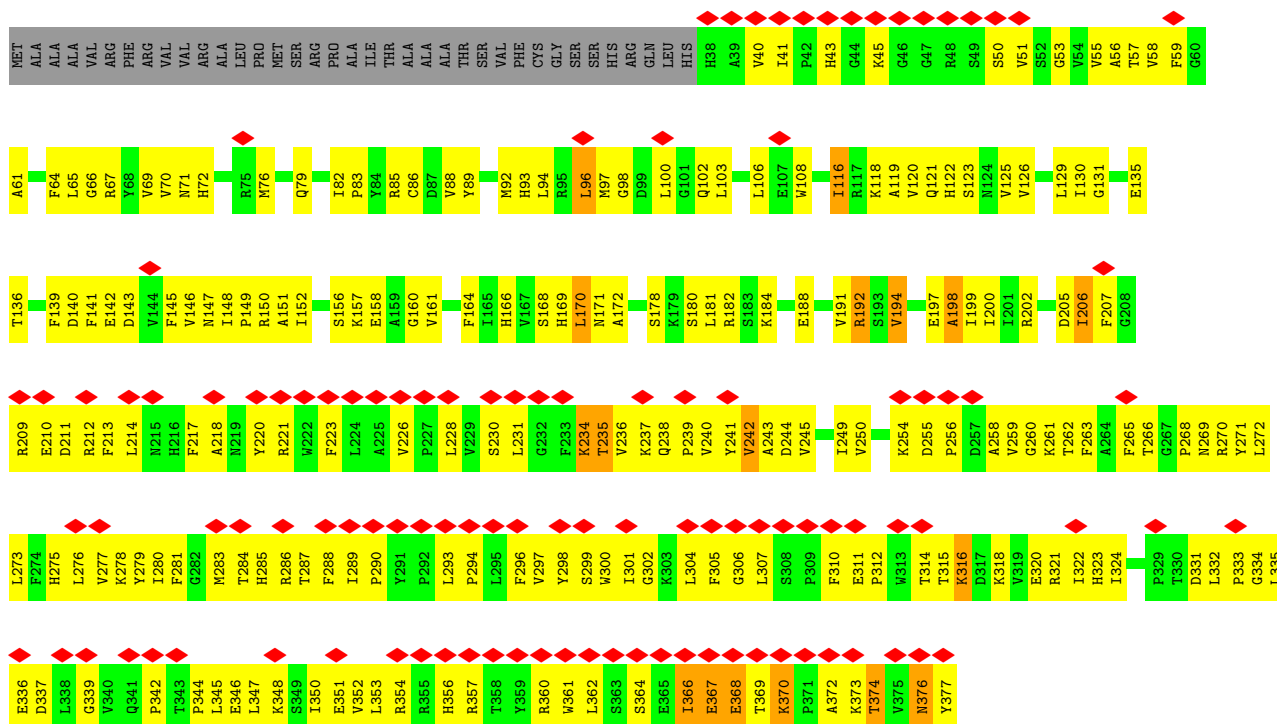




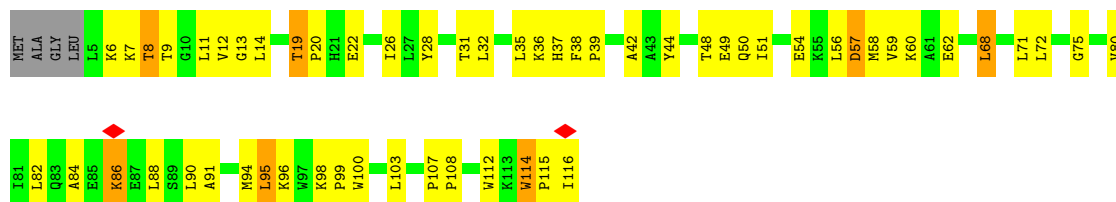
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



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

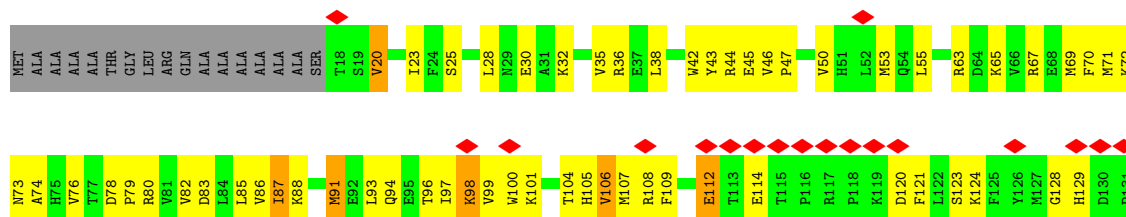


Chain V: 

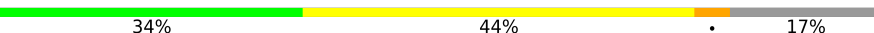


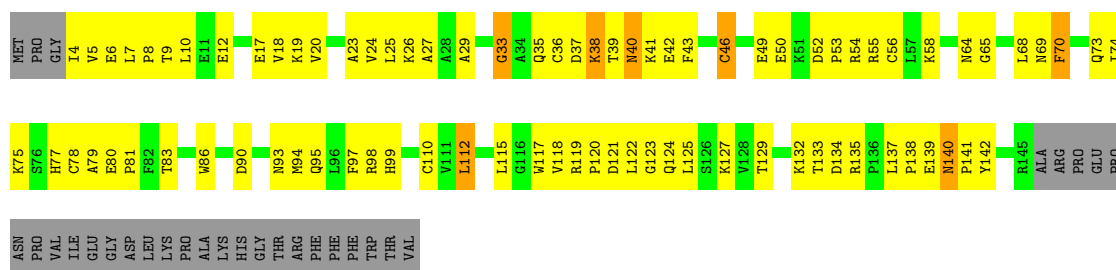
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W: 



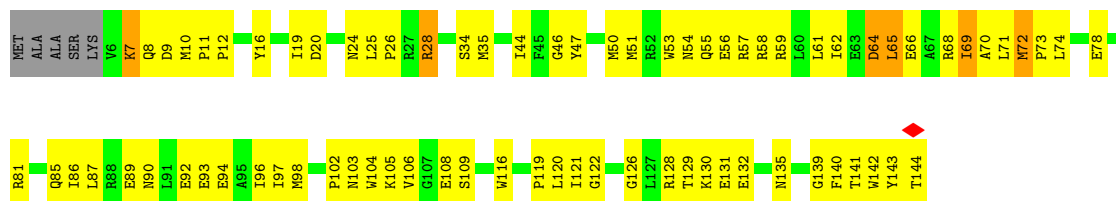
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X: 

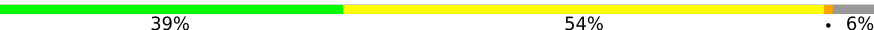


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z: 



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

Chain a: 



PRO	THR	ASP	THR	THR	THR	TYR	LYS	ASN	L35	Q36	H37	H38	D39	Y40	M41	T42	Y43	T44	F45	L46	D47	L48	M49	L50	D51	L52	S53	K54	F55	R56	L57	P58	Q59	P60	SER	SER	GLY	ARG	GLU	GLU	THR	PRO	ARG	THR	LYS	HIS		
MET	ALA	SER	LEU	LEU	LEU	ARG	GLY	GLY	ARG	ILE	ARG	ALA	LEU	LYS	ALA	VAL	LEU	GLU	ALA	ARG	VAL	PRO	GLY	LEU	SER	VAL	ARG	LEU	SER	THR	GLU	SER	GLY	LYS	SER	ALA	LYS	GLU	LYS	LEU	GLU	LEU	VAL	SER	GLN	THR	LYS	PRO

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11078	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	2.500	Depositor
Minimum map value	-0.577	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.3	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: EHZ, NDP, 3PE, FMN, FES, PC1, ZN, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.81	0/782	1.19	6/1066 (0.6%)
2	B	0.98	1/1278 (0.1%)	1.37	13/1730 (0.8%)
3	C	0.90	1/1687 (0.1%)	1.30	13/2297 (0.6%)
4	D	0.95	5/3169 (0.2%)	1.41	31/4286 (0.7%)
5	E	0.77	1/1675 (0.1%)	1.17	9/2282 (0.4%)
6	F	0.87	2/3363 (0.1%)	1.43	47/4543 (1.0%)
7	G	0.89	6/5374 (0.1%)	1.58	102/7281 (1.4%)
8	H	0.92	1/2600 (0.0%)	1.49	55/3550 (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%)	1.29	12/1324 (0.9%)
12	R	0.82	1/310 (0.3%)	1.21	2/414 (0.5%)
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	9/1335 (0.7%)
17	X	0.78	0/1191	1.34	18/1605 (1.1%)
18	Z	0.78	0/1183	1.22	13/1597 (0.8%)
19	a	0.88	0/553	1.21	4/745 (0.5%)
20	b	0.74	0/643	0.95	1/884 (0.1%)
21	q	0.70	0/44	1.02	0/59
22	r	0.87	1/421 (0.2%)	1.38	8/566 (1.4%)
23	s	0.43	0/233	0.75	1/317 (0.3%)
All	All	0.87	22/32938 (0.1%)	1.38	424/44621 (1.0%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	W	106	VAL	C-N	-8.61	1.22	1.33
11	Q	53	ILE	C-O	7.81	1.33	1.24
7	G	203	ASP	CA-C	6.76	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	600	GLU	CA-C	6.57	1.62	1.52
4	D	106	VAL	C-N	-6.56	1.24	1.33
2	B	110	PRO	C-O	-6.31	1.16	1.24
4	D	266	ARG	C-O	-6.28	1.16	1.24
7	G	127	ASP	CA-C	6.27	1.62	1.52
7	G	76	ARG	CA-C	6.05	1.61	1.53
5	E	93	PRO	N-CD	-5.87	1.39	1.47
7	G	361	VAL	CA-C	5.86	1.60	1.52
22	r	25	GLN	CA-C	5.82	1.60	1.52
8	H	60	PRO	N-CD	5.79	1.55	1.47
6	F	225	LEU	C-O	5.77	1.31	1.23
4	D	107	ARG	C-N	5.66	1.41	1.33
6	F	414	GLU	C-O	-5.54	1.17	1.24
4	D	392	PRO	C-O	-5.52	1.20	1.24
7	G	683	PRO	N-CD	-5.39	1.40	1.47
4	D	266	ARG	CA-C	-5.29	1.45	1.52
10	P	235	THR	CA-C	5.25	1.59	1.53
3	C	61	GLY	C-N	-5.03	1.27	1.33
12	R	89	PRO	N-CD	-5.03	1.40	1.47

All (424) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	142	VAL	N-CA-CB	19.30	132.46	110.65
4	D	142	VAL	N-CA-C	-19.04	92.53	110.42
7	G	174	THR	N-CA-C	-16.87	89.00	114.64
6	F	125	CYS	N-CA-C	-15.62	93.48	113.17
7	G	251	ILE	N-CA-C	13.37	126.88	108.17
7	G	77	MET	N-CA-C	-13.07	97.30	113.38
7	G	500	ILE	N-CA-C	-12.53	98.76	110.53
10	P	106	LEU	N-CA-C	12.22	128.75	109.07
6	F	449	ARG	N-CA-C	-11.64	98.67	111.36
7	G	204	MET	N-CA-C	-11.60	91.50	109.25
6	F	171	VAL	N-CA-C	-11.50	99.38	110.42
11	Q	60	ASP	N-CA-C	-11.32	90.33	109.24
7	G	599	THR	N-CA-C	11.29	126.15	112.38
16	W	87	ILE	N-CA-C	-11.08	99.78	110.42
8	H	259	PHE	N-CA-C	-11.03	99.34	111.36
15	V	57	ASP	N-CA-C	-11.02	99.28	111.07
9	I	164	VAL	N-CA-C	-10.60	100.18	113.22
9	I	77	LEU	N-CA-C	-10.53	99.61	111.71
2	B	195	PRO	N-CA-C	-10.40	98.01	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	139	MET	N-CA-C	-10.40	97.45	113.89
7	G	280	ASP	N-CA-C	10.33	122.54	111.28
19	a	4	GLU	N-CA-C	10.19	124.81	112.38
4	D	337	MET	N-CA-C	-10.17	100.18	111.07
9	I	161	ALA	N-CA-C	10.17	122.36	111.28
4	D	140	ASP	CB-CA-C	-10.16	98.11	111.42
10	P	366	ILE	N-CA-C	10.14	120.96	110.62
7	G	414	PHE	N-CA-C	-10.08	101.48	113.88
14	T	135	ALA	N-CA-C	-10.07	100.30	111.28
7	G	325	ARG	N-CA-C	-9.89	100.19	110.97
9	I	166	ALA	N-CA-C	-9.86	100.80	113.12
6	F	103	ASN	N-CA-C	-9.82	100.98	113.16
6	F	178	GLU	N-CA-C	-9.80	99.35	111.11
6	F	141	GLY	N-CA-C	-9.78	101.16	112.50
7	G	654	VAL	N-CA-C	9.74	123.26	111.09
6	F	144	VAL	N-CA-C	-9.69	101.42	110.53
7	G	337	ALA	N-CA-C	-9.57	100.81	114.12
8	H	52	ALA	N-CA-C	-9.57	100.83	111.07
6	F	418	GLN	N-CA-C	-9.56	100.82	111.14
17	X	70	PHE	N-CA-C	-9.54	99.66	111.11
17	X	112	LEU	N-CA-C	-9.45	100.93	111.14
4	D	427	PRO	N-CA-C	-9.44	95.68	110.50
7	G	692	LYS	N-CA-C	-9.30	100.52	112.23
7	G	694	PHE	N-CA-C	9.30	121.41	111.28
14	T	133	ILE	N-CA-C	9.27	119.81	110.82
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	-9.22	100.67	110.36
7	G	389	THR	N-CA-C	-9.17	96.20	109.96
7	G	640	ASP	N-CA-C	-9.16	101.37	111.36
5	E	85	ALA	N-CA-C	-9.15	101.39	111.36
19	a	57	VAL	N-CA-C	-9.00	105.16	113.71
7	G	133	GLN	N-CA-CB	8.84	121.58	110.45
8	H	60	PRO	N-CA-CB	8.77	108.61	102.65
7	G	212	LYS	N-CA-C	-8.77	94.61	108.90
10	P	96	LEU	N-CA-C	8.67	121.68	111.71
16	W	20	VAL	N-CA-C	8.66	120.74	108.36
9	I	154	TYR	N-CA-CB	-8.65	99.25	111.62
7	G	365	ASN	N-CA-C	-8.64	102.30	112.92
3	C	70	LYS	N-CA-C	8.54	121.66	111.33
10	P	373	LYS	N-CA-C	8.54	121.96	110.35
13	S	18	GLU	N-CA-C	8.50	123.26	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
17	X	99	HIS	N-CA-C	-8.41	102.19	111.36
8	H	141	SER	N-CA-C	-8.41	102.07	111.07
3	C	108	LYS	N-CA-C	8.40	120.06	111.07
11	Q	54	THR	N-CA-C	8.32	123.26	109.46
7	G	452	LEU	N-CA-C	-8.30	102.24	111.28
6	F	171	VAL	N-CA-CB	8.28	120.24	110.55
7	G	558	GLN	N-CA-C	-8.25	102.24	111.07
8	H	196	ALA	N-CA-C	8.21	127.95	109.81
8	H	311	THR	N-CA-C	-8.18	102.61	112.59
7	G	691	ILE	N-CA-C	8.17	123.66	111.89
6	F	298	GLU	N-CA-C	8.17	120.19	111.28
3	C	196	PRO	N-CA-C	8.17	124.88	113.53
16	W	96	THR	N-CA-C	-8.16	102.32	111.14
7	G	534	VAL	N-CA-C	-8.14	104.66	111.91
6	F	191	TYR	N-CA-C	8.14	121.71	110.24
1	A	64	LEU	N-CA-C	-8.12	102.38	111.07
15	V	86	LYS	N-CA-C	-8.10	102.39	111.14
2	B	110	PRO	N-CA-C	8.08	124.55	113.65
7	G	484	ASP	N-CA-C	8.07	120.99	111.71
7	G	500	ILE	N-CA-CB	8.05	120.88	110.57
8	H	271	LEU	N-CA-C	-8.05	102.45	111.14
13	S	76	THR	N-CA-C	8.05	122.01	108.90
9	I	201	ILE	N-CA-C	-8.02	102.62	110.72
17	X	46	CYS	N-CA-C	-8.01	102.63	111.36
17	X	43	PHE	N-CA-C	-7.99	102.52	111.07
16	W	98	LYS	N-CA-C	-7.98	101.59	113.72
7	G	651	PRO	CB-CA-C	-7.93	98.47	111.56
10	P	206	ILE	N-CA-C	7.92	120.91	108.87
15	V	6	LYS	N-CA-C	-7.91	100.09	110.53
1	A	9	ILE	N-CA-C	-7.90	102.56	110.62
8	H	311	THR	N-CA-CB	7.85	123.48	110.92
7	G	389	THR	N-CA-CB	7.82	121.50	109.85
9	I	160	GLU	N-CA-C	7.81	124.18	111.37
7	G	270	VAL	N-CA-CB	-7.81	100.70	110.31
10	P	235	THR	CB-CA-C	-7.81	100.04	112.07
9	I	74	LEU	N-CA-C	-7.77	102.81	111.28
17	X	58	LYS	N-CA-C	-7.76	102.76	111.07
8	H	253	GLU	N-CA-C	7.71	121.94	112.54
4	D	141	TYR	CA-C-N	7.69	130.10	120.72
4	D	141	TYR	C-N-CA	7.69	130.10	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	58	ARG	N-CA-C	-7.67	103.00	111.36
2	B	153	PRO	CB-CA-C	-7.59	99.04	111.56
7	G	569	GLN	N-CA-C	7.59	121.98	108.24
7	G	56	VAL	N-CA-C	-7.57	103.07	110.72
8	H	201	THR	N-CA-C	-7.57	102.63	111.03
4	D	361	ALA	N-CA-C	-7.57	103.15	112.38
7	G	467	LYS	N-CA-C	-7.54	102.21	111.33
12	R	74	HIS	N-CA-C	7.54	121.13	110.50
9	I	119	CYS	N-CA-C	-7.54	103.14	111.36
7	G	277	MET	N-CA-C	7.50	120.62	109.59
9	I	158	CYS	N-CA-C	-7.48	103.13	111.28
2	B	183	ARG	N-CA-C	-7.46	104.42	113.97
8	H	223	PHE	CB-CA-C	-7.45	99.18	110.88
7	G	510	TRP	N-CA-CB	7.42	120.91	109.85
6	F	430	GLY	N-CA-C	7.42	121.63	112.73
4	D	350	LYS	CB-CA-C	-7.41	100.96	111.85
4	D	99	LEU	N-CA-C	7.38	120.96	109.07
8	H	309	ILE	N-CA-C	7.38	117.45	110.30
7	G	303	THR	N-CA-C	7.37	122.98	113.18
15	V	57	ASP	N-CA-CB	7.36	120.68	110.01
7	G	384	ASN	N-CA-C	-7.30	103.35	111.82
13	S	94	VAL	N-CA-C	7.30	117.43	110.42
7	G	661	GLU	N-CA-C	7.29	118.92	110.97
10	P	370	LYS	N-CA-C	7.25	119.31	109.24
7	G	374	THR	CB-CA-C	-7.23	99.86	111.28
3	C	195	HIS	CB-CA-C	7.23	117.33	110.17
8	H	50	ALA	N-CA-C	7.21	118.79	111.07
8	H	254	LEU	N-CA-C	-7.20	103.47	111.82
14	T	105	MET	N-CA-C	7.20	119.20	111.36
8	H	139	THR	N-CA-CB	7.18	120.42	110.01
7	G	497	VAL	N-CA-C	-7.16	103.31	110.62
6	F	81	LYS	N-CA-C	-7.12	103.59	111.36
15	V	68	LEU	N-CA-C	-7.12	103.51	111.28
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	217	GLU	N-CA-C	-7.10	101.68	110.41
7	G	150	ARG	N-CA-C	7.08	119.68	109.14
2	B	166	ASN	N-CA-C	-7.07	103.27	110.97
7	G	465	VAL	N-CA-CB	7.07	118.35	110.51
11	Q	162	ALA	N-CA-C	7.07	118.98	111.28
7	G	148	SER	N-CA-C	7.06	120.91	109.40
6	F	78	GLY	N-CA-C	-7.05	104.27	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	95	LEU	N-CA-C	-7.05	103.60	111.28
10	P	235	THR	CA-C-O	7.04	128.22	121.67
6	F	455	GLN	N-CA-C	7.04	118.60	111.07
6	F	169	LEU	N-CA-C	7.02	118.93	111.28
7	G	294	TYR	N-CA-C	-6.97	104.59	113.23
6	F	428	GLY	N-CA-C	-6.96	103.85	112.77
8	H	176	LEU	CA-C-N	-6.96	113.63	120.52
8	H	176	LEU	C-N-CA	-6.96	113.63	120.52
8	H	292	ASN	N-CA-C	6.96	118.94	111.36
18	Z	34	SER	N-CA-C	-6.94	103.64	111.07
18	Z	28	ARG	N-CA-C	6.93	119.82	108.52
6	F	418	GLN	N-CA-CB	6.92	120.10	110.07
6	F	148	ALA	N-CA-C	-6.91	103.83	111.36
7	G	582	VAL	N-CA-C	6.91	118.42	108.48
16	W	87	ILE	N-CA-CB	6.90	118.62	110.55
6	F	103	ASN	N-CA-CB	6.90	120.99	110.44
5	E	152	GLN	N-CA-C	-6.89	103.69	111.07
6	F	246	GLU	N-CA-C	-6.89	103.77	111.28
7	G	362	ASP	N-CA-C	6.88	125.46	110.80
14	T	145	VAL	N-CA-C	-6.88	103.77	110.72
7	G	300	GLN	N-CA-CB	6.85	122.42	112.08
8	H	300	LEU	N-CA-C	-6.83	104.20	112.54
7	G	133	GLN	N-CA-C	-6.82	101.21	110.68
7	G	268	GLY	N-CA-C	6.81	124.77	115.30
8	H	305	ILE	N-CA-C	-6.76	103.45	113.39
6	F	244	ASN	N-CA-C	-6.74	101.00	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
9	I	208	ASP	N-CA-C	6.71	121.62	113.17
7	G	434	SER	N-CA-C	-6.70	101.04	110.29
15	V	8	THR	N-CA-C	6.70	119.04	108.79
3	C	79	CYS	N-CA-C	-6.68	101.69	110.43
7	G	601	GLY	N-CA-C	6.67	124.90	115.30
8	H	93	HIS	CB-CA-C	6.67	117.89	108.76
16	W	105	HIS	N-CA-C	-6.66	104.98	113.23
4	D	184	ILE	N-CA-C	-6.65	103.84	110.62
7	G	640	ASP	N-CA-CB	6.65	120.00	110.16
3	C	125	PHE	N-CA-CB	-6.64	100.60	110.17
15	V	86	LYS	N-CA-CB	6.63	119.69	110.07
3	C	69	PRO	N-CA-C	-6.63	104.32	113.53
7	G	287	SER	N-CA-C	6.62	119.26	110.53
10	P	116	ILE	N-CA-C	-6.61	104.05	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	267	SER	N-CA-C	-6.60	104.16	111.36
17	X	129	THR	N-CA-C	6.58	120.76	110.17
7	G	435	PRO	N-CA-C	-6.56	100.20	110.50
11	Q	141	ASN	N-CA-CB	6.55	120.75	110.46
18	Z	65	LEU	N-CA-C	-6.55	104.22	111.36
8	H	223	PHE	N-CA-C	-6.53	104.09	111.07
8	H	182	ALA	N-CA-C	-6.52	104.09	111.07
2	B	97	LEU	N-CA-C	-6.51	101.49	110.35
7	G	605	GLN	N-CA-C	6.50	119.12	108.52
17	X	98	ARG	N-CA-C	6.48	120.44	112.54
4	D	388	GLY	N-CA-C	6.48	119.58	110.38
8	H	255	TYR	N-CA-CB	6.46	119.38	110.01
9	I	66	LEU	N-CA-C	-6.45	104.33	111.36
7	G	250	SER	N-CA-C	6.45	116.79	108.34
22	r	24	LEU	N-CA-C	6.45	119.59	110.50
13	S	16	LEU	N-CA-C	-6.44	98.40	108.90
4	D	140	ASP	N-CA-C	-6.44	96.48	107.23
4	D	84	PHE	N-CA-C	-6.44	104.31	111.71
15	V	49	GLU	N-CA-C	-6.42	104.28	111.28
8	H	177	PRO	N-CA-C	-6.42	101.57	111.13
8	H	271	LEU	N-CA-CB	6.41	119.36	110.07
7	G	95	PRO	N-CA-C	-6.40	101.13	110.80
12	R	81	GLY	N-CA-C	-6.40	106.89	115.21
6	F	370	LEU	N-CA-C	-6.40	104.39	111.36
11	Q	59	LEU	N-CA-C	-6.39	100.72	110.30
6	F	178	GLU	N-CA-CB	6.38	119.45	109.94
9	I	205	ILE	N-CA-C	-6.38	104.28	110.72
3	C	125	PHE	N-CA-C	6.36	119.47	110.50
15	V	91	ALA	N-CA-C	-6.36	104.35	111.28
7	G	273	ILE	N-CA-C	-6.34	98.38	107.77
15	V	71	LEU	N-CA-C	6.34	118.19	111.28
7	G	176	CYS	N-CA-C	6.33	119.66	110.42
6	F	144	VAL	N-CA-CB	6.29	118.63	110.57
7	G	356	ASP	N-CA-CB	6.28	119.35	110.12
17	X	99	HIS	N-CA-CB	6.28	119.45	110.16
7	G	383	SER	N-CA-C	-6.28	106.84	114.75
6	F	101	PHE	N-CA-C	6.25	118.90	111.33
1	A	101	GLY	N-CA-C	-6.25	105.25	112.50
8	H	52	ALA	N-CA-CB	6.24	119.06	110.01
11	Q	141	ASN	N-CA-C	-6.24	105.67	113.28
4	D	233	HIS	N-CA-C	6.23	119.00	111.40
2	B	113	ASP	N-CA-CB	6.22	119.48	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	141	TYR	N-CA-C	6.22	120.87	113.16
7	G	420	LYS	N-CA-C	6.21	118.84	111.33
8	H	76	THR	N-CA-C	-6.21	104.51	111.28
19	a	26	ILE	N-CA-C	-6.20	104.64	113.07
8	H	269	THR	N-CA-C	6.19	118.03	111.28
22	r	26	LEU	N-CA-CB	-6.19	101.13	110.35
10	P	368	GLU	N-CA-CB	6.19	119.83	110.30
18	Z	69	ILE	N-CA-CB	6.18	117.37	110.51
7	G	451	ILE	N-CA-C	-6.18	104.97	113.00
13	S	61	VAL	N-CA-C	-6.17	99.59	108.42
6	F	192	ASP	N-CA-C	6.17	119.00	109.07
4	D	291	VAL	N-CA-C	-6.14	103.42	111.09
7	G	418	ILE	N-CA-C	-6.13	103.46	112.04
10	P	118	LYS	N-CA-C	6.12	118.92	111.82
7	G	325	ARG	N-CA-CB	6.11	118.83	109.91
6	F	415	ILE	N-CA-C	-6.10	104.40	110.62
8	H	185	TRP	N-CA-C	-6.08	104.00	112.45
8	H	276	SER	N-CA-C	6.08	118.87	111.82
8	H	202	GLU	N-CA-C	-6.07	105.85	113.20
6	F	212	LEU	N-CA-C	-6.06	104.68	111.28
7	G	353	ALA	N-CA-C	-6.06	104.60	112.23
13	S	87	VAL	N-CA-C	-6.05	104.45	110.62
8	H	103	LEU	N-CA-C	-6.05	104.77	111.36
8	H	7	LEU	N-CA-C	-6.04	104.33	111.03
7	G	508	ALA	N-CA-C	6.03	117.86	111.28
18	Z	72	MET	CA-C-N	-6.03	112.97	119.24
18	Z	72	MET	C-N-CA	-6.03	112.97	119.24
8	H	24	GLU	N-CA-C	-6.01	104.09	112.45
22	r	108	LYS	N-CA-C	6.01	117.91	111.36
18	Z	65	LEU	N-CA-CB	6.00	119.04	110.16
7	G	638	THR	N-CA-C	-6.00	100.18	109.24
2	B	196	PRO	N-CA-C	-5.96	101.86	111.03
17	X	38	LYS	N-CA-C	-5.94	104.72	111.07
6	F	291	GLU	N-CA-C	5.93	118.20	110.43
7	G	387	LEU	CB-CA-C	-5.92	101.74	111.68
18	Z	44	ILE	N-CA-C	-5.90	104.75	110.42
9	I	116	CYS	N-CA-C	-5.89	105.59	112.89
17	X	97	PHE	N-CA-C	5.88	118.64	111.82
2	B	135	GLY	CA-C-O	-5.88	117.88	122.52
6	F	127	ASP	N-CA-C	5.87	118.46	111.71
15	V	19	THR	N-CA-CB	5.86	120.80	110.37
8	H	116	ILE	N-CA-C	-5.85	104.80	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	94	ASP	N-CA-CB	-5.85	105.17	111.66
3	C	209	LEU	N-CA-CB	-5.84	100.66	110.83
4	D	352	PRO	N-CA-C	5.84	117.82	110.70
13	S	86	GLU	N-CA-CB	5.84	118.80	110.16
10	P	122	HIS	N-CA-C	5.84	120.10	112.92
6	F	255	CYS	N-CA-C	-5.82	104.53	111.69
7	G	480	ALA	N-CA-C	-5.82	105.02	111.36
7	G	639	LEU	N-CA-C	5.81	118.56	111.82
8	H	315	PRO	O-C-N	5.81	123.88	121.15
10	P	367	GLU	CB-CA-C	-5.79	99.54	110.67
17	X	36	CYS	CB-CA-C	-5.79	102.53	111.74
6	F	102	MET	CB-CA-C	-5.79	101.39	110.94
7	G	672	ALA	N-CA-C	-5.79	104.97	111.28
11	Q	164	PHE	N-CA-CB	5.79	119.79	110.42
1	A	105	GLU	N-CA-C	-5.78	104.97	111.28
4	D	414	ASP	N-CA-C	-5.76	101.43	110.36
4	D	258	VAL	N-CA-C	-5.75	104.06	110.62
10	P	234	LYS	CB-CA-C	-5.75	103.40	111.80
6	F	393	ASN	N-CA-C	-5.74	104.93	111.07
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
7	G	289	LYS	N-CA-C	5.71	117.50	111.28
8	H	252	PRO	N-CA-CB	-5.71	98.03	103.51
11	Q	124	MET	CA-C-N	-5.70	114.89	122.98
11	Q	124	MET	C-N-CA	-5.70	114.89	122.98
13	S	73	GLN	N-CA-C	-5.69	100.43	109.59
6	F	176	ALA	N-CA-C	5.68	118.20	111.33
10	P	119	ALA	N-CA-C	-5.68	105.01	111.14
8	H	126	LYS	N-CA-C	5.67	117.46	111.28
5	E	119	THR	N-CA-C	-5.67	105.86	112.89
7	G	540	ASN	CA-C-N	-5.67	114.55	120.38
7	G	540	ASN	C-N-CA	-5.67	114.55	120.38
7	G	59	GLN	N-CA-C	5.65	117.99	107.99
7	G	599	THR	CA-C-N	-5.64	114.14	122.83
7	G	599	THR	C-N-CA	-5.64	114.14	122.83
6	F	457	HIS	N-CA-CB	-5.64	100.92	110.50
6	F	416	SER	N-CA-C	5.64	117.87	111.11
2	B	112	TYR	N-CA-C	5.62	122.77	110.80
6	F	294	VAL	CA-C-N	-5.60	113.99	119.76
6	F	294	VAL	C-N-CA	-5.60	113.99	119.76
17	X	40	ASN	N-CA-C	-5.60	104.86	110.97
18	Z	64	ASP	N-CA-C	5.59	119.82	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	191	LEU	N-CA-C	-5.59	105.27	111.36
6	F	304	ALA	CB-CA-C	-5.58	110.12	116.54
5	E	183	PRO	N-CA-C	-5.57	102.19	111.26
22	r	94	ALA	N-CA-C	-5.57	101.61	109.96
6	F	118	ASP	N-CA-C	-5.54	102.08	110.28
2	B	201	LEU	N-CA-C	-5.54	105.14	111.07
7	G	530	TYR	N-CA-C	-5.52	102.11	110.28
4	D	200	PHE	CA-CB-CG	5.51	119.31	113.80
7	G	615	LEU	N-CA-C	-5.51	106.32	113.16
19	a	25	TYR	N-CA-C	-5.51	107.80	114.75
8	H	141	SER	N-CA-CB	5.51	117.99	110.01
7	G	313	LEU	N-CA-C	5.50	118.51	109.72
7	G	127	ASP	CA-C-O	5.48	128.95	121.89
2	B	98	ALA	CB-CA-C	-5.47	108.67	115.89
7	G	150	ARG	N-CA-CB	-5.46	102.77	111.62
7	G	363	SER	N-CA-C	-5.46	100.28	109.07
4	D	132	ALA	N-CA-C	-5.46	106.62	113.72
10	P	86	CYS	N-CA-C	-5.46	103.18	110.55
14	T	135	ALA	N-CA-CB	5.44	118.12	110.12
7	G	420	LYS	N-CA-CB	-5.43	101.92	110.06
4	D	231	GLY	N-CA-C	-5.40	103.14	110.43
18	Z	50	MET	N-CA-C	-5.40	105.39	111.28
7	G	682	ASP	CA-C-N	-5.40	114.20	119.76
7	G	682	ASP	C-N-CA	-5.40	114.20	119.76
7	G	404	GLY	N-CA-C	5.38	121.34	113.48
5	E	48	PRO	N-CA-C	5.38	120.83	113.84
10	P	374	THR	N-CA-C	5.37	117.48	108.73
11	Q	163	ASN	CB-CA-C	-5.37	99.26	109.95
7	G	510	TRP	N-CA-C	-5.36	101.92	109.96
17	X	27	ALA	N-CA-C	-5.36	105.10	111.69
14	T	92	LYS	N-CA-C	-5.35	106.34	112.92
4	D	141	TYR	N-CA-CB	-5.35	102.26	110.44
8	H	284	GLN	N-CA-C	-5.35	105.53	111.36
18	Z	55	GLN	N-CA-C	-5.35	105.45	111.28
4	D	201	PHE	N-CA-C	-5.33	105.55	111.36
4	D	391	VAL	CA-C-N	-5.33	115.83	119.66
4	D	391	VAL	C-N-CA	-5.33	115.83	119.66
6	F	199	ARG	N-CA-C	5.33	117.42	109.59
10	P	339	GLY	N-CA-C	5.32	122.66	115.00
9	I	54	THR	N-CA-C	-5.30	104.91	111.33
8	H	46	LEU	N-CA-C	-5.30	106.58	113.16
4	D	391	VAL	N-CA-C	5.30	113.95	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	252	PRO	CA-N-CD	5.29	119.41	112.00
8	H	310	PHE	N-CA-C	5.29	119.35	113.01
8	H	94	PRO	N-CA-C	5.28	118.61	111.22
11	Q	164	PHE	N-CA-C	-5.28	106.81	113.20
7	G	362	ASP	CA-CB-CG	5.28	117.88	112.60
9	I	160	GLU	N-CA-CB	-5.27	100.75	109.72
17	X	33	GLY	N-CA-C	-5.26	107.79	114.16
7	G	356	ASP	N-CA-C	-5.25	105.55	111.28
7	G	277	MET	N-CA-CB	-5.25	101.62	109.71
5	E	74	GLN	N-CA-C	-5.25	107.53	114.04
11	Q	72	ILE	N-CA-C	-5.24	108.39	113.53
10	P	260	GLY	N-CA-C	-5.24	108.39	115.36
4	D	363	VAL	N-CA-C	5.24	116.31	111.81
6	F	300	ILE	N-CA-CB	5.24	119.31	110.56
22	r	25	GLN	N-CA-C	5.24	118.93	112.54
3	C	164	TRP	N-CA-C	5.22	117.06	111.36
15	V	84	ALA	N-CA-C	5.22	116.66	111.07
8	H	199	ASP	CB-CA-C	-5.21	102.69	111.24
5	E	48	PRO	CB-CA-C	-5.21	104.45	111.85
7	G	600	GLU	CB-CA-C	-5.21	102.98	111.06
22	r	110	GLN	CA-C-N	-5.21	113.56	118.97
22	r	110	GLN	C-N-CA	-5.21	113.56	118.97
13	S	85	ASP	N-CA-C	5.21	117.86	111.82
7	G	435	PRO	CB-CA-C	-5.20	105.89	111.56
10	P	316	LYS	N-CA-C	-5.20	104.87	111.11
22	r	107	SER	N-CA-C	-5.20	102.16	109.96
7	G	63	PHE	CA-C-O	-5.19	115.03	121.06
8	H	101	GLY	N-CA-C	5.19	118.52	112.50
10	P	194	VAL	N-CA-CB	5.19	118.36	110.58
8	H	146	MET	N-CA-C	-5.18	105.53	111.07
20	b	82	LYS	N-CA-C	-5.16	103.72	110.53
7	G	172	ILE	N-CA-C	-5.16	98.61	109.34
7	G	458	GLY	N-CA-C	-5.16	108.21	115.32
7	G	713	ALA	N-CA-C	-5.16	105.55	111.07
7	G	556	THR	N-CA-C	-5.15	101.58	109.41
2	B	98	ALA	N-CA-C	5.15	117.67	109.02
8	H	196	ALA	CA-C-N	-5.14	113.46	119.32
8	H	196	ALA	C-N-CA	-5.14	113.46	119.32
7	G	569	GLN	CB-CA-C	-5.14	104.24	112.05
10	P	198	ALA	N-CA-C	-5.13	100.16	108.52
3	C	156	VAL	N-CA-C	-5.13	104.09	111.17
5	E	181	ASN	N-CA-C	-5.13	99.43	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	387	LEU	N-CA-C	-5.13	98.34	107.98
1	A	2	ASN	CA-C-N	-5.12	113.01	120.29
1	A	2	ASN	C-N-CA	-5.12	113.01	120.29
3	C	109	SER	N-CA-C	5.12	118.16	109.76
16	W	91	MET	N-CA-C	-5.11	105.89	111.82
6	F	60	GLY	N-CA-C	-5.11	106.00	114.48
9	I	95	PRO	N-CA-C	5.11	121.21	113.81
5	E	166	LYS	N-CA-C	-5.09	104.61	111.54
23	s	38	HIS	N-CA-C	5.08	118.58	112.38
8	H	277	TYR	N-CA-C	5.08	117.87	110.10
3	C	221	GLU	N-CA-C	-5.08	102.36	108.25
7	G	393	GLY	N-CA-C	-5.08	107.74	115.66
17	X	112	LEU	N-CA-CB	5.08	117.43	110.07
7	G	280	ASP	N-CA-CB	-5.06	102.68	110.12
10	P	376	ASN	CB-CA-C	-5.06	102.25	110.85
9	I	160	GLU	CB-CA-C	5.05	119.23	110.84
4	D	224	ALA	N-CA-C	5.05	117.17	111.11
10	P	170	LEU	N-CA-C	5.04	117.03	110.43
8	H	254	LEU	N-CA-CB	5.04	118.09	110.28
16	W	112	GLU	N-CA-C	5.03	116.84	111.36
18	Z	130	LYS	N-CA-C	-5.02	105.69	111.07
14	T	140	CYS	N-CA-C	5.01	116.66	109.04
17	X	140	ASN	CA-C-N	-5.01	114.62	119.78
17	X	140	ASN	C-N-CA	-5.01	114.62	119.78
4	D	224	ALA	CA-C-O	-5.01	115.54	120.90
8	H	90	PRO	CA-C-O	-5.01	117.52	121.38
14	T	140	CYS	CB-CA-C	-5.01	104.14	109.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	762	0	823	70	0
2	B	1247	0	1258	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1641	0	1596	136	0
4	D	3095	0	3066	312	0
5	E	1635	0	1626	174	0
6	F	3288	0	3243	341	0
7	G	5287	0	5323	545	0
8	H	2525	0	2613	325	0
9	I	1398	0	1359	146	0
10	P	2730	0	2747	222	0
11	Q	957	0	949	81	0
12	R	305	0	296	37	0
13	S	667	0	683	70	0
14	T	604	0	596	91	0
15	V	915	0	954	86	0
16	W	970	0	991	89	0
17	X	1164	0	1154	103	0
18	Z	1152	0	1148	107	0
19	a	540	0	550	43	0
20	b	620	0	617	93	0
21	q	44	0	35	6	0
22	r	413	0	429	39	0
23	s	226	0	214	14	0
24	B	8	0	0	5	0
24	F	8	0	0	10	0
24	G	16	0	0	5	0
24	I	16	0	0	16	0
25	B	35	0	44	3	0
26	E	4	0	0	4	0
26	G	4	0	0	4	0
27	F	31	0	19	3	0
28	P	48	0	26	4	0
29	R	1	0	0	0	0
30	W	32	0	0	7	0
31	b	46	0	69	27	0
All	All	32434	0	32428	2800	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (2800) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:142:VAL:HG21	4:D:185:MET:SD	1.68	1.34
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.27
4:D:142:VAL:CG2	4:D:185:MET:SD	2.23	1.25
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	1.42	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	1.19
15:V:44:TYR:CE1	15:V:48:THR:HG21	1.77	1.17
6:F:382:CYS:SG	24:F:502:SF4:FE3	1.38	1.12
9:I:123:CYS:SG	24:I:301:SF4:FE1	1.40	1.12
6:F:379:CYS:SG	24:F:502:SF4:FE4	1.43	1.09
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.09
17:X:53:PRO:HD2	18:Z:116:TRP:CD1	1.88	1.08
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.08
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.27	1.08
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.08
17:X:4:ILE:HG22	17:X:5:VAL:H	0.96	1.08
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.08
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.07
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
12:R:88:HIS:HB2	12:R:89:PRO:HD2	1.08	1.07
12:R:88:HIS:CB	12:R:89:PRO:HD2	1.84	1.07
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.07
11:Q:160:TYR:CZ	11:Q:164:PHE:HZ	1.72	1.07
9:I:152:CYS:SG	24:I:301:SF4:FE2	1.46	1.06
20:b:20:VAL:HA	31:b:201:3PE:H282	1.27	1.06
13:S:23:LEU:HD12	13:S:23:LEU:O	1.54	1.06
14:T:138:LEU:HD12	14:T:138:LEU:O	1.55	1.06
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.31	1.05
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.05
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.05
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.37	1.05
15:V:44:TYR:CE1	15:V:48:THR:CG2	2.39	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
2:B:82:ILE:HG23	8:H:57:MET:SD	1.97	1.04
5:E:179:CYS:SG	26:E:301:FES:FE2	1.48	1.04
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.33	1.04
7:G:401:LEU:HD11	7:G:466:LEU:HD21	1.40	1.04
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.03
6:F:266:GLY:CA	6:F:271:SER:HA	1.86	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:142:TYR:CD1	8:H:289:LEU:HD12	1.94	1.03
20:b:20:VAL:HG13	31:b:201:3PE:H2A1	1.06	1.03
3:C:102:HIS:HE1	15:V:48:THR:HG22	1.22	1.02
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.22	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.75	1.02
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.02
16:W:32:LYS:HG2	30:W:201:EHZ:C19	1.90	1.02
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.96	1.01
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.86	1.00
11:Q:160:TYR:CZ	11:Q:164:PHE:CZ	2.49	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
9:I:155:CYS:SG	24:I:301:SF4:FE4	1.52	1.00
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.00
2:B:105:MET:HE2	4:D:200:PHE:HE2	1.24	0.99
4:D:89:PRO:HG2	8:H:204:GLU:OE2	1.62	0.99
6:F:266:GLY:HA3	6:F:271:SER:CA	1.90	0.99
15:V:44:TYR:CZ	15:V:48:THR:HG21	1.97	0.99
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	0.99
5:E:179:CYS:HG	26:E:301:FES:FE2	0.70	0.99
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.99
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.99
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	0.99
2:B:82:ILE:HG12	8:H:57:MET:CE	1.93	0.98
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	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
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	0.98
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.98
16:W:55:LEU:HB3	16:W:107:MET:CE	1.94	0.98
18:Z:58:ARG:NH2	20:b:49:THR:HG21	1.78	0.98
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.97
17:X:4:ILE:HG22	17:X:5:VAL:N	1.77	0.97
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.47	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
6:F:379:CYS:HG	24:F:502:SF4:FE4	0.74	0.97
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	1.78	0.96
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.96
7:G:92:CYS:SG	26:G:803:FES:S1	2.62	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:Q:160:TYR:CE2	11:Q:164:PHE:CE2	2.53	0.96
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.46	0.96
10:P:376:ASN:OD1	10:P:377:TYR:N	1.98	0.95
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.95
4:D:142:VAL:HG22	4:D:185:MET:SD	2.03	0.95
2:B:100:CYS:SG	24:B:301:SF4:FE4	1.59	0.95
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.95
13:S:16:LEU:HD11	13:S:51:LEU:HD11	1.46	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.95
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.95
6:F:382:CYS:HG	24:F:502:SF4:FE3	0.66	0.95
5:E:240:PRO:HA	6:F:60:GLY:HA3	1.44	0.95
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.95
20:b:20:VAL:HG13	31:b:201:3PE:C2A	1.96	0.95
4:D:90:ALA:HB2	8:H:205:SER:HA	1.46	0.94
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.94
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.48	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.94
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.94
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.44	0.94
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.32	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
9:I:152:CYS:HG	24:I:301:SF4:FE2	0.69	0.94
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
9:I:113:CYS:SG	24:I:302:SF4:FE3	1.59	0.94
10:P:333:PRO:HB2	10:P:337:ASP:HB2	1.47	0.93
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.93
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.93
11:Q:160:TYR:CE2	11:Q:164:PHE:HE2	1.86	0.93
10:P:262:THR:H	10:P:332:LEU:HD12	1.34	0.93
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.93
10:P:93:HIS:CD2	10:P:94:LEU:CD1	2.52	0.93
18:Z:86:ILE:HG23	18:Z:128:ARG:HE	1.33	0.92
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.92
22:r:9:GLN:HA	22:r:12:ARG:HD3	1.50	0.92
17:X:4:ILE:CG2	17:X:5:VAL:H	1.82	0.92
12:R:88:HIS:HB2	12:R:89:PRO:CD	1.97	0.92
15:V:75:GLY:HA2	22:r:103:ARG:HD2	1.51	0.91
16:W:55:LEU:HB3	16:W:107:MET:HE1	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:20:VAL:HA	31:b:201:3PE:C28	2.01	0.91
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.86	0.90
7:G:176:CYS:HG	24:G:802:SF4:FE4	0.62	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.90
10:P:93:HIS:NE2	10:P:94:LEU:CD1	2.35	0.90
6:F:425:CYS:HG	24:F:502:SF4:FE1	0.62	0.90
7:G:226:CYS:HG	24:G:802:SF4:FE1	0.71	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
20:b:20:VAL:CG1	31:b:201:3PE:H2A1	2.01	0.89
6:F:110:PRO:HB3	6:F:152:ARG:CZ	2.03	0.89
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.89
8:H:93:HIS:CD2	19:a:27:HIS:HD1	1.91	0.89
6:F:266:GLY:HA3	6:F:271:SER:HA	0.94	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
17:X:18:VAL:HG21	18:Z:74:LEU:HD11	1.54	0.89
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.89
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.88	0.88
7:G:32:ILE:HG23	7:G:98:LYS:HD2	1.54	0.88
4:D:99:LEU:CD2	4:D:109:CYS:SG	2.62	0.88
10:P:96:LEU:HD12	10:P:97:MET:N	1.88	0.88
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.56	0.88
2:B:81:LEU:HG	8:H:53:MET:HE1	1.54	0.88
13:S:16:LEU:HD22	13:S:19:ILE:HD11	1.53	0.88
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.09	0.88
7:G:97:MET:HB2	7:G:100:TRP:CD1	2.09	0.87
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.87
10:P:192:ARG:HH22	10:P:198:ALA:HB3	1.36	0.87
20:b:60:ASP:OD1	20:b:61:GLY:N	2.07	0.87
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.87
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.86
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.86
14:T:79:ILE:HB	14:T:145:VAL:HG13	1.55	0.86
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.56	0.86
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.86
13:S:16:LEU:HD12	13:S:16:LEU:O	1.76	0.86
4:D:99:LEU:HD23	4:D:109:CYS:HA	1.57	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
7:G:78:CYS:SG	26:G:803:FES:FE2	1.68	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:162:CYS:SG	24:I:302:SF4:FE4	1.68	0.86
16:W:55:LEU:HD22	16:W:107:MET:HE2	1.58	0.86
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.85
6:F:44:ASN:HD21	6:F:51:TRP:HA	1.41	0.85
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.59	0.85
10:P:206:ILE:H	28:P:401:NDP:H71N	1.24	0.85
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.95	0.85
15:V:56:LEU:HD12	15:V:57:ASP:N	1.92	0.85
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.84
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.84
17:X:29:ALA:HB2	18:Z:71:LEU:HD11	1.58	0.84
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.84
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.84
7:G:126:LEU:CD1	12:R:89:PRO:HB2	2.07	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
4:D:266:ARG:HB2	9:I:65:GLU:OE2	1.77	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
2:B:105:MET:CE	4:D:200:PHE:HE2	1.90	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	1.40	0.84
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.84
7:G:78:CYS:HG	26:G:803:FES:FE2	0.53	0.83
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.83
17:X:37:ASP:OD2	20:b:70:PRO:HD3	1.77	0.83
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.83
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.61	0.83
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.83
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.79	0.83
8:H:93:HIS:CE1	19:a:24:ALA:HA	2.13	0.83
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.92	0.83
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.83
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.82
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.82
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.60	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.82
3:C:217:ARG:NH1	16:W:112:GLU:HB2	1.95	0.82
2:B:89:SER:O	8:H:54:LYS:HD3	1.79	0.82
6:F:117:ALA:HB1	6:F:131:MET:SD	2.19	0.82
20:b:20:VAL:CA	31:b:201:3PE:H282	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.45	0.82
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.82
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.62	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
7:G:401:LEU:CD1	7:G:466:LEU:HD21	2.09	0.81
8:H:246:LEU:HD12	8:H:246:LEU:O	1.80	0.81
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.81
16:W:55:LEU:CD2	16:W:107:MET:HE2	2.10	0.81
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.96	0.81
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
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
6:F:342:LEU:HB3	6:F:347:THR:HG23	1.63	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
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
2:B:89:SER:O	8:H:54:LYS:CD	2.29	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.80
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.80
8:H:181:MET:CE	8:H:304:HIS:ND1	2.45	0.80
8:H:251:LEU:O	8:H:251:LEU:CD1	2.28	0.80
9:I:123:CYS:HG	24:I:301:SF4:FE1	0.51	0.80
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.80
2:B:105:MET:HE2	4:D:200:PHE:CE2	2.14	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
7:G:73:GLY:HA2	26:G:803:FES:S1	2.21	0.80
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.46	0.80
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.63	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
14:T:87:LEU:HD21	14:T:104:PHE:HZ	1.47	0.79
14:T:93:ILE:HG21	14:T:110:LEU:HD22	1.63	0.79
6:F:174:ARG:HA	23:s:52:LEU:HD21	1.64	0.79
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
8:H:142:TYR:OH	8:H:288:LEU:HD22	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:162:CYS:HG	24:I:302:SF4:FE4	0.51	0.79
16:W:42:TRP:CZ2	16:W:93:LEU:HB2	2.16	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.79
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.79
3:C:102:HIS:CE1	15:V:48:THR:HG22	2.14	0.79
4:D:89:PRO:CG	8:H:204:GLU:OE2	2.31	0.79
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.79
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79
4:D:89:PRO:HG2	8:H:204:GLU:CD	2.07	0.79
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.79
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.65	0.79
8:H:17:MET:SD	8:H:229:THR:OG1	2.41	0.79
9:I:68:ARG:HH22	18:Z:26:PRO:HD2	1.44	0.79
4:D:280:ALA:CB	15:V:11:LEU:HG	2.13	0.79
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.78
9:I:113:CYS:HG	24:I:302:SF4:FE3	0.49	0.78
14:T:113:LEU:HD22	16:W:71:MET:HE2	1.63	0.78
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.23	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	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	1.64	0.78
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.65	0.78
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.63	0.78
14:T:87:LEU:HD22	14:T:104:PHE:CE1	2.19	0.78
17:X:124:GLN:O	20:b:70:PRO:HB2	1.84	0.78
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.18	0.78
20:b:66:VAL:HG13	20:b:72:ASP:HB2	1.65	0.78
7:G:117:MET:HE3	7:G:143:SER:N	1.98	0.78
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.78
17:X:133:THR:HG23	20:b:58:ARG:HH12	1.47	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.78
4:D:128:THR:H	4:D:131:GLN:HE21	1.32	0.77
5:E:178:ALA:HA	6:F:125:CYS:SG	2.24	0.77
14:T:83:VAL:CG2	14:T:126:PHE:HZ	1.97	0.77
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
2:B:96:GLY:HA2	2:B:101:ALA:HB2	1.67	0.77
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.66	0.77
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.65	0.77
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.77
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.65	0.77
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.77
3:C:217:ARG:HH12	16:W:112:GLU:HB2	1.50	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.77
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.50	0.77
4:D:99:LEU:HD22	4:D:109:CYS:SG	2.24	0.77
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.77
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.00	0.76
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.76
17:X:20:VAL:HG22	17:X:24:VAL:HG21	1.66	0.76
4:D:348:LEU:O	18:Z:11:PRO:HB3	1.85	0.76
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.76
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.67	0.76
2:B:89:SER:O	8:H:54:LYS:HE2	1.85	0.76
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.13	0.76
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
13:S:51:LEU:HD13	13:S:95:LEU:HD21	1.68	0.76
4:D:271:ARG:HD2	8:H:279:ARG:O	1.86	0.76
5:E:189:ASP:CG	6:F:163:TYR:HB3	2.11	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
14:T:93:ILE:HG23	14:T:110:LEU:HD13	1.66	0.76
10:P:143:ASP:HA	10:P:147:ASN:HB2	1.67	0.76
16:W:42:TRP:CD2	16:W:93:LEU:HD12	2.21	0.76
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.68	0.76
12:R:89:PRO:HG3	12:R:106:TYR:CE1	2.20	0.76
13:S:19:ILE:HG13	13:S:95:LEU:HD11	1.69	0.75
3:C:102:HIS:HE1	15:V:48:THR:CG2	1.99	0.75
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.75
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.75
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.75
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.75
25:B:302:PC1:H371	8:H:49:PHE:HB3	1.66	0.75
7:G:651:PRO:HG3	13:S:57:GLU:H	1.51	0.75
11:Q:160:TYR:CD2	11:Q:164:PHE:HE2	2.04	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.75
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.67	0.75
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.75
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.75
11:Q:167:ASN:O	11:Q:168:LYS:CD	2.35	0.75
8:H:91:MET:O	8:H:92:PRO:C	2.26	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.75
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.75
16:W:28:LEU:HG	16:W:32:LYS:HE3	1.69	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.74
18:Z:58:ARG:NH2	20:b:49:THR:CG2	2.50	0.74
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.74
8:H:93:HIS:HE1	19:a:24:ALA:HA	1.51	0.74
16:W:55:LEU:HB3	16:W:107:MET:HE2	1.66	0.74
4:D:99:LEU:HD21	4:D:109:CYS:SG	2.26	0.74
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.88	0.74
10:P:336:GLU:HG3	10:P:342:PRO:HD3	1.67	0.74
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.74
14:T:117:GLU:HA	14:T:120:MET:HE3	1.68	0.74
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.74
6:F:425:CYS:SG	24:F:502:SF4:FE1	1.78	0.74
7:G:674:LEU:HD11	13:S:46:LYS:HE2	1.69	0.74
14:T:88:LYS:HG3	14:T:98:LEU:HD22	1.70	0.74
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.03	0.74
14:T:94:ASP:HB3	14:T:98:LEU:HB2	1.68	0.74
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.68	0.73
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.73
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.70	0.73
14:T:103:HIS:CG	14:T:106:LYS:HD2	2.23	0.73
20:b:31:ILE:HA	20:b:34:MET:HE2	1.69	0.73
6:F:210:THR:HB	6:F:224:ARG:HB2	1.70	0.73
7:G:176:CYS:SG	24:G:802:SF4:FE4	1.78	0.73
18:Z:93:GLU:O	18:Z:97:ILE:HG13	1.88	0.73
2:B:112:TYR:OH	9:I:91:GLY:CA	2.29	0.73
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.69	0.73
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73
5:E:240:PRO:HG3	6:F:57:LEU:O	1.88	0.73
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.73
4:D:260:GLU:HG3	18:Z:25:LEU:HD22	1.69	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:160:ILE:HD12	4:D:286:TYR:HE1	1.54	0.73
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.73
4:D:90:ALA:HB2	8:H:205:SER:CA	2.18	0.73
16:W:32:LYS:HE2	30:W:201:EHZ:C19	2.18	0.73
18:Z:65:LEU:O	18:Z:69:ILE:HG12	1.89	0.73
5:E:39:VAL:HG11	7:G:163:LYS:NZ	2.04	0.73
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
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.70	0.72
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.72
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
11:Q:167:ASN:O	11:Q:168:LYS:HD2	1.88	0.72
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
10:P:169:HIS:H	10:P:184:LYS:HE3	1.54	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
12:R:89:PRO:CG	12:R:106:TYR:CZ	2.72	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
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.72
14:T:120:MET:HG2	16:W:44:ARG:HH11	1.54	0.72
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.72
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.71	0.71
9:I:200:GLU:OE2	21:q:93:MET:SD	2.48	0.71
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	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
5:E:240:PRO:CA	6:F:60:GLY:HA3	2.20	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
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.70	0.71
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.71
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.71
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.71
10:P:192:ARG:NH1	10:P:192:ARG:HA	2.05	0.71
16:W:101:LYS:NZ	16:W:109:PHE:CE2	2.58	0.71
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.71	0.71
8:H:113:VAL:HG22	8:H:136:VAL:HG23	1.72	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
8:H:42:PRO:HD2	8:H:45:ILE:HG12	1.72	0.71
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.26	0.71
17:X:53:PRO:HD2	18:Z:116:TRP:HD1	1.49	0.71
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
10:P:170:LEU:O	10:P:171:ASN:OD1	2.09	0.71
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.56	0.71
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.24	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
18:Z:144:THR:HA	19:a:45:TRP:HZ3	1.55	0.71
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.74	0.70
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.70
4:D:141:TYR:O	4:D:144:MET:SD	2.49	0.70
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.73	0.70
2:B:116:ARG:O	8:H:39:ILE:HG22	1.91	0.70
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.55	0.70
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.73	0.70
9:I:155:CYS:HG	24:I:301:SF4:FE4	1.08	0.70
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.55	0.70
17:X:133:THR:HG23	20:b:58:ARG:NH1	2.05	0.70
2:B:82:ILE:HA	8:H:57:MET:HE1	1.74	0.70
2:B:89:SER:O	8:H:54:LYS:CE	2.40	0.70
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.70
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.27	0.70
5:E:237:PRO:HG3	6:F:49:HIS:CD2	2.27	0.70
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.70
6:F:314:LEU:HB3	6:F:329:LYS:HD3	1.72	0.70
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.70
16:W:32:LYS:CG	30:W:201:EHZ:C19	2.69	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.70
2:B:95:PHE:HE2	2:B:131:MET:SD	2.15	0.70
2:B:136:THR:HG21	2:B:177:VAL:HG22	1.73	0.70
7:G:127:ASP:HA	12:R:106:TYR:OH	1.90	0.70
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.69
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.22	0.69
15:V:56:LEU:HD12	15:V:56:LEU:C	2.16	0.69
18:Z:86:ILE:HG23	18:Z:128:ARG:NE	2.06	0.69
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.21	0.69
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.73	0.69
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.69
14:T:100:VAL:HB	14:T:142:GLN:HB2	1.74	0.69
16:W:101:LYS:HZ1	16:W:109:PHE:HE2	1.36	0.69
20:b:19:LEU:HD21	31:b:201:3PE:H342	1.73	0.69
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
10:P:171:ASN:OD1	10:P:171:ASN:O	2.11	0.69
4:D:253:LEU:HB2	22:r:23:LYS:CD	2.23	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:5:ASN:HD21	19:a:23:THR:HG23	1.58	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
9:I:53:ALA:HB1	20:b:14:ALA:HB2	1.73	0.69
14:T:87:LEU:HD22	14:T:104:PHE:HE1	1.58	0.69
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.75	0.69
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.28	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
7:G:179:CYS:HG	24:G:802:SF4:FE3	1.07	0.68
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.68
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.23	0.68
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.68
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
14:T:138:LEU:HD13	14:T:144:ILE:CG1	2.23	0.68
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.68
17:X:50:GLU:HG3	17:X:56:CYS:SG	2.33	0.68
20:b:20:VAL:HG22	31:b:201:3PE:H282	1.74	0.68
4:D:89:PRO:HG2	8:H:204:GLU:CG	2.23	0.68
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.75	0.68
8:H:33:LEU:HD23	22:r:25:GLN:HG2	1.76	0.68
8:H:85:LEU:HD21	8:H:108:THR:HB	1.74	0.68
11:Q:160:TYR:CE2	11:Q:164:PHE:CZ	2.80	0.68
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.75	0.68
3:C:107:PHE:CD1	3:C:133:SER:HB2	2.28	0.68
4:D:92:HIS:HB3	4:D:458:PHE:HE2	1.59	0.68
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.29	0.68
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.68
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.57	0.68
10:P:191:VAL:HA	10:P:194:VAL:HG22	1.73	0.68
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.68
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.08	0.68
22:r:20:LEU:C	22:r:20:LEU:HD12	2.18	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.68
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.76	0.68
10:P:192:ARG:NH2	10:P:200:ILE:HD11	2.09	0.68
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.76	0.68
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	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:175:LEU:O	8:H:179:TRP:HB3	1.93	0.68
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.58	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.28	0.67
1:A:105:GLU:CG	1:A:111:LEU:HG	2.25	0.67
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.75	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	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
7:G:126:LEU:HD11	12:R:89:PRO:HB2	1.75	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
2:B:94:THR:HB	2:B:104:MET:HE1	1.74	0.67
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.67
17:X:53:PRO:HG2	18:Z:116:TRP:NE1	2.09	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
10:P:197:GLU:HB3	10:P:259:VAL:CG2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.76	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
13:S:16:LEU:HB3	13:S:69:TYR:HD1	1.58	0.67
5:E:147:ILE:HG23	5:E:151:LEU:HD13	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
17:X:90:ASP:OD2	19:a:62:VAL:HG11	1.94	0.67
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.05	0.67
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.77	0.67
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.67
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.09	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
9:I:93:LEU:O	21:q:93:MET:HG2	1.94	0.66
10:P:94:LEU:HA	10:P:97:MET:HE3	1.77	0.66
10:P:192:ARG:HH22	10:P:198:ALA:CB	2.07	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
8:H:42:PRO:HD2	8:H:45:ILE:CG1	2.25	0.66
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.74	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
3:C:141:ARG:NH1	4:D:410:TYR:HE1	1.93	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.28	0.66
14:T:87:LEU:CD2	14:T:104:PHE:CZ	2.78	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.77	0.66
8:H:207:LEU:O	8:H:208:VAL:C	2.38	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
9:I:35:THR:CG2	22:r:107:SER:HA	2.26	0.66
9:I:80:GLU:OE2	22:r:26:LEU:CD1	2.44	0.66
6:F:41:ILE:HG23	6:F:253:THR:HG21	1.76	0.66
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.66
13:S:24:CYS:SG	13:S:61:VAL:O	2.53	0.66
14:T:83:VAL:HG22	14:T:126:PHE:CZ	2.31	0.66
16:W:42:TRP:CH2	16:W:93:LEU:HA	2.31	0.66
16:W:121:PHE:HA	16:W:124:LYS:HE2	1.75	0.66
3:C:98:PHE:CA	15:V:90:LEU:HD11	2.19	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:169:HIS:H	10:P:184:LYS:CE	2.09	0.66
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.66
15:V:44:TYR:CE1	15:V:48:THR:HG23	2.30	0.66
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.66
3:C:79:CYS:O	3:C:80:LEU:HB2	1.96	0.66
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.66
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.77	0.65
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.65
10:P:199:ILE:HD11	10:P:258:ALA:O	1.96	0.65
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.78	0.65
8:H:130:PHE:HD2	8:H:207:LEU:HD21	1.61	0.65
8:H:283:ASP:OD1	8:H:284:GLN:N	2.29	0.65
10:P:59:PHE:HB2	10:P:130:ILE:HD11	1.78	0.65
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.77	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
13:S:16:LEU:HB3	13:S:69:TYR:CD1	2.32	0.65
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.26	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
4:D:260:GLU:CG	18:Z:25:LEU:HD22	2.27	0.65
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.65
13:S:58:CYS:HB2	13:S:61:VAL:HG12	1.78	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.65
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.65
20:b:20:VAL:HG22	31:b:201:3PE:H261	1.78	0.65
10:P:236:VAL:CG1	10:P:270:ARG:HH21	2.10	0.65
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.78	0.65
2:B:93:MET:HE1	2:B:131:MET:HE2	1.78	0.65
4:D:145:MET:HA	4:D:148:GLU:HG3	1.77	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.65
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.65
9:I:79:ARG:HG2	22:r:12:ARG:HH21	1.62	0.65
2:B:173:TYR:O	3:C:203:LEU:HD22	1.97	0.65
10:P:191:VAL:HG13	10:P:192:ARG:NH2	2.12	0.65
10:P:226:VAL:HG21	10:P:281:PHE:CZ	2.32	0.65
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.65
5:E:79:LEU:HB2	5:E:80:PRO:HD3	1.78	0.65
14:T:118:ILE:HG23	14:T:122:MET:HE3	1.78	0.65
17:X:123:GLY:HA2	18:Z:66:GLU:OE2	1.97	0.65
2:B:146:ARG:O	2:B:147:LYS:C	2.39	0.64
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:88:VAL:HG12	10:P:92:MET:HE2	1.80	0.64
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.64
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.32	0.64
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.64
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.77	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.79	0.64
17:X:53:PRO:HG2	18:Z:116:TRP:HE1	1.62	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.64
8:H:33:LEU:CD2	22:r:25:GLN:HG2	2.26	0.64
11:Q:163:ASN:OD1	11:Q:164:PHE:N	2.31	0.64
14:T:138:LEU:O	14:T:138:LEU:CD1	2.40	0.64
17:X:132:LYS:HB3	20:b:59:ASP:HB3	1.79	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.64
17:X:65:GLY:HA2	17:X:68:LEU:HD12	1.78	0.64
18:Z:86:ILE:HA	18:Z:128:ARG:HH21	1.62	0.64
6:F:228:PRO:HG3	11:Q:160:TYR:CD2	2.33	0.64
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.64
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.64
14:T:83:VAL:HG23	14:T:126:PHE:HZ	1.62	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.63	0.64
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.33	0.64
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.64
14:T:87:LEU:HD21	14:T:104:PHE:CZ	2.32	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.78	0.64
17:X:37:ASP:OD1	17:X:38:LYS:N	2.31	0.64
2:B:136:THR:CG2	2:B:177:VAL:HG22	2.29	0.63
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.63
2:B:92:PRO:HD2	2:B:120:VAL:HG12	1.80	0.63
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:333:PRO:HB2	10:P:337:ASP:CB	2.25	0.63
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.63
18:Z:65:LEU:O	18:Z:68:ARG:HG2	1.98	0.63
2:B:94:THR:CB	2:B:104:MET:HE1	2.27	0.63
4:D:260:GLU:HG3	18:Z:25:LEU:CD2	2.28	0.63
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.63
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.63
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.63
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.63
16:W:101:LYS:NZ	16:W:109:PHE:HE2	1.94	0.63
2:B:70:ARG:HG3	2:B:73:TYR:H	1.63	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
10:P:93:HIS:NE2	10:P:94:LEU:HD11	2.14	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
13:S:15:GLY:HA3	13:S:17:ARG:HH22	1.63	0.63
13:S:16:LEU:HA	13:S:69:TYR:HA	1.79	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
4:D:142:VAL:HG13	4:D:207:ARG:NH1	2.14	0.63
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.63
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.79	0.63
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	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
16:W:55:LEU:CB	16:W:107:MET:CE	2.75	0.63
22:r:109:ASP:O	22:r:110:GLN:HG2	1.99	0.63
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.63
5:E: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:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.63
8:H:312:ALA:HB2	20:b:38:TYR:HB3	1.80	0.63
12:R:89:PRO:HG2	12:R:106:TYR:CZ	2.33	0.63
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.63
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.80	0.63
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.99	0.63
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.29	0.63
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.28	0.63
1:A:52:SER:HB2	1:A:54:LYS:HG2	1.79	0.62
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.62
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.62
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.62
8:H:195:ARG:O	8:H:199:ASP:HB2	1.99	0.62
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.34	0.62
16:W:83:ASP:O	16:W:86:VAL:HG22	1.99	0.62
17:X:122:LEU:HD23	20:b:82:LYS:HG2	1.80	0.62
20:b:16:GLU:HG3	31:b:201:3PE:C2	2.29	0.62
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.62
16:W:55:LEU:CB	16:W:107:MET:HE2	2.30	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.79	0.62
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.35	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.81	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
14:T:103:HIS:ND1	14:T:140:CYS:SG	2.73	0.62
2:B:194:CYS:O	24:B:301:SF4:S2	2.58	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.29	0.62
8:H:306:SER:HG	8:H:310:PHE:HE2	1.30	0.62
10:P:240:VAL:HB	10:P:266:THR:O	2.00	0.62
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.34	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
7:G:399:VAL:CG2	7:G:462:PHE:HZ	2.12	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.62
18:Z:58:ARG:CZ	20:b:49:THR:HG21	2.30	0.62
22:r:20:LEU:HD12	22:r:21:GLN:N	2.14	0.62
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.81	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.65	0.62
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.26	0.62
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.48	0.62
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.82	0.62
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.35	0.62
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.82	0.62
7:G:651:PRO:CD	13:S:56:ARG:HB3	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.35	0.62
8:H:307:LEU:HD11	18:Z:47:TYR:CD1	2.34	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.61
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.61
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.61
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.61
20:b:11:ASN:O	20:b:15:LYS:N	2.31	0.61
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.61	0.61
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.36	0.61
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.61
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.82	0.61
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.61
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.61
7:G:617:ARG:NH1	16:W:129:HIS:HA	2.14	0.61
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.61
17:X:69:ASN:O	17:X:73:GLN:HG3	2.00	0.61
18:Z:28:ARG:HG3	18:Z:28:ARG:O	1.99	0.61
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.82	0.61
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.63	0.61
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.82	0.61
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.30	0.61
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.61
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.61
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.81	0.61
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.61
4:D:202:TRP:CZ3	4:D:261:MET:HG3	2.36	0.61
5:E:71:GLU:HB2	23:s:59:GLN:HB3	1.82	0.61
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.61
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
14:T:138:LEU:HD12	14:T:138:LEU:C	2.24	0.61
7:G:82:ILE:CG2	7:G:100:TRP:HB3	2.30	0.61
10:P:191:VAL:HG13	10:P:192:ARG:HH21	1.66	0.61
12:R:98:GLU:CD	12:R:98:GLU:H	2.06	0.61
2:B:93:MET:HB2	2:B:128:ALA:CB	2.30	0.61
8:H:311:THR:O	18:Z:51:MET:HG3	2.01	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.61
5:E:182:ALA:O	5:E:183:PRO:C	2.42	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
6:F:416:SER:O	6:F:419:ILE:HG22	2.01	0.61
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	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
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.61
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.61
10:P:169:HIS:HD2	10:P:181:LEU:HD11	1.65	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.61
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.61
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.02	0.60
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.60
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.60
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.62	0.60
10:P:192:ARG:HA	10:P:192:ARG:CZ	2.31	0.60
14:T:103:HIS:HB2	14:T:106:LYS:HB2	1.83	0.60
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.32	0.60
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.66	0.60
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.60
12:R:89:PRO:CG	12:R:106:TYR:CE1	2.83	0.60
16:W:42:TRP:CZ2	16:W:93:LEU:CB	2.83	0.60
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.60
10:P:263:PHE:HD2	10:P:333:PRO:O	1.84	0.60
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.60
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.60
10:P:299:SER:HB3	10:P:316:LYS:HE3	1.83	0.60
16:W:97:ILE:HG23	16:W:98:LYS:HG3	1.82	0.60
18:Z:143:TYR:O	18:Z:144:THR:C	2.45	0.60
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.60
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
13:S:19:ILE:HG13	13:S:95:LEU:CD1	2.31	0.60
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.60
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:315:THR:O	10:P:316:LYS:C	2.45	0.60
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.67	0.60
2:B:144:ALA:O	2:B:145:LEU:C	2.45	0.60
9:I:80:GLU:OE2	22:r:26:LEU:HD11	2.01	0.60
16:W:53:MET:SD	16:W:106:VAL:HG21	2.42	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
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.60
10:P:136:THR:CG2	10:P:139:PHE:HB2	2.31	0.60
13:S:16:LEU:CB	13:S:69:TYR:HD1	2.15	0.60
14:T:83:VAL:HG22	14:T:126:PHE:HZ	1.66	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
4:D:202:TRP:CH2	4:D:261:MET:HG3	2.37	0.60
7:G:304:GLU:OE2	10:P:41:ILE:HG12	2.01	0.60
10:P:262:THR:N	10:P:332:LEU:HD12	2.12	0.60
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.60
3:C:70:LYS:O	15:V:103:LEU:HD12	2.02	0.59
17:X:37:ASP:HA	17:X:40:ASN:HB2	1.84	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	1.85	0.59
17:X:20:VAL:HG12	17:X:25:LEU:HD21	1.84	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.65	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	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
20:b:8:PHE:HA	20:b:11:ASN:ND2	2.18	0.59
1:A:68:GLU:CD	1:A:98:LEU:HG	2.28	0.59
4:D:95:LEU:HG	4:D:97:LEU:HG	1.85	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
10:P:318:LYS:O	10:P:322:ILE:HG13	2.02	0.59
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.32	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
17:X:33:GLY:CA	18:Z:70:ALA:HB1	2.32	0.59
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.59
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
6:F:119:GLU:HB3	6:F:124:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
8:H:142:TYR:CG	8:H:289:LEU:HD12	2.37	0.59
18:Z:105:LYS:O	18:Z:106:VAL:C	2.46	0.59
23:s:57:LEU:HG	23:s:58:PRO:HD2	1.83	0.59
10:P:96:LEU:HD12	10:P:96:LEU:C	2.28	0.59
20:b:6:SER:O	20:b:9:LEU:HB3	2.03	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.59
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.30	0.59
10:P:178:SER:O	10:P:182:ARG:HG2	2.02	0.59
13:S:23:LEU:O	13:S:23:LEU:CD1	2.41	0.59
18:Z:122:GLY:O	18:Z:126:GLY:N	2.34	0.59
4:D:375:MET:HE1	7:G:126:LEU:CA	2.33	0.59
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.59
14:T:123:GLU:OE1	16:W:44:ARG:NH1	2.36	0.59
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.85	0.59
17:X:78:CYS:SG	17:X:110:CYS:HB3	2.42	0.59
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.59
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.59
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.33	0.58
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.84	0.58
2:B:105:MET:CE	4:D:200:PHE:CE2	2.80	0.58
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.36	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
4:D:388:GLY:HA3	4:D:417:SER:OG	2.02	0.58
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.84	0.58
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.67	0.58
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.85	0.58
10:P:357:ARG:HD3	10:P:361:TRP:O	2.03	0.58
13:S:47:ALA:O	13:S:49:PRO:HD3	2.03	0.58
4:D:99:LEU:CD2	4:D:109:CYS:HA	2.32	0.58
6:F:44:ASN:HB3	6:F:134:ASP:HB2	1.84	0.58
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.85	0.58
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.83	0.58
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.85	0.58
17:X:29:ALA:HB2	18:Z:71:LEU:CD1	2.31	0.58
6:F:382:CYS:SG	24:F:502:SF4:S1	3.02	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
10:P:57:THR:HG23	10:P:123:SER:CB	2.33	0.58
17:X:134:ASP:O	17:X:135:ARG:C	2.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.68	0.58
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.58
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.58
4:D:99:LEU:HB3	4:D:101:LEU:CD1	2.34	0.58
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.85	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.17	0.58
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.58
23:s:35:LEU:HB3	23:s:38:HIS:HB2	1.85	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
8:H:201:THR:OG1	8:H:202:GLU:N	2.36	0.58
10:P:57:THR:HG23	10:P:123:SER:HB2	1.86	0.58
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.04	0.58
2:B:115:ASP:HA	2:B:119:VAL:O	2.04	0.58
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.04	0.58
4:D:128:THR:H	4:D:131:GLN:NE2	2.00	0.58
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.58
5:E:164:PRO:C	5:E:166:LYS:H	2.11	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.58
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.84	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
10:P:245:VAL:O	10:P:249:ILE:HG13	2.04	0.58
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.58
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.86	0.57
17:X:133:THR:O	20:b:58:ARG:NH1	2.36	0.57
2:B:164:CYS:SG	24:B:301:SF4:S4	3.02	0.57
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.39	0.57
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.57
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.86	0.57
8:H:85:LEU:CD2	8:H:108:THR:HB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.86	0.57
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.39	0.57
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.57
10:P:220:TYR:HA	10:P:223:PHE:HD2	1.67	0.57
14:T:90:TYR:CE2	14:T:92:LYS:HB3	2.39	0.57
3:C:186:ILE:HG13	3:C:187:LEU:N	2.17	0.57
6:F:48:ARG:NH1	6:F:48:ARG:HA	2.19	0.57
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
8:H:142:TYR:CE1	8:H:289:LEU:HD12	2.39	0.57
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.57
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.57
20:b:69:HIS:CD2	20:b:70:PRO:HD2	2.37	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:126:LEU:HD12	12:R:89:PRO:HB2	1.83	0.57
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.57
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.85	0.57
14:T:90:TYR:CE2	14:T:92:LYS:CB	2.87	0.57
2:B:99:CYS:C	2:B:101:ALA:N	2.59	0.57
2:B:110:PRO:HB3	8:H:33:LEU:O	2.03	0.57
4:D:89:PRO:HG2	8:H:204:GLU:HG2	1.85	0.57
4:D:166:ARG:CZ	18:Z:8:GLN:HG2	2.34	0.57
10:P:192:ARG:CZ	10:P:198:ALA:HB3	2.34	0.57
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.57
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.29	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
8:H:307:LEU:HD11	18:Z:47:TYR:CG	2.39	0.57
13:S:16:LEU:HD11	13:S:51:LEU:CD1	2.29	0.57
2:B:153:PRO:HB2	2:B:155:PRO:HD2	1.85	0.57
2:B:170:TYR:OH	4:D:131:GLN:O	2.22	0.57
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.57
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.57
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.86	0.57
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.57
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.57
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:212:GLU:O	4:D:216:ARG:HG2	2.04	0.57
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.57
6:F:39:ASP:HA	6:F:261:TRP:HZ2	1.70	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.05	0.57
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.57
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.84	0.57
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.88	0.57
10:P:320:GLU:O	10:P:324:ILE:HG12	2.05	0.57
1:A:60:ILE:O	1:A:61:THR:C	2.46	0.56
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.05	0.56
2:B:100:CYS:HG	24:B:301:SF4:FE4	1.22	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
4:D:266:ARG:NH1	9:I:60:ILE:HA	2.20	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
8:H:69:SER:C	8:H:71:PHE:H	2.12	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
17:X:52:ASP:OD2	17:X:55:ARG:HG3	2.04	0.56
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.58	0.56
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.56
10:P:188:GLU:O	10:P:192:ARG:HG2	2.05	0.56
16:W:42:TRP:CZ2	30:W:201:EHZ:O1	2.58	0.56
1:A:105:GLU:HG2	1:A:111:LEU:HG	1.87	0.56
3:C:80:LEU:HD21	4:D:157:LYS:O	2.05	0.56
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.30	0.56
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.86	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:213:ILE:HG23	6:F:235:VAL:HA	1.86	0.56
6:F:293:SER:N	6:F:338:ASP:OD1	2.38	0.56
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.05	0.56
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.70	0.56
14:T:134:ASP:OD1	14:T:134:ASP:O	2.23	0.56
16:W:104:THR:O	16:W:108:ARG:HG3	2.05	0.56
2:B:194:CYS:HB2	9:I:153:ILE:O	2.05	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:92:GLU:O	18:Z:96:ILE:HG13	2.05	0.56
2:B:93:MET:HE1	2:B:95:PHE:CE2	2.40	0.56
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.56
14:T:90:TYR:HE2	14:T:92:LYS:CB	2.19	0.56
14:T:130:ILE:HD11	14:T:148:ILE:HD11	1.86	0.56
18:Z:7:LYS:HB2	18:Z:7:LYS:NZ	2.20	0.56
1:A:113:TRP:HH2	8:H:287:HIS:CD2	2.23	0.56
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.36	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.41	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.21	0.56
11:Q:167:ASN:O	11:Q:168:LYS:HG2	2.04	0.56
14:T:83:VAL:CG2	14:T:126:PHE:CZ	2.83	0.56
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.87	0.56
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	2.03	0.56
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.87	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.56
7:G:401:LEU:HD11	7:G:462:PHE:HE2	1.71	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.40	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
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.40	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
8:H:202:GLU:O	8:H:203:GLY:C	2.49	0.56
2:B:69:SER:O	2:B:70:ARG:C	2.48	0.56
2:B:154:GLU:O	10:P:89:TYR:OH	2.21	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.56
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.56
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.56
11:Q:165:SER:HB3	11:Q:168:LYS:O	2.06	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:95:PHE:CE2	2:B:131:MET:SD	2.99	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:382:ARG:HD2	13:S:56:ARG:CD	2.36	0.56
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.46	0.56
10:P:64:PHE:HE1	10:P:209:ARG:O	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.56
16:W:42:TRP:CZ2	16:W:93:LEU:CA	2.89	0.56
4:D:266:ARG:NH2	9:I:59:ARG:O	2.38	0.55
6:F:293:SER:HB3	6:F:338:ASP:OD2	2.06	0.55
10:P:140:ASP:OD1	10:P:142:GLU:HB2	2.05	0.55
17:X:54:ARG:HD3	18:Z:116:TRP:CE3	2.40	0.55
2:B:97:LEU:HD21	2:B:141:MET:HG2	1.88	0.55
3:C:184:ARG:HA	16:W:91:MET:SD	2.46	0.55
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.55
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.55
17:X:33:GLY:HA3	18:Z:70:ALA:HB1	1.88	0.55
20:b:16:GLU:HG3	31:b:201:3PE:O21	2.06	0.55
1:A:102:LEU:CD1	1:A:111:LEU:HD11	2.37	0.55
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.71	0.55
4:D:279:THR:HA	15:V:12:VAL:HG13	1.87	0.55
5:E:139:CYS:CB	5:E:144:SER:HB3	2.35	0.55
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.07	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.88	0.55
20:b:8:PHE:CG	20:b:9:LEU:N	2.74	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55
11:Q:160:TYR:OH	11:Q:164:PHE:HZ	1.89	0.55
17:X:39:THR:HG23	17:X:40:ASN:N	2.20	0.55
17:X:124:GLN:C	17:X:125:LEU:HD12	2.32	0.55
2:B:174:SER:HA	3:C:203:LEU:CD2	2.37	0.55
7:G:35:PHE:O	7:G:101:ASN:HA	2.07	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.55
10:P:145:PHE:O	10:P:149:PRO:HG2	2.05	0.55
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.06	0.55
4:D:84:PHE:HB2	4:D:97:LEU:HB2	1.87	0.55
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
5:E:162:THR:HG22	5:E:166:LYS:HA	1.89	0.55
6:F:170:GLN:HB3	23:s:48:LEU:HD22	1.89	0.55
6:F:382:CYS:SG	24:F:502:SF4:S4	3.05	0.55
9:I:75:SER:O	22:r:12:ARG:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.71	0.55
10:P:376:ASN:OD1	10:P:376:ASN:C	2.50	0.55
16:W:25:SER:HB3	16:W:30:GLU:HB3	1.88	0.55
18:Z:56:GLU:HA	18:Z:59:ARG:HH11	1.72	0.55
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	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:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
10:P:236:VAL:HG13	10:P:270:ARG:HH21	1.71	0.55
16:W:23:ILE:HG13	16:W:80:ARG:HG2	1.87	0.55
22:r:7:VAL:O	22:r:11:LEU:HG	2.06	0.55
22:r:9:GLN:O	22:r:12:ARG:HB2	2.06	0.55
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.89	0.55
6:F:67:GLU:O	6:F:71:LYS:HG2	2.06	0.55
6:F:339:PHE:O	6:F:343:VAL:HG23	2.07	0.55
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.49	0.55
16:W:35:VAL:HG21	30:W:201:EHZ:N2	2.22	0.55
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.87	0.55
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.55
5:E:39:VAL:HG21	7:G:163:LYS:HZ2	1.72	0.55
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.46	0.55
8:H:69:SER:C	8:H:71:PHE:N	2.61	0.55
10:P:71:ASN:HA	10:P:97:MET:SD	2.47	0.55
10:P:98:GLY:HA3	10:P:103:LEU:HG	1.87	0.55
16:W:53:MET:HB2	16:W:55:LEU:HG	1.89	0.55
20:b:20:VAL:CG2	31:b:201:3PE:H282	2.37	0.55
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.88	0.54
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.32	0.54
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.54
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.07	0.54
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.54
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.37	0.54
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.54
14:T:87:LEU:HD22	14:T:104:PHE:CZ	2.41	0.54
14:T:128:PHE:CE2	14:T:130:ILE:HG13	2.42	0.54
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.37	0.54
6:F:119:GLU:HG3	6:F:127:ASP:OD2	2.07	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
7:G:617:ARG:HH12	16:W:128:GLY:C	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:I:123:CYS:SG	24:I:301:SF4:S3	3.06	0.54
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.54
19:a:58:ASN:HB2	19:a:61:TYR:CD2	2.43	0.54
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.23	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
6:F:299:LEU:CD1	6:F:300:ILE:HG23	2.37	0.54
6:F:300:ILE:HD11	6:F:311:TRP:HD1	1.72	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
8:H:130:PHE:CD2	8:H:207:LEU:HD11	2.41	0.54
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.54
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.54
19:a:31:ASN:HD21	19:a:36:LYS:HB2	1.71	0.54
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.14	0.54
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.43	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.73	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
10:P:300:TRP:O	10:P:304:LEU:HG	2.08	0.54
15:V:50:GLN:HE22	22:r:94:ALA:H	1.56	0.54
17:X:64:ASN:O	17:X:68:LEU:HG	2.07	0.54
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.54
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.42	0.54
5:E:164:PRO:C	5:E:166:LYS:N	2.64	0.54
5:E:199:ASP:O	5:E:203:ILE:HG13	2.08	0.54
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.54
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.90	0.54
4:D:92:HIS:HB3	4:D:458:PHE:CE2	2.41	0.54
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.90	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.73	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
9:I:50:MET:HE1	20:b:13:TRP:CD1	2.42	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
10:P:316:LYS:O	10:P:320:GLU:HG2	2.08	0.54
2:B:126:ARG:HG3	8:H:213:VAL:O	2.08	0.54
3:C:217:ARG:HH12	16:W:112:GLU:CB	2.19	0.54
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:232:VAL:HG23	4:D:356:ILE:HD13	1.88	0.54
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.33	0.54
5:E:180:VAL:CG1	5:E:224:CYS:SG	2.96	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
8:H:133:LEU:O	8:H:136:VAL:HG12	2.08	0.54
10:P:172:ALA:H	10:P:202:ARG:NH2	2.06	0.54
10:P:207:PHE:CE1	10:P:214:LEU:HD22	2.43	0.54
14:T:97:LYS:HG3	14:T:97:LYS:O	2.08	0.54
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.54
5:E:39:VAL:HG11	7:G:163:LYS:HZ3	1.73	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.54
9:I:80:GLU:CB	22:r:26:LEU:HD11	2.38	0.54
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.54
20:b:8:PHE:O	20:b:9:LEU:C	2.50	0.54
3:C:80:LEU:HD22	4:D:157:LYS:HB3	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
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.90	0.54
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.23	0.54
1:A:110:GLY:O	1:A:111:LEU:HB2	2.08	0.54
3:C:100:ARG:HH12	15:V:86:LYS:NZ	2.06	0.54
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.89	0.54
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.54
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.90	0.54
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.54
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.91	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.90	0.54
8:H:51:ASP:OD1	8:H:51:ASP:C	2.51	0.54
1:A:73:LEU:O	8:H:160:TYR:OH	2.25	0.53
4:D:253:LEU:HD11	22:r:18:GLN:HG3	1.90	0.53
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	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:163:LYS:HB3	7:G:211:GLU:OE1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.53
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.37	0.53
10:P:58:VAL:O	10:P:83:PRO:HD2	2.09	0.53
10:P:142:GLU:HA	10:P:146:VAL:HG12	1.90	0.53
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.53
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.53
5:E:139:CYS:C	5:E:144:SER:HB3	2.33	0.53
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.53
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.53
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.53
10:P:85:ARG:HE	28:P:401:NDP:C2A	2.21	0.53
14:T:103:HIS:HD1	14:T:140:CYS:HG	1.50	0.53
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.53
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.73	0.53
6:F:80:MET:HE2	6:F:95:THR:HG21	1.89	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:617:ARG:NH1	16:W:128:GLY:C	2.66	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
9:I:62:MET:SD	18:Z:35:MET:HG2	2.47	0.53
13:S:16:LEU:HD13	13:S:19:ILE:CD1	2.38	0.53
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.90	0.53
4:D:145:MET:O	4:D:148:GLU:N	2.41	0.53
4:D:368:ARG:HA	4:D:371:MET:HG2	1.89	0.53
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.53
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
8:H:264:LEU:HD21	19:a:12:MET:HE2	1.90	0.53
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.53
12:R:98:GLU:HA	12:R:113:GLN:CD	2.33	0.53
13:S:30:SER:O	13:S:31:GLN:C	2.49	0.53
2:B:126:ARG:NH1	8:H:61:MET:SD	2.76	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
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.53
6:F:329:LYS:HA	6:F:332:CYS:SG	2.49	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.38	0.53
9:I:80:GLU:OE2	22:r:26:LEU:HD13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:370:LYS:HG3	10:P:370:LYS:O	2.08	0.53
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	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
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.53
4:D:92:HIS:O	4:D:93:GLY:C	2.50	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	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:85:LEU:HD13	6:F:262:PHE:CE2	2.44	0.53
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.73	0.53
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.53
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.53
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.44	0.53
1:A:112:GLU:C	1:A:113:TRP:CG	2.86	0.53
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.53
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.53
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
10:P:353:LEU:HA	10:P:356:HIS:HD2	1.74	0.53
14:T:118:ILE:HG23	14:T:122:MET:CE	2.37	0.53
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.69	0.53
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.22	0.53
4:D:210:MET:O	4:D:211:PHE:C	2.51	0.53
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.53
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.91	0.53
6:F:235:VAL:HG22	6:F:236:PHE:HD2	1.68	0.53
6:F:294:VAL:HG12	6:F:337:MET:HB2	1.90	0.53
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.24	0.53
7:G:364:ASP:C	7:G:364:ASP:OD1	2.52	0.53
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.53
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.53
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.91	0.53
9:I:68:ARG:HH22	18:Z:26:PRO:CD	2.18	0.53
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	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
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.27	0.53
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.53
9:I:80:GLU:HB3	22:r:26:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:265:PHE:HD1	10:P:334:GLY:HA3	1.74	0.53
14:T:100:VAL:O	14:T:141:PRO:HD2	2.09	0.53
20:b:59:ASP:HA	20:b:63:MET:HE2	1.89	0.53
2:B:136:THR:HG21	4:D:118:ARG:HG2	1.90	0.52
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.64	0.52
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.52
6:F:411:SER:HA	6:F:414:GLU:CD	2.34	0.52
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.92	0.52
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.52
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.52
19:a:42:GLN:O	19:a:43:TYR:C	2.50	0.52
1:A:21:ALA:HB2	8:H:218:GLY:HA3	1.90	0.52
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.52
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.52
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.45	0.52
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.85	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.52
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.52
10:P:305:PHE:CG	10:P:314:THR:HG22	2.45	0.52
5:E:39:VAL:HG21	7:G:163:LYS:NZ	2.25	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
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.52
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.52
10:P:283:MET:HE2	10:P:366:ILE:HG22	1.92	0.52
10:P:336:GLU:CG	10:P:342:PRO:HD3	2.38	0.52
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.52
20:b:66:VAL:HG11	20:b:70:PRO:HA	1.92	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.09	0.52
3:C:104:ASN:O	22:r:97:PRO:HD3	2.10	0.52
3:C:170:TRP:CZ2	16:W:91:MET:HE1	2.44	0.52
4:D:235:ASP:OD2	18:Z:8:GLN:NE2	2.40	0.52
5:E:65:ILE:HA	5:E:68:ASN:ND2	2.24	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:372:PHE:H	7:G:532:PRO:HB2	1.74	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.52
14:T:130:ILE:CG2	14:T:131:PRO:HD2	2.40	0.52
17:X:80:GLU:HB3	17:X:81:PRO:HD3	1.91	0.52
1:A:3:LEU:HA	8:H:96:ILE:CD1	2.40	0.52
2:B:92:PRO:HD3	2:B:119:VAL:HG13	1.91	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
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
17:X:77:HIS:HD2	17:X:115:LEU:HD21	1.74	0.52
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.42	0.52
2:B:81:LEU:HD22	25:B:302:PC1:H262	1.92	0.52
4:D:137:ASP:OD1	4:D:148:GLU:HG2	2.09	0.52
6:F:126:LYS:HG3	6:F:275:LEU:CB	2.39	0.52
7:G:617:ARG:HH12	16:W:129:HIS:N	2.07	0.52
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.35	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
2:B:127:GLN:H	2:B:127:GLN:CD	2.18	0.52
4:D:101:LEU:HG	4:D:106:VAL:HA	1.91	0.52
4:D:381:HIS:HE1	9:I:161:ALA:O	1.93	0.52
5:E:177:GLY:O	26:E:301:FES:S1	2.68	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.10	0.52
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.75	0.52
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.52
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.52
1:A:19:LEU:O	1:A:20:VAL:C	2.50	0.52
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.52
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.52
7:G:541:PRO:HB2	7:G:561:PRO:HD3	1.91	0.52
10:P:236:VAL:HG11	10:P:270:ARG:HH21	1.75	0.52
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.52
14:T:79:ILE:CG2	14:T:145:VAL:HG13	2.40	0.52
16:W:94:GLN:HA	16:W:97:ILE:HG22	1.92	0.52
17:X:25:LEU:HB3	18:Z:71:LEU:HD22	1.91	0.52
19:a:2:TRP:O	19:a:3:PHE:C	2.53	0.52
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.52
1:A:102:LEU:HD11	1:A:111:LEU:HD11	1.91	0.52
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.45	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
9:I:155:CYS:SG	24:I:301:SF4:S2	3.08	0.52
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	2.98	0.52
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.43	0.52
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.90	0.52
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
10:P:192:ARG:NH1	10:P:198:ALA:HB3	2.25	0.52
20:b:48:ALA:O	20:b:49:THR:C	2.53	0.52
1:A:113:TRP:CH2	8:H:287:HIS:HD2	2.27	0.51
5:E:196:THR:O	5:E:197:PRO:C	2.54	0.51
6:F:331:VAL:O	6:F:335:VAL:HG23	2.10	0.51
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
7:G:399:VAL:HG21	7:G:462:PHE:CZ	2.44	0.51
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	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
18:Z:61:LEU:O	18:Z:64:ASP:OD1	2.29	0.51
3:C:73:GLN:NE2	15:V:112:TRP:HE1	2.07	0.51
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.92	0.51
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.51
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.51
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.91	0.51
4:D:218:SER:CB	4:D:224:ALA:HB1	2.41	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.93	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.11	0.51
6:F:259:GLY:O	6:F:263:ALA:N	2.40	0.51
7:G: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:142:TYR:CA	8:H:289:LEU:CD1	2.74	0.51
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.51
1:A:105:GLU:HG3	1:A:111:LEU:HG	1.91	0.51
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.25	0.51
5:E:188:ASN:O	5:E:189:ASP:HB3	2.10	0.51
6:F:225:LEU:HB2	11:Q:160:TYR:CZ	2.45	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
10:P:157:LYS:O	10:P:158:GLU:C	2.53	0.51
13:S:16:LEU:O	13:S:16:LEU:CD1	2.52	0.51
17:X:18:VAL:CG2	18:Z:74:LEU:HD11	2.33	0.51
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.93	0.51
1:A:106:TRP:CD1	1:A:111:LEU:HD12	2.45	0.51
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.92	0.51
6:F:40:ARG:HB3	6:F:289:GLU:CD	2.36	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.51
8:H:222:LEU:O	8:H:223:PHE:C	2.50	0.51
9:I:68:ARG:HH21	18:Z:26:PRO:HD2	1.68	0.51
9:I:71:GLY:O	22:r:15:ALA:HB1	2.11	0.51
4:D:259:GLU:C	4:D:261:MET:H	2.18	0.51
4:D:299:GLN:HB3	22:r:104:TRP:CE3	2.45	0.51
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.75	0.51
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.51
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.51
14:T:140:CYS:HB2	14:T:143:GLU:CG	2.40	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
16:W:65:LYS:HE3	16:W:69:MET:HE2	1.92	0.51
17:X:25:LEU:O	17:X:29:ALA:N	2.44	0.51
20:b:11:ASN:OD1	20:b:12:ALA:N	2.44	0.51
20:b:20:VAL:HG22	31:b:201:3PE:C27	2.41	0.51
20:b:22:SER:OG	31:b:201:3PE:H3A1	2.11	0.51
3:C:241:PHE:H	7:G:146:PHE:HE1	1.58	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
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.40	0.51
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.41	0.51
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.51
15:V:44:TYR:CD1	15:V:48:THR:HG23	2.46	0.51
2:B:81:LEU:CG	8:H:53:MET:HE1	2.34	0.51
2:B:125:PRO:HB3	2:B:148:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:217:GLU:CD	11:Q:166:TRP:HE1	2.18	0.51
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.41	0.51
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.51
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
7:G:639:LEU:HD23	7:G:639:LEU:C	2.36	0.51
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.51
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.51
10:P:305:PHE:HB2	10:P:314:THR:HG22	1.92	0.51
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.11	0.51
10:P:374:THR:HG23	10:P:374:THR:O	2.11	0.51
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.51
17:X:133:THR:CG2	20:b:58:ARG:NH1	2.74	0.51
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.50
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.45	0.50
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.50
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.50
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.45	0.50
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.91	0.50
10:P:108:TRP:CZ2	28:P:401:NDP:H2A	2.46	0.50
11:Q:167:ASN:C	11:Q:168:LYS:HG2	2.36	0.50
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.50
7:G:651:PRO:HD2	13:S:56:ARG:HD2	1.94	0.50
10:P:234:LYS:HG2	10:P:234:LYS:O	2.10	0.50
14:T:87:LEU:HD23	14:T:122:MET:CE	2.41	0.50
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.46	0.50
6:F:392:MET:HE2	6:F:416:SER:HA	1.93	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:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
17:X:38:LYS:O	17:X:42:GLU:HG3	2.11	0.50
17:X:137:LEU:HG	17:X:138:PRO:HD2	1.92	0.50
20:b:20:VAL:HG22	31:b:201:3PE:C28	2.39	0.50
20:b:23:PHE:HE1	31:b:201:3PE:H3A2	1.76	0.50
2:B:99:CYS:C	2:B:101:ALA:H	2.19	0.50
2:B:171:TYR:HE1	4:D:120:THR:HG22	1.76	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
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:212:ARG:O	10:P:213:PHE:C	2.55	0.50
14:T:105:MET:HB2	14:T:139:MET:SD	2.51	0.50
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.50
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.93	0.50
5:E:70:PRO:HB3	23:s:60:PRO:HG3	1.92	0.50
6:F:49:HIS:O	6:F:50:ASP:C	2.54	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
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.94	0.50
8:H:230:ASN:O	8:H:231:ILE:C	2.53	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
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.50
14:T:130:ILE:HG23	14:T:131:PRO:CD	2.40	0.50
19:a:3:PHE:O	19:a:6:LEU:HG	2.11	0.50
4:D:97:LEU:HD23	4:D:111:PRO:HA	1.94	0.50
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.50
8:H:172:MET:SD	18:Z:46:GLY:HA2	2.52	0.50
16:W:97:ILE:C	16:W:99:VAL:H	2.18	0.50
2:B:84:TRP:HA	2:B:87:ARG:HG2	1.93	0.50
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.50
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	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:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.50
10:P:150:ARG:O	10:P:151:ALA:C	2.55	0.50
14:T:140:CYS:O	14:T:144:ILE:HG13	2.12	0.50
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.50
10:P:207:PHE:HE1	10:P:214:LEU:HD22	1.76	0.50
17:X:29:ALA:CB	18:Z:71:LEU:HD11	2.38	0.50
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.50
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.50
2:B:99:CYS:O	2:B:101:ALA:N	2.44	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.50
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.50
4:D:460:GLU:O	4:D:463:ARG:HG2	2.11	0.50
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.50

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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	0.50
7:G:272:ARG:HH11	7:G:274:LEU:HD23	1.77	0.50
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.50
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.50
8:H:17:MET:CE	8:H:225:MET:HB3	2.41	0.50
10:P:70:VAL:HG12	10:P:97:MET:SD	2.52	0.50
13:S:42:VAL:O	13:S:46:LYS:HG3	2.12	0.50
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.50
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.50
18:Z:129:THR:HG22	18:Z:131:GLU:H	1.77	0.50
19:a:4:GLU:O	19:a:7:PRO:HD2	2.11	0.50
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.42	0.49
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.49
4:D:289:SER:N	4:D:293:LEU:HG	2.26	0.49
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.49
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.94	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
10:P:135:GLU:CG	10:P:140:ASP:HA	2.41	0.49
14:T:138:LEU:HD13	14:T:144:ILE:CD1	2.42	0.49
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.49
5:E:55:THR:O	5:E:56:PRO:C	2.54	0.49
6:F:342:LEU:HD12	6:F:349:LEU:CA	2.42	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:192:ARG:CZ	10:P:200:ILE:HD11	2.42	0.49
13:S:24:CYS:N	13:S:58:CYS:SG	2.85	0.49
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.49
2:B:171:TYR:CE1	4:D:120:THR:HG22	2.45	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.95	0.49
4:D:145:MET:O	4:D:146:CYS:C	2.54	0.49
5:E:245:GLN:HB3	6:F:256:ARG:O	2.11	0.49
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.27	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.48	0.49
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.49
20:b:23:PHE:HZ	31:b:201:3PE:H351	1.76	0.49
20:b:23:PHE:CE1	31:b:201:3PE:H3A2	2.47	0.49
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.30	0.49
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.49
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:383:THR:O	6:F:384:PRO:C	2.55	0.49
7:G:126:LEU:HD11	12:R:89:PRO:CB	2.41	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.12	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
10:P:367:GLU:HG2	10:P:368:GLU:N	2.26	0.49
11:Q:160:TYR:CD2	11:Q:164:PHE:CE2	2.91	0.49
16:W:32:LYS:CD	30:W:201:EHZ:C19	2.90	0.49
17:X:49:GLU:HB3	17:X:138:PRO:HG3	1.93	0.49
18:Z:66:GLU:HA	18:Z:69:ILE:HG12	1.93	0.49
18:Z:140:PHE:O	18:Z:141:THR:C	2.56	0.49
20:b:20:VAL:HG22	31:b:201:3PE:C26	2.42	0.49
1:A:54:LYS:O	1:A:58:VAL:HG23	2.11	0.49
3:C:73:GLN:HE21	15:V:112:TRP:HE1	1.60	0.49
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49
4:D:207:ARG:O	4:D:208:GLU:C	2.54	0.49
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.93	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
6:F:427:LEU:HB2	27:F:501:FMN:C7M	2.43	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	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:238:GLN:HB2	10:P:270:ARG:HG2	1.94	0.49
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.49
17:X:73:GLN:OE1	17:X:117:TRP:HZ2	1.96	0.49
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.49
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.26	0.49
3:C:224:GLU:OE2	10:P:45:LYS:HB3	2.13	0.49
4:D:259:GLU:C	4:D:261:MET:N	2.69	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.49
14:T:88:LYS:NZ	14:T:96:GLU:H	2.11	0.49
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.13	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
10:P:64:PHE:CZ	10:P:211:ASP:HB3	2.48	0.49
10:P:235:THR:O	10:P:236:VAL:C	2.56	0.49
10:P:315:THR:H	10:P:318:LYS:HB3	1.76	0.49
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.42	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
8:H:93:HIS:HE1	19:a:24:ALA:CA	2.20	0.49
16:W:42:TRP:CE2	16:W:93:LEU:HD12	2.47	0.49
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.49
9:I:49:ASP:O	9:I:50:MET:C	2.55	0.49
9:I:106:TYR:O	9:I:107:PRO:C	2.55	0.49
9:I:114:ILE:HD13	12:R:106:TYR:CD1	2.48	0.49
13:S:36:PHE:CZ	13:S:44:LEU:HD11	2.36	0.49
15:V:56:LEU:HA	15:V:59:VAL:HB	1.94	0.49
17:X:4:ILE:CG2	17:X:5:VAL:N	2.50	0.49
1:A:18:ILE:O	1:A:21:ALA:HB3	2.13	0.49
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.49
4:D:279:THR:HA	15:V:12:VAL:CG1	2.43	0.49
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.49
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.49
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.49
6:F:379:CYS:SG	24:F:502:SF4:S1	3.11	0.49
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.49
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.49
17:X:115:LEU:HD13	17:X:117:TRP:CZ3	2.48	0.49
2:B:127:GLN:NE2	8:H:215:TYR:O	2.46	0.48
4:D:142:VAL:CG2	4:D:185:MET:CE	2.90	0.48
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.48
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.48
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.48
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.48
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.48
17:X:112:LEU:HD13	17:X:118:VAL:HG22	1.95	0.48
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.95	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.48
10:P:228:LEU:HD11	10:P:288:PHE:HZ	1.78	0.48
17:X:69:ASN:O	17:X:70:PHE:C	2.56	0.48
1:A:109:LYS:HD2	1:A:112:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.48
6:F:126:LYS:HG3	6:F:275:LEU:HB3	1.94	0.48
7:G:34:VAL:HG11	7:G:96:VAL:HG22	1.94	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.48
8:H:66:THR:HA	8:H:124:ASN:OD1	2.13	0.48
8:H:253:GLU:HB3	19:a:21:VAL:HG22	1.94	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
10:P:59:PHE:CB	10:P:130:ILE:HD11	2.42	0.48
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.48
16:W:46:VAL:N	16:W:47:PRO:HD2	2.29	0.48
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.48
1:A:72:LEU:HB3	8:H:151:LEU:HD21	1.95	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.48
8:H:172:MET:HE1	18:Z:46:GLY:HA3	1.95	0.48
10:P:197:GLU:HB3	10:P:259:VAL:HG23	1.93	0.48
14:T:90:TYR:HE2	14:T:92:LYS:HB3	1.78	0.48
17:X:7:LEU:HD13	18:Z:87:LEU:HB3	1.96	0.48
2:B:174:SER:HB2	4:D:123:LEU:HD21	1.95	0.48
3:C:176:PHE:CE1	16:W:87:ILE:HG21	2.48	0.48
3:C:234:LEU:O	4:D:387:GLU:HG3	2.13	0.48
5:E:143:ASP:O	5:E:144:SER:C	2.55	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
9:I:171:PRO:HB3	21:q:93:MET:CE	2.38	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
6:F:343:VAL:O	6:F:344:GLN:C	2.54	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
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.13	0.48
18:Z:85:GLN:O	18:Z:89:GLU:HG3	2.14	0.48
1:A:113:TRP:CH2	8:H:287:HIS:HB2	2.49	0.48
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.49	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
4:D:202:TRP:CH2	9:I:72:MET:HG2	2.48	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48
5:E:221:ARG:HH21	5:E:227:ALA:HB2	1.79	0.48
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:104:PHE:CZ	14:T:118:ILE:HG21	2.48	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.96	0.48
17:X:17:GLU:HB3	17:X:19:LYS:HG3	1.96	0.48
19:a:37:ARG:CB	19:a:48:MET:HE2	2.43	0.48
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.95	0.48
1:A:81:THR:O	20:b:46:ASN:ND2	2.47	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.12	0.48
3:C:100:ARG:HH12	15:V:86:LYS:HZ1	1.62	0.48
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.49	0.48
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.49	0.48
5:E:45:GLU:CD	5:E:45:GLU:H	2.21	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:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
9:I:53:ALA:CB	20:b:14:ALA:HB2	2.42	0.48
10:P:79:GLN:NE2	10:P:102:GLN:O	2.47	0.48
20:b:68:SER:O	20:b:69:HIS:C	2.56	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.48
6:F:270:ASN:ND2	6:F:338:ASP:HB3	2.29	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
11:Q:64:LEU:HD12	16:W:85:LEU:HD21	1.95	0.48
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.48
12:R:89:PRO:HG2	12:R:106:TYR:CE2	2.49	0.48
14:T:119:ILE:HG13	14:T:135:ALA:HB1	1.95	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
2:B:115:ASP:O	2:B:116:ARG:C	2.55	0.48
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.73	0.48
13:S:50:ASN:O	13:S:51:LEU:C	2.57	0.48
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.48
1:A:102:LEU:HG	1:A:106:TRP:HE1	1.79	0.47
3:C:151:PRO:HG2	16:W:23:ILE:HG23	1.96	0.47
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.14	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.47
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.47
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.47
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
9:I:49:ASP:O	9:I:53:ALA:N	2.41	0.47
17:X:80:GLU:O	17:X:81:PRO:C	2.56	0.47
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.47
5:E:142:ARG:O	5:E:143:ASP:HB2	2.13	0.47
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.14	0.47
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	0.47
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.47
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.79	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
10:P:294:PRO:HB3	10:P:296:PHE:HD1	1.79	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
18:Z:62:ILE:HD12	20:b:81:LEU:CD2	2.43	0.47
3:C:209:LEU:HD21	16:W:108:ARG:NH1	2.29	0.47
4:D:142:VAL:HG13	4:D:207:ARG:HH12	1.78	0.47
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.49	0.47
6:F:110:PRO:O	6:F:238:CYS:HB3	2.14	0.47
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.47
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.14	0.47
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.95	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
7:G:688:GLN:HA	7:G:693:ASP:CB	2.44	0.47
10:P:304:LEU:O	10:P:307:LEU:HB3	2.14	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
24:B:301:SF4:S4	4:D:138:ARG:HD3	2.54	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.48	0.47
6:F:299:LEU:HD11	6:F:300:ILE:HG23	1.95	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.48	0.47
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.47
10:P:311:GLU:O	10:P:312:PRO:C	2.57	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.47
2:B:117:PHE:HA	8:H:39:ILE:HG21	1.95	0.47
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.47
4:D:279:THR:HG23	15:V:13:GLY:CA	2.23	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
6:F:425:CYS:SG	24:F:502:SF4:S4	3.13	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
10:P:170:LEU:HG	10:P:171:ASN:N	2.28	0.47
16:W:120:ASP:OD1	16:W:121:PHE:N	2.46	0.47
20:b:23:PHE:HE1	31:b:201:3PE:H371	1.80	0.47
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.45	0.47
5:E:145:ASP:O	5:E:146:SER:C	2.56	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
15:V:116:ILE:O	15:V:116:ILE:CG2	2.61	0.47
2:B:99:CYS:O	2:B:102:VAL:N	2.45	0.47
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.47	0.47
3:C:70:LYS:HB2	15:V:99:PRO:O	2.14	0.47
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.29	0.47
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.47
6:F:281:HIS:HB3	6:F:358:ASP:CG	2.40	0.47
7:G:82:ILE:HG21	7:G:100:TRP:HB3	1.96	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
7:G:541:PRO:HB2	7:G:561:PRO:CG	2.44	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
8:H:93:HIS:NE2	19:a:27:HIS:ND1	2.56	0.47
9:I:209:TYR:CG	12:R:86:LEU:HD21	2.50	0.47
10:P:55:VAL:HG12	10:P:123:SER:HA	1.96	0.47
10:P:76:MET:HE1	10:P:254:LYS:CE	2.45	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
13:S:58:CYS:HB2	13:S:61:VAL:CG1	2.43	0.47
16:W:32:LYS:O	16:W:36:ARG:HG3	2.15	0.47
16:W:46:VAL:O	16:W:50:VAL:HG23	2.14	0.47
17:X:39:THR:CG2	17:X:40:ASN:N	2.77	0.47
17:X:64:ASN:HD21	18:Z:81:ARG:NH1	2.12	0.47
17:X:139:GLU:O	17:X:140:ASN:C	2.57	0.47
19:a:22:SER:O	19:a:23:THR:C	2.57	0.47
20:b:69:HIS:CD2	20:b:71:GLN:H	2.33	0.47
1:A:108:GLN:C	1:A:110:GLY:N	2.72	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.48	0.47
18:Z:87:LEU:HD21	18:Z:119:PRO:HG3	1.97	0.47
23:s:55:PHE:O	23:s:56:ARG:C	2.57	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
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.03	0.47
10:P:287:THR:HG23	10:P:289:ILE:HD11	1.97	0.47
15:V:56:LEU:HD12	15:V:57:ASP:CA	2.44	0.47
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.40	0.47
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.47
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.96	0.47
4:D:299:GLN:OE1	22:r:104:TRP:HB2	2.14	0.47
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.47
6:F:44:ASN:ND2	6:F:133:HIS:O	2.48	0.47
6:F:251:SER:N	6:F:252:PRO:HD2	2.30	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
10:P:207:PHE:CD2	10:P:241:TYR:HD1	2.33	0.47
12:R:88:HIS:HE1	12:R:91:VAL:HG22	1.80	0.47
1:A:87:MET:HE3	1:A:87:MET:HB3	1.84	0.46
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.46
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.46
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.96	0.46
17:X:20:VAL:CG2	17:X:24:VAL:HG21	2.40	0.46
17:X:115:LEU:HD13	17:X:117:TRP:CZ2	2.51	0.46
22:r:109:ASP:O	22:r:110:GLN:OE1	2.32	0.46
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.49	0.46
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.97	0.46
2:B:140:LYS:O	2:B:143:PRO:HD2	2.14	0.46
4:D:264:ASN:O	9:I:65:GLU:OE1	2.32	0.46
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.97	0.46
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.50	0.46
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.98	0.46
7:G:275:PRO:HB3	7:G:286:ILE:HG23	1.96	0.46
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	0.46
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.96	0.46
10:P:209:ARG:O	10:P:210:GLU:HB2	2.15	0.46
16:W:50:VAL:HA	16:W:55:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.44	0.46
19:a:49:GLU:CD	19:a:52:ARG:HH11	2.22	0.46
3:C:134:LEU:H	3:C:134:LEU:HD12	1.80	0.46
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.46
7:G:496:MET:O	7:G:500:ILE:HG13	2.15	0.46
13:S:19:ILE:HD12	13:S:94:VAL:CG1	2.44	0.46
14:T:87:LEU:CD2	14:T:104:PHE:HZ	2.12	0.46
16:W:32:LYS:CE	30:W:201:EHZ:C19	2.90	0.46
17:X:35:GLN:HG3	17:X:70:PHE:HE1	1.80	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.58	0.46
2:B:116:ARG:HA	8:H:37:PRO:HA	1.97	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
6:F:39:ASP:CA	6:F:261:TRP:HZ2	2.28	0.46
6:F:213:ILE:CG2	6:F:224:ARG:HH21	2.27	0.46
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
10:P:235:THR:HG22	10:P:323:HIS:O	2.15	0.46
10:P:276:LEU:O	10:P:280:ILE:HG13	2.15	0.46
15:V:22:GLU:O	15:V:26:ILE:HG12	2.16	0.46
3:C:141:ARG:NH1	4:D:410:TYR:CE1	2.81	0.46
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.24	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
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
9:I:53:ALA:O	9:I:54:THR:C	2.56	0.46
14:T:114:ASP:OD1	16:W:67:ARG:NH1	2.48	0.46
23:s:52:LEU:HB3	23:s:56:ARG:HH11	1.81	0.46
2:B:94:THR:HB	2:B:104:MET:CE	2.45	0.46
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.46
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
5:E:143:ASP:O	5:E:146:SER:N	2.49	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
10:P:245:VAL:HA	10:P:265:PHE:CD2	2.49	0.46
14:T:117:GLU:HG2	16:W:43:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:72:LEU:C	15:V:72:LEU:CD1	2.89	0.46
2:B:93:MET:HB2	2:B:128:ALA:HB2	1.97	0.46
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.46
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.46
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.51	0.46
6:F:51:TRP:HZ2	23:s:36:GLN:HG3	1.80	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.46
10:P:131:GLY:HA3	28:P:401:NDP:O3D	2.15	0.46
15:V:56:LEU:HD13	15:V:60:LYS:HE2	1.98	0.46
18:Z:135:ASN:HD21	19:a:52:ARG:NH1	2.14	0.46
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.81	0.46
6:F:35:LEU:HG	6:F:39:ASP:HB2	1.97	0.46
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.46
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.97	0.46
10:P:157:LYS:O	10:P:160:GLY:N	2.49	0.46
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	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:107:MET:O	2:B:112:TYR:O	2.32	0.46
3:C:75:VAL:HG23	3:C:83:LEU:HD11	1.98	0.46
4:D:198:THR:HA	8:H:32:GLN:HG2	1.98	0.46
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.46
4:D:368:ARG:NH2	9:I:165:ASP:HB2	2.31	0.46
7:G:82:ILE:HG23	7:G:100:TRP:HB3	1.96	0.46
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.46
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.46
10:P:261:LYS:HB2	10:P:263:PHE:CE1	2.51	0.46
14:T:87:LEU:CD2	14:T:122:MET:HE1	2.46	0.46
16:W:99:VAL:HG13	16:W:99:VAL:O	2.15	0.46
18:Z:140:PHE:CE1	19:a:45:TRP:HB2	2.51	0.46
19:a:58:ASN:HB2	19:a:61:TYR:CE2	2.50	0.46
20:b:28:LEU:O	20:b:32:MET:HG2	2.16	0.46
20:b:45:ILE:N	20:b:80:TRP:HH2	2.14	0.46
5:E:134:CYS:SG	5:E:139:CYS:SG	3.06	0.46
6:F:51:TRP:CB	6:F:133:HIS:O	2.64	0.46
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.46
7:G:176:CYS:SG	24:G:802:SF4:S1	3.14	0.46
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.46
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.46
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.46
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.81	0.46
10:P:66:GLY:O	10:P:69:VAL:N	2.48	0.46
14:T:119:ILE:CD1	14:T:138:LEU:HD11	2.43	0.46
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.28	0.46
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.45
6:F:137:LYS:HG2	6:F:249:ALA:HB1	1.98	0.45
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.45
9:I:123:CYS:SG	24:I:301:SF4:S4	3.13	0.45
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.45
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.32	0.45
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.98	0.45
4:D:142:VAL:HG21	4:D:185:MET:CE	2.41	0.45
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.99	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
5:E:163:THR:O	5:E:166:LYS:HD3	2.16	0.45
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.45
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.45
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.45
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
10:P:285:HIS:CE1	10:P:364:SER:HB3	2.51	0.45
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.50	0.45
16:W:97:ILE:C	16:W:99:VAL:N	2.73	0.45
17:X:33:GLY:HA3	18:Z:70:ALA:CB	2.46	0.45
2:B:99:CYS:O	2:B:100:CYS:C	2.57	0.45
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.45
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.45
6:F:227:PRO:HB2	6:F:228:PRO:HD3	1.99	0.45
6:F:398:ARG:HH12	6:F:408:GLU:CD	2.24	0.45
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.45
8:H:140:ILE:HG13	8:H:141:SER:N	2.30	0.45
10:P:259:VAL:H	10:P:261:LYS:HG2	1.81	0.45
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.45
14:T:87:LEU:CD2	14:T:104:PHE:CE1	2.94	0.45
15:V:56:LEU:HD11	15:V:57:ASP:OD1	2.17	0.45
18:Z:86:ILE:CG2	18:Z:128:ARG:HE	2.16	0.45
2:B:136:THR:HG21	2:B:177:VAL:CG2	2.44	0.45
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.45
5:E:59:TYR:O	5:E:62:ILE:HB	2.17	0.45
5:E:184:MET:HG3	5:E:192:TYR:O	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
10:P:220:TYR:HA	10:P:223:PHE:CD2	2.50	0.45
10:P:315:THR:HB	10:P:318:LYS:HB2	1.98	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
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.45
7:G:97:MET:HB2	7:G:100:TRP:NE1	2.30	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.45
7:G:401:LEU:HD11	7:G:462:PHE:CE2	2.51	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.31	0.45
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.45
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.45
10:P:170:LEU:HD12	10:P:171:ASN:H	1.81	0.45
11:Q:160:TYR:CE1	11:Q:164:PHE:HZ	2.25	0.45
3:C:243:ALA:C	7:G:105:ASN:ND2	2.75	0.45
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
5:E:162:THR:CG2	5:E:166:LYS:HA	2.46	0.45
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.45
6:F:224:ARG:HG2	11:Q:164:PHE:CZ	2.52	0.45
6:F:249:ALA:O	6:F:252:PRO:HD2	2.17	0.45
7:G:163:LYS:HE2	12:R:97:LYS:NZ	2.31	0.45
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:382:ARG:HD2	13:S:56:ARG:HD3	1.99	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
10:P:218:ALA:HB2	10:P:280:ILE:CG2	2.47	0.45
13:S:42:VAL:HB	13:S:46:LYS:HE3	1.98	0.45
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.16	0.45
2:B:126:ARG:C	2:B:128:ALA:H	2.24	0.45
3:C:79:CYS:O	3:C:80:LEU:CB	2.60	0.45
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.45
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.74	0.45
5:E:45:GLU:O	5:E:50:THR:HG21	2.15	0.45
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.45
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.45
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.32	0.45
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.45
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.98	0.45
14:T:90:TYR:O	14:T:91:ASP:HB2	2.17	0.45
14:T:117:GLU:HA	14:T:120:MET:CE	2.41	0.45
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.45
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.51	0.45
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.32	0.45
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.45
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.45
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.45	0.45
5:E:81:VAL:O	5:E:82:LEU:C	2.60	0.45
5:E:163:THR:HG23	5:E:168:PHE:O	2.17	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.99	0.45
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.45
10:P:192:ARG:HH12	10:P:198:ALA:HB3	1.80	0.45
10:P:209:ARG:CA	10:P:352:VAL:HG22	2.47	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
14:T:83:VAL:HG21	14:T:145:VAL:HG22	1.99	0.45
14:T:130:ILE:CG2	14:T:131:PRO:CD	2.95	0.45
18:Z:66:GLU:HA	18:Z:69:ILE:CG1	2.46	0.45
1:A:109:LYS:HA	1:A:112:GLU:CD	2.42	0.45
2:B:99:CYS:HB3	4:D:141:TYR:CD2	2.52	0.45
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.98	0.45
3:C:170:TRP:CE2	16:W:91:MET:HE1	2.52	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
4:D:84:PHE:CE2	4:D:91:ALA:HB2	2.51	0.45
5:E:52:PHE:O	5:E:99:LYS:HG3	2.17	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
6:F:299:LEU:CD1	6:F:300:ILE:N	2.67	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.45
7:G:341:ILE:HD12	7:G:555:ILE:CG1	2.47	0.45
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.45
9:I:93:LEU:O	21:q:93:MET:CG	2.65	0.45
14:T:133:ILE:HG23	14:T:134:ASP:N	2.32	0.45
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.45
2:B:124:SER:HB3	2:B:125:PRO:HD2	1.99	0.45
4:D:100:GLU:C	4:D:101:LEU:HD12	2.41	0.45
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.82	0.45
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.45
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.52	0.45
6:F:382:CYS:HA	7:G:74:ASN:O	2.17	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.45
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.45
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.45
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.45
14:T:82:ARG:NH2	14:T:126:PHE:HD1	2.15	0.45
16:W:71:MET:C	16:W:73:ASN:N	2.70	0.45
3:C:73:GLN:NE2	15:V:107:PRO:HB3	2.31	0.44
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.44
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.44
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.44
8:H:295:PRO:HB3	31:b:201:3PE:H382	1.98	0.44
9:I:50:MET:O	9:I:51:LYS:C	2.60	0.44
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.44
18:Z:98:MET:HB2	18:Z:104:TRP:CE2	2.52	0.44
2:B:80:ASP:O	2:B:81:LEU:C	2.59	0.44
3:C:98:PHE:HB2	15:V:94:MET:CE	2.47	0.44
4:D:78:THR:O	4:D:79:ASN:C	2.59	0.44
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.83	0.44
5:E:90:GLY:HA3	5:E:126:VAL:HG12	1.99	0.44
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.98	0.44
16:W:45:GLU:O	16:W:46:VAL:C	2.58	0.44
16:W:71:MET:O	16:W:72:LYS:C	2.59	0.44
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.44
17:X:46:CYS:SG	17:X:135:ARG:NH1	2.90	0.44
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:68:ARG:O	18:Z:69:ILE:C	2.60	0.44
20:b:23:PHE:HD2	31:b:201:3PE:H281	1.81	0.44
22:r:109:ASP:O	22:r:110:GLN:CG	2.64	0.44
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.81	0.44
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.17	0.44
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.44
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.48	0.44
10:P:55:VAL:HA	10:P:79:GLN:O	2.18	0.44
10:P:245:VAL:HA	10:P:265:PHE:HD2	1.82	0.44
12:R: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
23:s:52:LEU:O	23:s:56:ARG:HG2	2.17	0.44
2:B:71:ALA:O	2:B:75:VAL:N	2.47	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.17	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.97	0.44
6:F:119:GLU:HB3	6:F:124:THR:HG22	2.00	0.44
6:F:126:LYS:O	6:F:129:GLU:HG2	2.18	0.44
6:F:292:MET:O	6:F:293:SER:OG	2.33	0.44
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.31	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.44
9:I:42:LYS:HD3	9:I:42:LYS:HA	1.84	0.44
10:P:305:PHE:CB	10:P:314:THR:HG22	2.47	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
13:S:20:ARG:HG3	13:S:54:LEU:CB	2.43	0.44
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.44
14:T:79:ILE:O	14:T:83:VAL:HG23	2.17	0.44
14:T:133:ILE:O	14:T:136:GLU:N	2.46	0.44
17:X:40:ASN:O	17:X:41:LYS:C	2.58	0.44
17:X:52:ASP:OD1	18:Z:116:TRP:HB2	2.18	0.44
1:A:106:TRP:HH2	20:b:19:LEU:HD11	1.83	0.44
3:C:55:LYS:HE2	3:C:55:LYS:HB3	1.83	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.44
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.57	0.44
6:F:427:LEU:HB2	27:F:501:FMN:HM73	2.00	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
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
9:I:79:ARG:HG2	22:r:12:ARG:NH2	2.29	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.98	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
5:E:222:PHE:H	5:E:225:GLU:CD	2.25	0.44
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	2.00	0.44
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44
8:H:99:ASN:OD1	19:a:40:ARG:HG3	2.18	0.44
9:I:78:PHE:HB2	22:r:12:ARG:CG	2.48	0.44
10:P:156:SER:HB2	10:P:161:VAL:CG2	2.47	0.44
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.44
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.44
2:B:90:LEU:O	2:B:119:VAL:HA	2.18	0.44
3:C:136:PHE:O	3:C:137:ASN:C	2.60	0.44
4:D:91:ALA:O	4:D:92:HIS:C	2.60	0.44
4:D:258:VAL:O	4:D:261:MET:HB2	2.17	0.44
4:D:446:ASP:O	4:D:450:ILE:HG13	2.17	0.44
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.44
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.44
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.44
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.80	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.44
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.77	0.44
10:P:168:SER:O	10:P:202:ARG:HA	2.17	0.44
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
14:T:113:LEU:O	14:T:116:VAL:HB	2.17	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	2.00	0.44
1:A:18:ILE:HG12	8:H:222:LEU:CD2	2.48	0.44
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.48	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
7:G:607:LYS:HG2	11:Q:78:ARG:HH11	1.82	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.47	0.44
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.44
12:R:79:CYS:O	12:R:88:HIS:CE1	2.71	0.44
13:S:23:LEU:HB3	13:S:33:VAL:HG12	2.00	0.44
2:B:93:MET:CE	2:B:95:PHE:CE2	3.00	0.44
2:B:96:GLY:CA	2:B:101:ALA:HB2	2.40	0.44
2:B:146:ARG:NH2	3:C:211:TYR:CZ	2.86	0.44
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.44
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.44
4:D:348:LEU:HB3	18:Z:16:TYR:CE2	2.53	0.44
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.46	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.44
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.52	0.44
9:I:62:MET:SD	18:Z:35:MET:SD	3.16	0.44
10:P:130:ILE:N	10:P:130:ILE:HD12	2.33	0.44
18:Z:62:ILE:CD1	20:b:81:LEU:HD22	2.48	0.44
20:b:12:ALA:HB1	31:b:201:3PE:H261	2.00	0.44
3:C:70:LYS:O	15:V:103:LEU:HA	2.18	0.43
4:D:271:ARG:CD	8:H:279:ARG:O	2.62	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
6:F:225:LEU:N	11:Q:160:TYR:OH	2.38	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:303:THR:HB	7:G:614:GLY:HA3	1.99	0.43
7:G:362:ASP:HB2	13:S:71:PHE:CD1	2.52	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.96	0.43
8:H:200:LEU:HD21	8:H:282:TYR:HD1	1.83	0.43
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.43
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.43
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.43
13:S:30:SER:O	13:S:33:VAL:N	2.51	0.43
16:W:20:VAL:HG21	16:W:80:ARG:CZ	2.48	0.43
18:Z:72:MET:O	18:Z:73:PRO:C	2.59	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
5:E:192:TYR:OH	5:E:213:PRO:HD2	2.18	0.43
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.43
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.43
8:H:200:LEU:CD2	8:H:282:TYR:HD1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.43
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.43
15:V:56:LEU:C	15:V:56:LEU:CD1	2.85	0.43
18:Z:28:ARG:O	18:Z:28:ARG:CG	2.64	0.43
1:A:63:LEU:O	1:A:64:LEU:C	2.61	0.43
1:A:112:GLU:O	1:A:113:TRP:C	2.58	0.43
2:B:70:ARG:HG3	2:B:70:ARG:O	2.18	0.43
4:D:99:LEU:HB3	4:D:101:LEU:HD11	2.00	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
5:E:124:LYS:HB3	5:E:125:PRO:HD2	2.00	0.43
5:E:183:PRO:HB2	5:E:195:LEU:N	2.34	0.43
5:E:195:LEU:HD21	5:E:218:ARG:HG2	1.99	0.43
6:F:126:LYS:HE2	6:F:274:LYS:HZ3	1.83	0.43
7:G:466:LEU:O	7:G:467:LYS:C	2.61	0.43
8:H:93:HIS:CE1	19:a:24:ALA:CA	2.93	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.60	0.43
8:H:200:LEU:C	8:H:200:LEU:HD12	2.43	0.43
9:I:78:PHE:HB2	22:r:12:ARG:HG2	2.00	0.43
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.82	0.43
10:P:197:GLU:HB3	10:P:259:VAL:HG22	1.99	0.43
12:R:88:HIS:ND1	12:R:89:PRO:O	2.50	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.43
3:C:221:GLU:OE1	16:W:114:GLU:HB2	2.18	0.43
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.43
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
5:E:48:PRO:C	5:E:50:THR:N	2.74	0.43
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.43
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	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:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
8:H:63:PRO:HD2	8:H:66:THR:HG21	2.01	0.43
10:P:76:MET:HE1	10:P:254:LYS:HE2	2.01	0.43
15:V:56:LEU:CD1	15:V:57:ASP:OD1	2.67	0.43
17:X:7:LEU:CD1	18:Z:87:LEU:HB3	2.49	0.43
4:D:166:ARG:CD	18:Z:8:GLN:NE2	2.82	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:413:TRP:CH2	6:F:436:GLN:HG2	2.53	0.43
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.18	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	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:277:TYR:OH	9:I:66:LEU:HB3	2.17	0.43
10:P:170:LEU:O	10:P:171:ASN:CG	2.61	0.43
13:S:24:CYS:SG	13:S:61:VAL:HG12	2.58	0.43
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.52	0.43
2:B:82:ILE:CG1	8:H:57:MET:CE	2.82	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
3:C:139:ARG:NH2	4:D:406:GLU:OE2	2.48	0.43
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
4:D:232:VAL:CG2	4:D:356:ILE:HB	2.48	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
10:P:64:PHE:CE1	10:P:209:ARG:O	2.69	0.43
10:P:310:PHE:O	10:P:311:GLU:C	2.60	0.43
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.43
16:W:71:MET:O	16:W:74:ALA:N	2.39	0.43
18:Z:144:THR:OG1	19:a:48:MET:HE1	2.18	0.43
1:A:23:TRP:O	1:A:26:GLN:HG3	2.19	0.43
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.34	0.43
6:F:166:ALA:HB1	23:s:45:PHE:HD2	1.84	0.43
6:F:294:VAL:CG1	6:F:337:MET:HG3	2.48	0.43
7:G:279:GLU:HG3	11:Q:154:LYS:HG3	2.00	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
8:H:257:THR:O	8:H:260:MET:HB3	2.19	0.43
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.43
14:T:92:LYS:O	14:T:92:LYS:HG2	2.16	0.43
16:W:120:ASP:HB3	16:W:123:SER:OG	2.19	0.43
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.43
4:D:339:GLN:NE2	9:I:37:LYS:HZ2	2.16	0.43
5:E:81:VAL:HB	5:E:104:LEU:HD11	2.00	0.43
5:E:140:MET:HE1	6:F:366:ALA:HA	2.01	0.43
6:F:38:GLU:HG3	6:F:39:ASP:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:419:ILE:HG23	6:F:432:ALA:HB2	2.01	0.43
7:G:31:LEU:HA	7:G:31:LEU:HD23	1.79	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.43
7:G:466:LEU:HD13	7:G:500:ILE:HD13	2.00	0.43
7:G:617:ARG:NH1	16:W:129:HIS:N	2.66	0.43
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.54	0.43
8:H:123:SER:HB3	8:H:214:GLU:HG3	2.00	0.43
11:Q:104:ARG:HA	11:Q:104:ARG:HD3	1.88	0.43
14:T:109:GLY:O	14:T:110:LEU:C	2.61	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.43
5:E:163:THR:HG1	5:E:167:LEU:H	1.67	0.43
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.34	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43
8:H:42:PRO:HD2	8:H:45:ILE:CD1	2.49	0.43
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.43
17:X:10:LEU:H	17:X:10:LEU:HD12	1.84	0.43
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.43
19:a:55:SER:O	19:a:56:GLY:C	2.61	0.43
1:A:73:LEU:O	1:A:76:PRO:HD2	2.18	0.43
2:B:111:ARG:CZ	4:D:208:GLU:HG2	2.49	0.43
2:B:117:PHE:HA	8:H:39:ILE:CG2	2.49	0.43
4:D:339:GLN:HE21	9:I:37:LYS:HZ2	1.66	0.43
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.43
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
6:F:340:ASP:O	6:F:343:VAL:HB	2.19	0.43
6:F:416:SER:O	6:F:419:ILE:CG2	2.65	0.43
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.43
7:G:117:MET:SD	7:G:143:SER:HB2	2.59	0.43
7:G: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
9:I:152:CYS:SG	24:I:301:SF4:S3	3.17	0.43
10:P:237:LYS:HE3	10:P:322:ILE:O	2.19	0.43
10:P:259:VAL:N	10:P:261:LYS:HG2	2.33	0.43
10:P:306:GLY:HA2	10:P:312:PRO:HB3	2.01	0.43
17:X:41:LYS:HD2	20:b:56:PRO:HG3	2.01	0.43
18:Z:86:ILE:HA	18:Z:128:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:12:MET:HE2	19:a:12:MET:HB3	1.90	0.43
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.43
1:A:73:LEU:N	1:A:74:PRO:HD2	2.35	0.42
3:C:124:ARG:HD2	11:Q:140:LYS:HZ1	1.83	0.42
4:D:198:THR:HG23	8:H:275:ALA:O	2.18	0.42
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.42
5:E:137:THR:HG22	6:F:370:LEU:HD21	2.02	0.42
5:E:165:ASP:O	5:E:166:LYS:C	2.62	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
6:F:126:LYS:HG3	6:F:275:LEU:HB2	2.01	0.42
6:F:224:ARG:HD3	11:Q:164:PHE:CD1	2.55	0.42
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.42
7:G:496:MET:HG2	7:G:500:ILE:HD11	2.01	0.42
8:H:17:MET:HE1	8:H:225:MET:HE3	2.01	0.42
8:H:33:LEU:HD21	22:r:25:GLN:HG2	2.01	0.42
10:P:169:HIS:CD2	10:P:181:LEU:HD11	2.52	0.42
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.00	0.42
11:Q:160:TYR:CE1	11:Q:164:PHE:CZ	3.02	0.42
14:T:93:ILE:HD11	14:T:118:ILE:HD11	2.00	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.62	0.42
16:W:38:LEU:HG	16:W:70:PHE:HZ	1.84	0.42
18:Z:74:LEU:O	18:Z:78:GLU:HG3	2.19	0.42
20:b:15:LYS:O	20:b:15:LYS:HG3	2.18	0.42
20:b:23:PHE:CE1	31:b:201:3PE:H371	2.54	0.42
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	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:351:MET:O	18:Z:10:MET:HE3	2.18	0.42
6:F:398:ARG:NH1	6:F:408:GLU:CD	2.78	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.83	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.54	0.42
16:W:83:ASP:O	16:W:86:VAL:CG2	2.66	0.42
18:Z:58:ARG:HH22	20:b:49:THR:HG21	1.75	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42
1:A:25:PRO:HG3	8:H:60:PRO:CD	2.42	0.42
4:D:83:ASN:C	4:D:85:GLY:N	2.74	0.42
4:D:92:HIS:CE1	4:D:457:VAL:HA	2.53	0.42
6:F:291:GLU:OE2	6:F:292:MET:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.42
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.83	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
7:G:664:TYR:OH	13:S:23:LEU:HD11	2.20	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.53	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
9:I:162:CYS:SG	24:I:302:SF4:S2	3.17	0.42
10:P:376:ASN:O	10:P:377:TYR:C	2.61	0.42
16:W:120:ASP:OD1	16:W:120:ASP:C	2.61	0.42
17:X:52:ASP:OD1	18:Z:116:TRP:CB	2.67	0.42
22:r:12:ARG:HB3	22:r:20:LEU:CD2	2.49	0.42
5:E:179:CYS:C	5:E:181:ASN:N	2.77	0.42
6:F:47:GLY:N	6:F:133:HIS:ND1	2.68	0.42
6:F:50:ASP:O	6:F:55:GLY:HA3	2.19	0.42
6:F:333:GLU:HG2	6:F:334:THR:N	2.33	0.42
7:G:36:VAL:O	7:G:39:GLN:HG2	2.19	0.42
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.42
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.42
9:I:35:THR:HG22	22:r:107:SER:HA	1.97	0.42
13:S:16:LEU:HD13	13:S:19:ILE:HD11	2.02	0.42
17:X:29:ALA:CB	18:Z:71:LEU:CD1	2.98	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
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.42
1:A:52:SER:O	1:A:53:MET:C	2.61	0.42
2:B:94:THR:OG1	2:B:104:MET:HE1	2.20	0.42
3:C:101:ASP:OD1	15:V:86:LYS:HE3	2.19	0.42
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.42
5:E:94:ILE:HD13	7:G:209:TYR:CE2	2.53	0.42
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
8:H:196:ALA:C	8:H:198:PHE:N	2.77	0.42
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.85	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
10:P:207:PHE:O	10:P:241:TYR:HA	2.19	0.42
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.42
17:X:26:LYS:HD3	17:X:95:GLN:OE1	2.19	0.42
17:X:75:LYS:O	17:X:79:ALA:HB2	2.19	0.42
23:s:53:SER:HA	23:s:56:ARG:HG2	2.02	0.42
4:D:259:GLU:O	4:D:261:MET:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
5:E:221:ARG:HB2	5:E:225:GLU:HG2	2.01	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.42
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.20	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.42
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.42
10:P:220:TYR:CG	10:P:226:VAL:HG13	2.55	0.42
10:P:300:TRP:NE1	10:P:304:LEU:HD21	2.35	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
18:Z:108:GLU:O	18:Z:109:SER:C	2.61	0.42
2:B:126:ARG:O	2:B:128:ALA:N	2.50	0.42
6:F:261:TRP:CE2	6:F:265:PHE:CZ	3.08	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
8:H:8:THR:O	8:H:9:LEU:CB	2.68	0.42
8:H:68:MET:HG3	8:H:68:MET:O	2.19	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.42
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.42
11:Q:55:VAL:HG21	16:W:78:ASP:OD1	2.19	0.42
13:S:19:ILE:O	13:S:53:ILE:HD12	2.20	0.42
17:X:41:LYS:O	17:X:42:GLU:C	2.59	0.42
17:X:132:LYS:HB3	17:X:132:LYS:HE2	1.84	0.42
18:Z:102:PRO:O	18:Z:103:ASN:C	2.62	0.42
18:Z:120:LEU:HD12	18:Z:121:ILE:H	1.85	0.42
20:b:15:LYS:O	20:b:16:GLU:HB2	2.20	0.42
1:A:93:ILE:HD13	1:A:93:ILE:HA	1.90	0.42
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.42
6:F:47:GLY:C	6:F:49:HIS:H	2.27	0.42
6:F:235:VAL:O	6:F:236:PHE:C	2.62	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.42
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.42
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.42
10:P:242:VAL:HG13	10:P:243:ALA:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:354:ARG:HG3	10:P:362:LEU:CD2	2.48	0.42
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.42
14:T:80:LYS:O	14:T:84:LEU:HG	2.20	0.42
20:b:22:SER:OG	31:b:201:3PE:H3B1	2.20	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: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
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.42
4:D:144:MET:HG2	4:D:223:HIS:H	1.85	0.42
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.28	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
16:W:28:LEU:O	16:W:32:LYS:HG3	2.20	0.42
16:W:78:ASP:HA	16:W:79:PRO:HD3	1.94	0.42
17:X:52:ASP:O	17:X:53:PRO:C	2.61	0.42
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.42
20:b:69:HIS:HD2	20:b:70:PRO:CD	2.26	0.42
20:b:82:LYS:HB3	20:b:82:LYS:HE2	1.81	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.20	0.42
3:C:243:ALA:C	7:G:105:ASN:HD21	2.28	0.42
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.42
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.42
4:D:264:ASN:O	4:D:265:ASN:C	2.56	0.42
5:E:136:THR:HB	26:E:301:FES:S2	2.60	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42
6:F:410:ASP:OD1	6:F:411:SER:N	2.53	0.42
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.42
8:H:172:MET:HE3	8:H:176:LEU:CB	2.47	0.42
14:T:90:TYR:CD2	14:T:92:LYS:HB3	2.54	0.42
22:r:10:LYS:O	22:r:11:LEU:C	2.62	0.42
22:r:18:GLN:OE1	22:r:18:GLN:N	2.53	0.42
1:A:112:GLU:O	1:A:113:TRP:CD1	2.73	0.41
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.41
5:E:62:ILE:HG21	5:E:103:VAL:HG11	2.02	0.41
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41
10:P:228:LEU:HD11	10:P:288:PHE:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:331:ASP:CG	10:P:332:LEU:H	2.28	0.41
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.41
14:T:123:GLU:HG2	14:T:130:ILE:HD12	2.02	0.41
16:W:93:LEU:HD23	16:W:93:LEU:C	2.45	0.41
17:X:53:PRO:CD	18:Z:116:TRP:CD1	2.80	0.41
20:b:11:ASN:O	20:b:15:LYS:HG2	2.20	0.41
20:b:59:ASP:HA	20:b:63:MET:CE	2.51	0.41
22:r:113:LEU:HD12	22:r:113:LEU:HA	1.77	0.41
1:A:20:VAL:O	1:A:21:ALA:C	2.63	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
25:B:302:PC1:H372	8:H:53:MET:SD	2.60	0.41
3:C:48:PRO:HD3	4:D:162:GLN:OE1	2.20	0.41
4:D:266:ARG:CA	9:I:65:GLU:OE2	2.68	0.41
4:D:448:VAL:HG11	8:H:205:SER:HB2	2.02	0.41
5:E:69:TYR:HB3	5:E:70:PRO:CD	2.50	0.41
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.41
5:E:134:CYS:SG	5:E:175:CYS:HA	2.60	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:272:ARG:HH11	7:G:274:LEU:CD2	2.33	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.02	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.41
14:T:87:LEU:CD2	14:T:122:MET:CE	2.98	0.41
14:T:118:ILE:HD13	14:T:118:ILE:HA	1.83	0.41
16:W:76:VAL:HG13	16:W:82:VAL:HG22	2.02	0.41
17:X:70:PHE:CE1	17:X:117:TRP:CZ3	3.08	0.41
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.41
3:C:72:VAL:HG23	3:C:72:VAL:O	2.20	0.41
3:C:241:PHE:O	3:C:242:PRO:C	2.62	0.41
4:D:140:ASP:O	4:D:147:ASN:ND2	2.53	0.41
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.41
4:D:198:THR:N	4:D:199:PRO:CD	2.84	0.41
5:E:203:ILE:HG12	5:E:218:ARG:NH1	2.35	0.41
6:F:299:LEU:HD12	6:F:300:ILE:HG23	2.01	0.41
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	0.41
7:G:160:VAL:CG1	7:G:161:GLU:N	2.83	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:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.41
7:G:541:PRO:HB2	7:G:561:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.89	0.41
8:H:174:LEU:HD23	8:H:174:LEU:HA	1.81	0.41
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.41
9:I:152:CYS:SG	24:I:301:SF4:S1	3.17	0.41
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.21	0.41
11:Q:85:ASN:C	11:Q:87:MET:N	2.76	0.41
14:T:115:GLN:O	14:T:116:VAL:C	2.63	0.41
20:b:25:VAL:O	20:b:26:TRP:C	2.64	0.41
20:b:31:ILE:O	20:b:32:MET:C	2.63	0.41
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
4:D:376:GLU:HG2	7:G:121:LEU:CD1	2.51	0.41
6:F:119:GLU:CD	27:F:501:FMN:HN3	2.28	0.41
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.41
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.41
7:G:32:ILE:CG2	7:G:98:LYS:HA	2.50	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.55	0.41
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.41
10:P:231:LEU:HD11	10:P:290:PRO:HB2	2.03	0.41
12:R:81:GLY:HA3	12:R:88:HIS:CD2	2.55	0.41
19:a:49:GLU:OE2	19:a:49:GLU:HA	2.20	0.41
20:b:16:GLU:N	20:b:17:PRO:HD3	2.35	0.41
2:B:95:PHE:HE2	2:B:131:MET:CE	2.33	0.41
2:B:137:LEU:HD11	2:B:142:ALA:HA	2.03	0.41
3:C:141:ARG:HE	3:C:141:ARG:HB2	1.41	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.36	0.41
4:D:202:TRP:HZ2	9:I:73:THR:HG22	1.86	0.41
4:D:339:GLN:HE21	9:I:37:LYS:NZ	2.17	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
5:E:167:LEU:HD23	5:E:168:PHE:HE1	1.85	0.41
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.41
5:E:192:TYR:CD2	5:E:203:ILE:HD13	2.56	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:P:230:SER:O	10:P:231:LEU:C	2.64	0.41
10:P:243:ALA:O	10:P:244:ASP:C	2.63	0.41
10:P:265:PHE:N	10:P:265:PHE:CD1	2.87	0.41
10:P:316:LYS:C	10:P:316:LYS:HD3	2.46	0.41
10:P:362:LEU:HA	10:P:362:LEU:HD23	1.88	0.41
13:S:16:LEU:CB	13:S:69:TYR:CD1	2.97	0.41
13:S:20:ARG:HD2	13:S:22:HIS:NE2	2.35	0.41
19:a:49:GLU:O	19:a:50:ARG:C	2.62	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.02	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
4:D:201:PHE:HB2	8:H:32:GLN:HB3	2.03	0.41
4:D:265:ASN:C	4:D:267:ILE:H	2.29	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.41
5:E:48:PRO:HD3	5:E:94:ILE:CG2	2.51	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.41
8:H:206:GLU:O	8:H:207:LEU:HB2	2.20	0.41
17:X:70:PHE:O	17:X:74:ILE:HG13	2.20	0.41
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.84	0.41
5:E:61:ARG:O	5:E:65:ILE:HG13	2.21	0.41
5:E:225:GLU:O	5:E:226:PRO:C	2.60	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:280:GLY:O	6:F:356:VAL:HB	2.20	0.41
6:F:300:ILE:CD1	6:F:307:VAL:HG23	2.49	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.41
8:H:42:PRO:HD2	8:H:45:ILE:HD11	2.03	0.41
8:H:90:PRO:O	8:H:91:MET:C	2.60	0.41
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.35	0.41
18:Z:19:ILE:HG22	18:Z:20:ASP:N	2.36	0.41
20:b:61:GLY:O	20:b:63:MET:HG3	2.20	0.41
3:C:70:LYS:HD3	3:C:71:TYR:CZ	2.56	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
4:D:197:MET:HG3	8:H:32:GLN:NE2	2.36	0.41
4:D:261:MET:HE3	4:D:261:MET:HB3	1.90	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
5:E:142:ARG:HB3	5:E:182:ALA:HB3	2.03	0.41
5:E:145:ASP:OD1	5:E:145:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:337:MET:HE2	6:F:337:MET:HA	2.02	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.41
17:X:26:LYS:HE2	17:X:26:LYS:HB3	1.85	0.41
17:X:37:ASP:OD1	17:X:37:ASP:C	2.62	0.41
1:A:102:LEU:O	1:A:106:TRP:HD1	2.04	0.41
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.41
2:B:145:LEU:O	2:B:146:ARG:C	2.64	0.41
3:C:101:ASP:O	15:V:90:LEU:HD13	2.21	0.41
3:C:102:HIS:CE1	15:V:48:THR:CG2	2.89	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.03	0.41
4:D:240:LEU:O	4:D:241:LEU:C	2.62	0.41
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.41
5:E:138:PRO:CG	6:F:122:PRO:HB3	2.47	0.41
6:F:88:ARG:HA	6:F:88:ARG:HD3	1.85	0.41
6:F:311:TRP:CH2	6:F:333:GLU:HB3	2.55	0.41
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	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:187:ILE:HG23	8:H:198:PHE:CE2	2.56	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
8:H:306:SER:CB	8:H:310:PHE:HE2	2.34	0.41
9:I:50:MET:O	9:I:54:THR:N	2.37	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
10:P:135:GLU:HG3	10:P:140:ASP:HA	2.03	0.41
14:T:107:ASP:OD1	14:T:108:LEU:N	2.54	0.41
14:T:120:MET:O	14:T:121:ALA:C	2.63	0.41
18:Z:69:ILE:HG23	20:b:54:PRO:HD3	2.03	0.41
18:Z:90:ASN:O	18:Z:94:GLU:HB2	2.21	0.41
19:a:48:MET:HE3	19:a:48:MET:HB2	1.77	0.41
20:b:20:VAL:HA	31:b:201:3PE:C29	2.47	0.41
20:b:20:VAL:CG2	31:b:201:3PE:H261	2.49	0.41
22:r:24:LEU:HD23	22:r:24:LEU:HA	1.85	0.41
2:B:111:ARG:NE	4:D:208:GLU:HG2	2.35	0.41
2:B:138:THR:HG21	4:D:116:LEU:HA	2.02	0.41
2:B:163:SER:HB2	9:I:150:THR:O	2.20	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:47:ARG:HG3	4:D:160:ASN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.85	0.41
4:D:79:ASN:HB2	4:D:100:GLU:HB3	2.03	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
5:E:238:LYS:HB3	5:E:242:PHE:CG	2.56	0.41
7:G:32:ILE:HG22	7:G:33:GLU:N	2.36	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.41
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.55	0.41
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
8:H:264:LEU:HD23	8:H:264:LEU:HA	1.81	0.41
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.41
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.85	0.41
15:V:98:LYS:HG2	15:V:100:TRP:CZ2	2.55	0.41
17:X:53:PRO:HD2	18:Z:116:TRP:NE1	2.31	0.41
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.54	0.40
4:D:238:LEU:HA	18:Z:9:ASP:HB2	2.03	0.40
6:F:210:THR:CB	6:F:224:ARG:H	2.34	0.40
6:F:257:ARG:HG2	6:F:261:TRP:CE3	2.55	0.40
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.40
7:G:217:GLU:C	7:G:219:SER:N	2.79	0.40
7:G:277:MET:HE1	11:Q:153:PRO:HD3	2.03	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.40
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.42	0.40
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.86	0.40
8:H:89:LEU:HD12	8:H:89:LEU:HA	1.87	0.40
8:H:251:LEU:HD11	8:H:254:LEU:HB2	2.02	0.40
10:P:146:VAL:HG13	10:P:147:ASN:OD1	2.21	0.40
10:P:191:VAL:HG13	10:P:192:ARG:CZ	2.51	0.40
11:Q:55:VAL:HG21	16:W:80:ARG:HH11	1.86	0.40
15:V:96:LYS:HE2	15:V:96:LYS:HB2	1.95	0.40
4:D:240:LEU:N	18:Z:9:ASP:OD2	2.54	0.40
6:F:70:LEU:O	6:F:71:LYS:C	2.63	0.40
6:F:337:MET:O	6:F:338:ASP:OD1	2.38	0.40
8:H:87:VAL:HB	8:H:88:PRO:HD3	2.04	0.40
8:H:114:TYR:O	8:H:117:LEU:N	2.55	0.40
8:H:253:GLU:CB	19:a:21:VAL:HG22	2.52	0.40
8:H:253:GLU:O	8:H:257:THR:N	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:140:ASP:O	10:P:141:PHE:C	2.65	0.40
10:P:288:PHE:CZ	10:P:290:PRO:HB3	2.56	0.40
10:P:293:LEU:HD12	10:P:294:PRO:HD2	2.01	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
14:T:99:SER:HB2	14:T:102:SER:HB2	2.03	0.40
18:Z:140:PHE:C	18:Z:142:TRP:N	2.77	0.40
1:A:16:THR:O	1:A:20:VAL:HG23	2.22	0.40
1:A:102:LEU:HG	1:A:106:TRP:NE1	2.36	0.40
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.40
3:C:224:GLU:OE1	10:P:50:SER:OG	2.40	0.40
5:E:109:MET:HE2	7:G:196:GLY:CA	2.51	0.40
6:F:306:GLY:O	6:F:307:VAL:C	2.64	0.40
7:G:49:VAL:HG13	7:G:102:ILE:HG12	2.03	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.09	0.40
7:G:163:LYS:HD3	7:G:163:LYS:HA	1.84	0.40
7:G:314:LEU:HD23	7:G:583:ILE:HG13	2.02	0.40
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.55	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
17:X:23:ALA:HB2	17:X:95:GLN:HE22	1.82	0.40
19:a:9:LEU:O	19:a:10:ALA:C	2.64	0.40
22:r:20:LEU:C	22:r:20:LEU:CD1	2.89	0.40
1:A:1:MET:O	1:A:2:ASN:C	2.64	0.40
2:B:147:LYS:HD2	2:B:147:LYS:HA	1.74	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
4:D:259:GLU:HB3	18:Z:25:LEU:HD11	2.03	0.40
6:F:196:PHE:HD1	23:s:56:ARG:HH21	1.70	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.40
8:H:63:PRO:O	8:H:66:THR:HG22	2.21	0.40
8:H:153:VAL:HG11	8:H:241:ILE:HG23	2.03	0.40
10:P:56:ALA:HA	10:P:125:VAL:O	2.20	0.40
10:P:96:LEU:C	10:P:96:LEU:CD1	2.94	0.40
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.40
14:T:140:CYS:HB2	14:T:143:GLU:HB2	2.02	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
4:D:128:THR:HG22	4:D:131:GLN:CG	2.52	0.40
4:D:142:VAL:CG1	4:D:185:MET:SD	3.10	0.40
4:D:144:MET:HE2	4:D:144:MET:HB2	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:213:PHE:O	4:D:214:TYR:C	2.64	0.40
5:E:190:ASN:HD22	5:E:192:TYR:HE1	1.69	0.40
6:F:114:VAL:CG1	6:F:212:LEU:HD23	2.52	0.40
6:F:205:ILE:O	6:F:206:CYS:C	2.63	0.40
6:F:257:ARG:CG	6:F:261:TRP:CD2	2.93	0.40
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.40
8:H:204:GLU:O	8:H:208:VAL:HA	2.21	0.40
10:P:315:THR:HB	10:P:318:LYS:H	1.85	0.40
11:Q:57:GLU:O	11:Q:58:LYS:C	2.65	0.40
13:S:23:LEU:HB3	13:S:33:VAL:CG1	2.51	0.40
18:Z:10:MET:HE2	18:Z:10:MET:HB3	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	89/115 (77%)	82 (92%)	7 (8%)	0	100	100
2	B	154/224 (69%)	142 (92%)	10 (6%)	2 (1%)	9	41
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%)	190 (91%)	18 (9%)	0	100	100
6	F	424/464 (91%)	405 (96%)	19 (4%)	0	100	100
7	G	685/727 (94%)	630 (92%)	55 (8%)	0	100	100
8	H	310/318 (98%)	291 (94%)	18 (6%)	1 (0%)	36	70
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	R	39/116 (34%)	38 (97%)	1 (3%)	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	4/145 (3%)	3 (75%)	1 (25%)	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	3981/5036 (79%)	3747 (94%)	231 (6%)	3 (0%)	49	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	127	GLN
8	H	92	PRO
2	B	195	PRO

5.3.2 Protein sidechains ⓘ

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	341/370 (92%)	340 (100%)	1 (0%)	86	85
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	87
8	H	278/280 (99%)	278 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	P	297/325 (91%)	295 (99%)	2 (1%)	76	79
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68	76
12	R	31/96 (32%)	31 (100%)	0	100	100
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	71
14	T	69/135 (51%)	68 (99%)	1 (1%)	59	71
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	129 (100%)	0	100	100
18	Z	120/123 (98%)	119 (99%)	1 (1%)	73	77
19	a	56/60 (93%)	56 (100%)	0	100	100
20	b	70/73 (96%)	70 (100%)	0	100	100
21	q	6/131 (5%)	6 (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	3493/4292 (81%)	3484 (100%)	9 (0%)	84	85

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

Mol	Chain	Res	Type
5	E	244	VAL
6	F	337	MET
7	G	271	MET
10	P	192	ARG
10	P	242	VAL
11	Q	96	LYS
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 (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	54	HIS
3	C	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	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
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

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Mol	Chain	Res	Type
7	G	569	GLN
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	169	GLN
8	H	258	ASN
8	H	287	HIS
10	P	43	HIS
10	P	71	ASN
10	P	154	GLN
10	P	166	HIS
10	P	216	HIS
10	P	251	ASN
10	P	269	ASN
10	P	275	HIS
10	P	323	HIS
10	P	341	GLN
10	P	356	HIS
11	Q	51	GLN
11	Q	88	GLN
15	V	41	HIS
15	V	50	GLN
16	W	54	GLN
17	X	30	HIS
17	X	77	HIS
18	Z	135	ASN
19	a	31	ASN
20	b	69	HIS
20	b	71	GLN
20	b	83	ASN
22	r	9	GLN
22	r	21	GLN
22	r	110	GLN
23	s	59	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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
28	NDP	P	401	-	49,52,52	1.19	5 (10%)	66,80,80	1.67	11 (16%)
31	3PE	b	201	-	45,45,50	1.12	5 (11%)	48,50,55	1.23	3 (6%)
24	SF4	B	301	2	0,12,12	-	-	-		
24	SF4	G	802	7	0,12,12	-	-	-		
24	SF4	I	301	9	0,12,12	-	-	-		
27	FMN	F	501	-	33,33,33	1.39	5 (15%)	48,50,50	1.21	7 (14%)
30	EHZ	W	201	-	27,31,37	1.90	7 (25%)	37,41,47	1.86	11 (29%)
26	FES	G	803	7	0,4,4	-	-	-		
25	PC1	B	302	-	34,34,53	1.15	2 (5%)	40,42,61	1.12	2 (5%)
24	SF4	F	502	6	0,12,12	-	-	-		
24	SF4	I	302	9	0,12,12	-	-	-		
26	FES	E	301	5	0,4,4	-	-	-		
24	SF4	G	801	7	0,12,12	-	-	-		

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
28	NDP	P	401	-	-	3/34/77/77	0/5/5/5
31	3PE	b	201	-	-	19/49/49/54	-
24	SF4	B	301	2	-	-	0/6/5/5
27	FMN	F	501	-	-	3/18/18/18	0/3/3/3
24	SF4	G	802	7	-	-	0/6/5/5
24	SF4	I	301	9	-	-	0/6/5/5
30	EHZ	W	201	-	-	21/39/39/45	-
26	FES	G	803	7	-	-	0/1/1/1
25	PC1	B	302	-	-	8/38/38/57	-
24	SF4	F	502	6	-	-	0/6/5/5
24	SF4	I	302	9	-	-	0/6/5/5
26	FES	E	301	5	-	-	0/1/1/1
24	SF4	G	801	7	-	-	0/6/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	W	201	EHZ	C15-N2	5.38	1.45	1.33
30	W	201	EHZ	C12-N1	5.14	1.45	1.33
27	F	501	FMN	C9A-C5A	4.85	1.49	1.41
28	P	401	NDP	C5A-C4A	4.27	1.47	1.39
25	B	302	PC1	O31-C31	4.17	1.45	1.33
25	B	302	PC1	O21-C21	4.10	1.45	1.34
28	P	401	NDP	C6N-C5N	3.31	1.39	1.33
31	b	201	3PE	O21-C21	3.10	1.43	1.34
27	F	501	FMN	C8-C7	3.09	1.48	1.40
31	b	201	3PE	O31-C31	3.08	1.42	1.33
27	F	501	FMN	C4-N3	-2.68	1.33	1.38
30	W	201	EHZ	O4-C15	-2.55	1.18	1.23
30	W	201	EHZ	P1-O7	2.55	1.64	1.54
28	P	401	NDP	C5A-C6A	2.48	1.48	1.41
30	W	201	EHZ	C9-S1	2.40	1.81	1.76
28	P	401	NDP	C5A-N7A	-2.39	1.34	1.39
28	P	401	NDP	C8A-N7A	2.38	1.36	1.31
30	W	201	EHZ	O3-C12	-2.35	1.18	1.23
27	F	501	FMN	C5A-N5	-2.31	1.35	1.39
31	b	201	3PE	O21-C2	-2.26	1.40	1.46
30	W	201	EHZ	P1-OP3	-2.24	1.46	1.54
31	b	201	3PE	O31-C3	-2.19	1.40	1.45
31	b	201	3PE	P-O12	-2.11	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	501	FMN	C4A-N5	2.00	1.34	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	W	201	EHZ	C8-C9-S1	6.35	121.48	113.63
28	P	401	NDP	C5A-C4A-N3A	-6.09	118.80	126.75
28	P	401	NDP	N3A-C4A-N9A	4.77	134.94	127.08
31	b	201	3PE	O21-C21-C22	4.05	120.23	111.50
25	B	302	PC1	O21-C21-C22	4.05	120.23	111.50
28	P	401	NDP	C2A-N3A-C4A	3.89	120.94	111.75
28	P	401	NDP	PN-O3-PA	-3.64	120.34	132.83
28	P	401	NDP	C4A-C5A-N7A	-3.25	106.66	110.62
28	P	401	NDP	N3A-C2A-N1A	-3.22	123.56	128.60
30	W	201	EHZ	C13-C12-N1	3.09	121.63	116.42
30	W	201	EHZ	C14-C13-C12	-3.02	107.33	112.36
25	B	302	PC1	O31-C31-C32	2.93	121.10	111.91
30	W	201	EHZ	OP3-P1-O9	-2.89	99.35	110.68
30	W	201	EHZ	C7-C8-C9	-2.84	107.42	113.89
28	P	401	NDP	C5A-N7A-C8A	2.80	107.49	103.51
28	P	401	NDP	C4A-N9A-C8A	2.75	108.71	105.73
27	F	501	FMN	C4A-C10-N1	-2.57	118.76	124.73
31	b	201	3PE	O31-C31-C32	2.49	119.72	111.91
27	F	501	FMN	C4-C4A-N5	2.45	121.72	118.23
27	F	501	FMN	O4-C4-C4A	-2.41	120.20	126.60
30	W	201	EHZ	C5-C6-C7	-2.37	108.02	114.85
30	W	201	EHZ	C10-S1-C9	2.26	108.92	101.87
28	P	401	NDP	C6A-C5A-N7A	2.24	136.19	132.02
28	P	401	NDP	N9A-C8A-N7A	-2.22	110.88	113.91
27	F	501	FMN	O2-C2-N1	-2.21	118.16	121.83
27	F	501	FMN	C4A-C10-N10	2.20	119.69	116.48
30	W	201	EHZ	C11-N1-C12	-2.17	118.82	122.84
28	P	401	NDP	C3D-C2D-C1D	2.17	105.54	101.43
31	b	201	3PE	O12-P-O14	-2.15	101.60	112.24
30	W	201	EHZ	O2-C9-S1	-2.14	119.83	122.61
27	F	501	FMN	C10-N1-C2	2.14	121.17	116.90
30	W	201	EHZ	O3-C12-N1	-2.11	119.03	123.01
30	W	201	EHZ	O6-P1-O9	2.10	112.36	106.47
27	F	501	FMN	C4A-C4-N3	2.01	118.29	113.19

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	F	501	FMN	C5'-O5'-P-O2P
27	F	501	FMN	C5'-O5'-P-O3P
28	P	401	NDP	C2B-O2B-P2B-O2X
30	W	201	EHZ	O1-C7-C8-C9
30	W	201	EHZ	C6-C7-C8-C9
30	W	201	EHZ	C7-C8-C9-S1
30	W	201	EHZ	S1-C10-C11-N1
30	W	201	EHZ	C11-C10-S1-C9
30	W	201	EHZ	C16-C17-C20-O6
30	W	201	EHZ	C20-O6-P1-O7
30	W	201	EHZ	C20-O6-P1-O9
30	W	201	EHZ	C20-O6-P1-OP3
31	b	201	3PE	C1-O11-P-O12
31	b	201	3PE	C1-O11-P-O14
31	b	201	3PE	O22-C21-O21-C2
31	b	201	3PE	C22-C21-O21-C2
31	b	201	3PE	C2B-C2C-C2D-C2E
31	b	201	3PE	C32-C31-O31-C3
31	b	201	3PE	C39-C3A-C3B-C3C
31	b	201	3PE	O32-C31-O31-C3
31	b	201	3PE	C1-O11-P-O13
25	B	302	PC1	C22-C21-O21-C2
31	b	201	3PE	C27-C28-C29-C2A
25	B	302	PC1	O22-C21-O21-C2
31	b	201	3PE	C1-C2-C3-O31
27	F	501	FMN	C5'-O5'-P-O1P
31	b	201	3PE	O11-C1-C2-C3
30	W	201	EHZ	N2-C15-C16-C17
31	b	201	3PE	C24-C25-C26-C27
30	W	201	EHZ	C3-C4-C5-C6
30	W	201	EHZ	C5-C6-C7-O1
25	B	302	PC1	C32-C31-O31-C3
30	W	201	EHZ	O2-C9-S1-C10
31	b	201	3PE	O11-C1-C2-O21
25	B	302	PC1	O32-C31-O31-C3
31	b	201	3PE	C11-O13-P-O11
31	b	201	3PE	C11-O13-P-O12
28	P	401	NDP	O4D-C1D-N1N-C6N
25	B	302	PC1	C11-C12-N-C15
31	b	201	3PE	O21-C2-C3-O31
30	W	201	EHZ	O4-C15-C16-O5
30	W	201	EHZ	C19-C17-C20-O6
31	b	201	3PE	C3-C2-O21-C21

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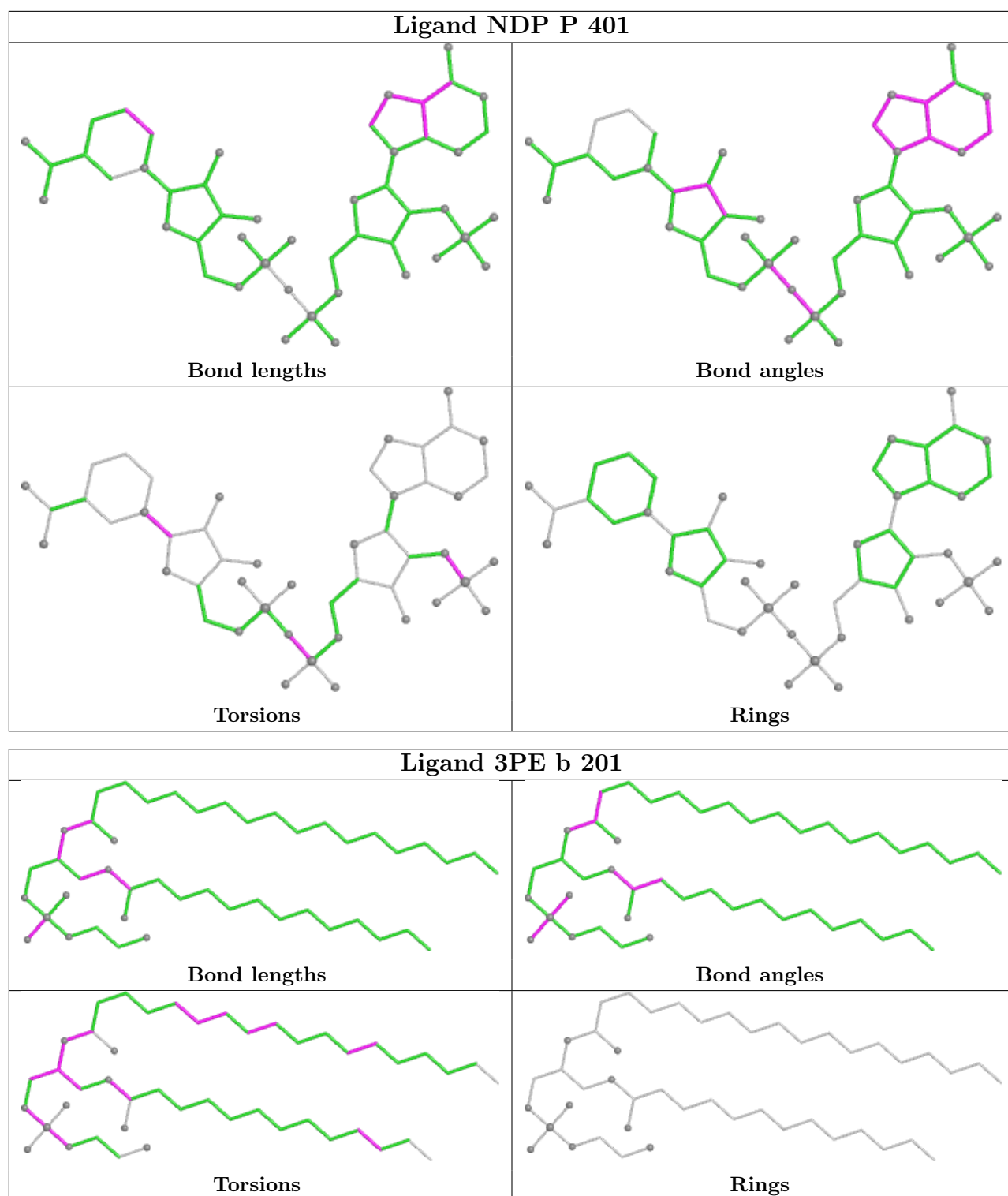
Mol	Chain	Res	Type	Atoms
30	W	201	EHZ	C2-C3-C4-C5
28	P	401	NDP	PN-O3-PA-O2A
25	B	302	PC1	C11-C12-N-C14
25	B	302	PC1	C11-C12-N-C13
30	W	201	EHZ	N2-C15-C16-O5
31	b	201	3PE	C25-C26-C27-C28
30	W	201	EHZ	C18-C17-C20-O6
30	W	201	EHZ	C15-C16-C17-C18
30	W	201	EHZ	O5-C16-C17-C18
30	W	201	EHZ	O4-C15-C16-C17
25	B	302	PC1	O21-C21-C22-C23

There are no ring outliers.

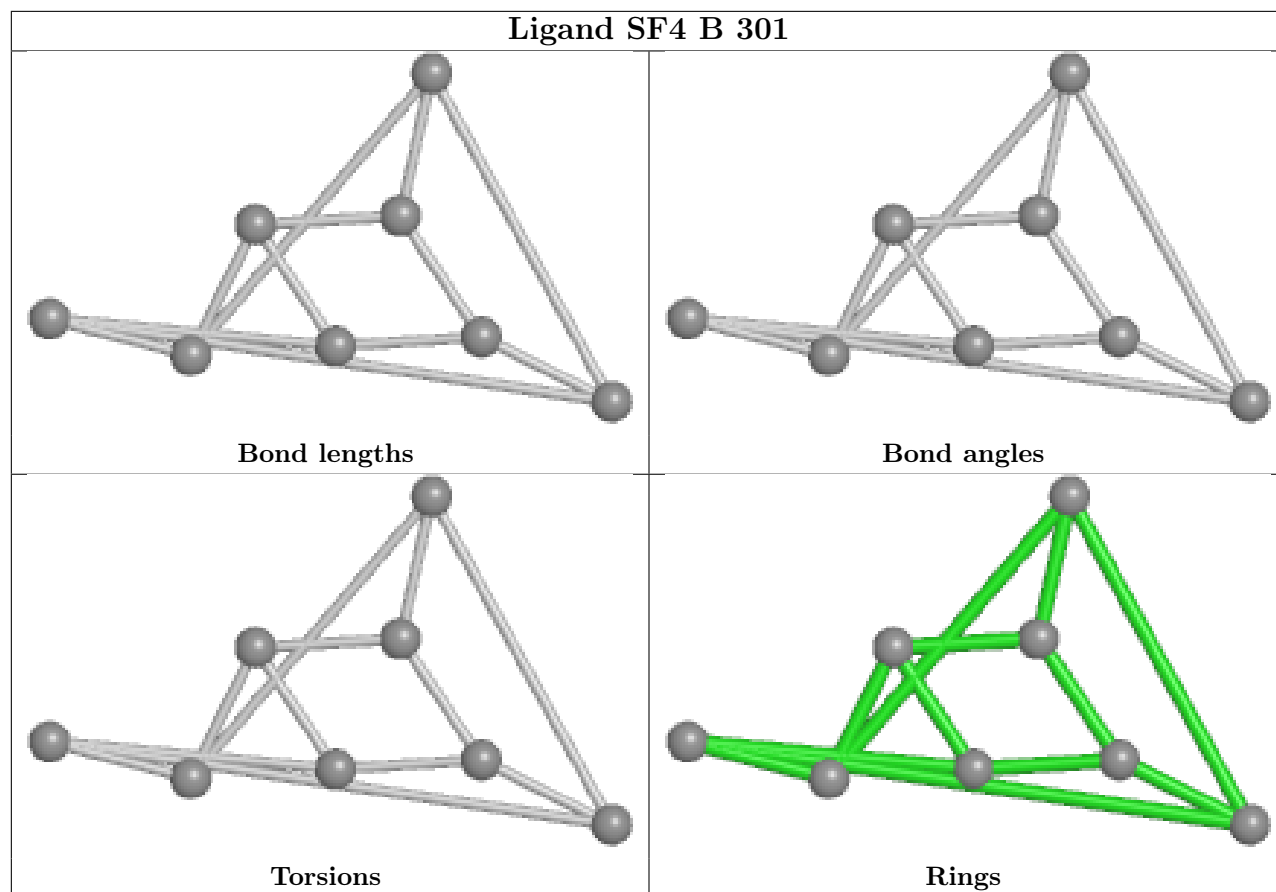
12 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	P	401	NDP	4	0
31	b	201	3PE	27	0
24	B	301	SF4	5	0
24	G	802	SF4	5	0
24	I	301	SF4	11	0
27	F	501	FMN	3	0
30	W	201	EHZ	7	0
26	G	803	FES	4	0
25	B	302	PC1	3	0
24	F	502	SF4	10	0
24	I	302	SF4	5	0
26	E	301	FES	4	0

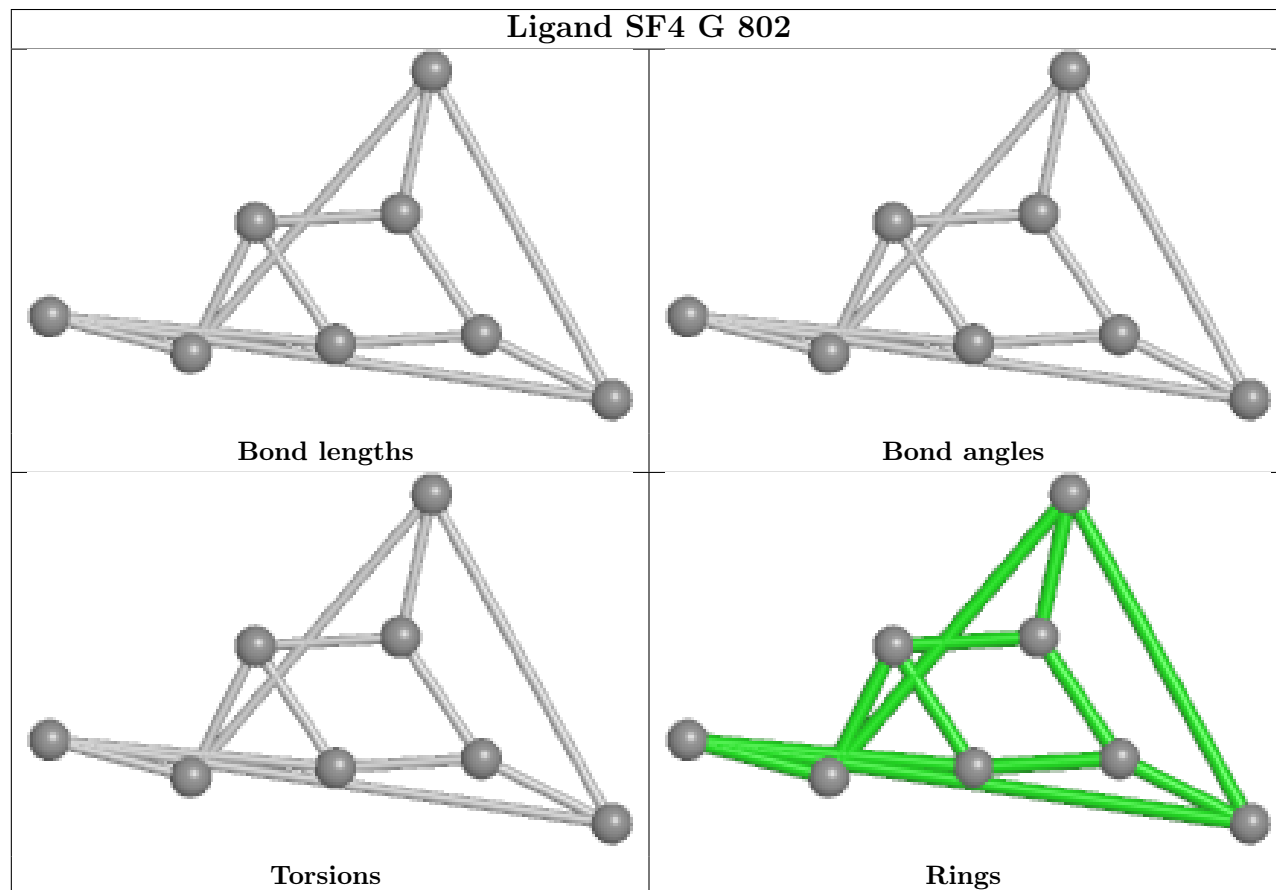
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

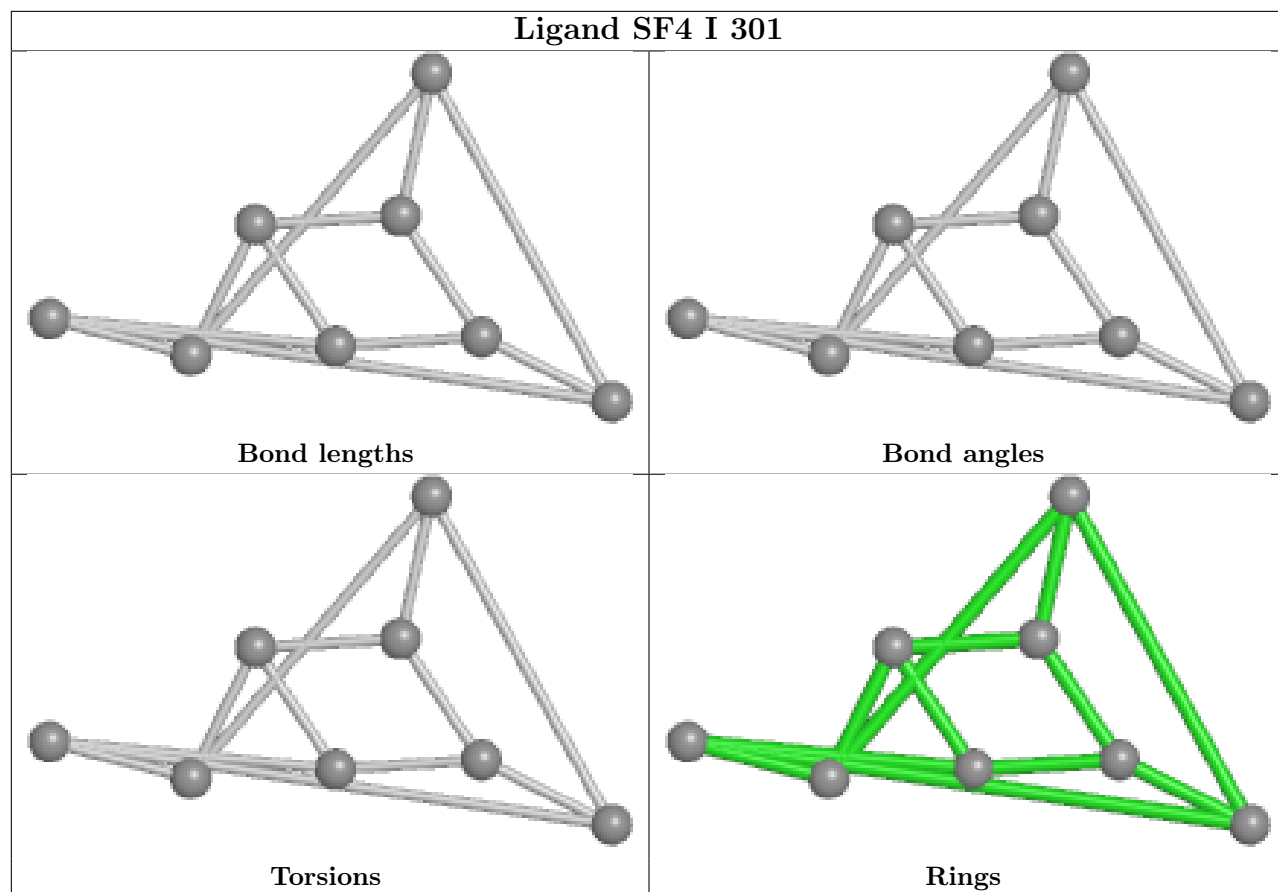


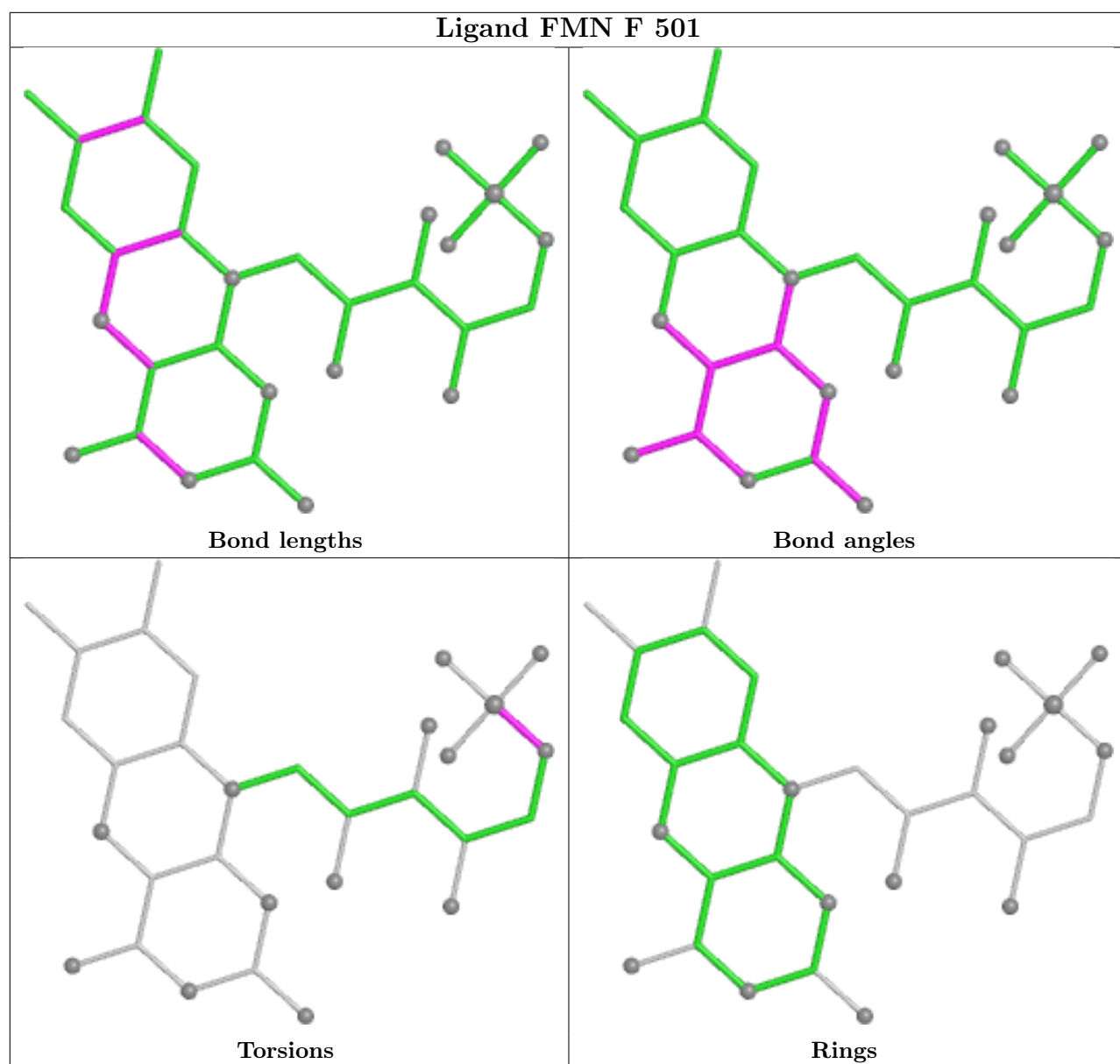
Ligand SF4 B 301

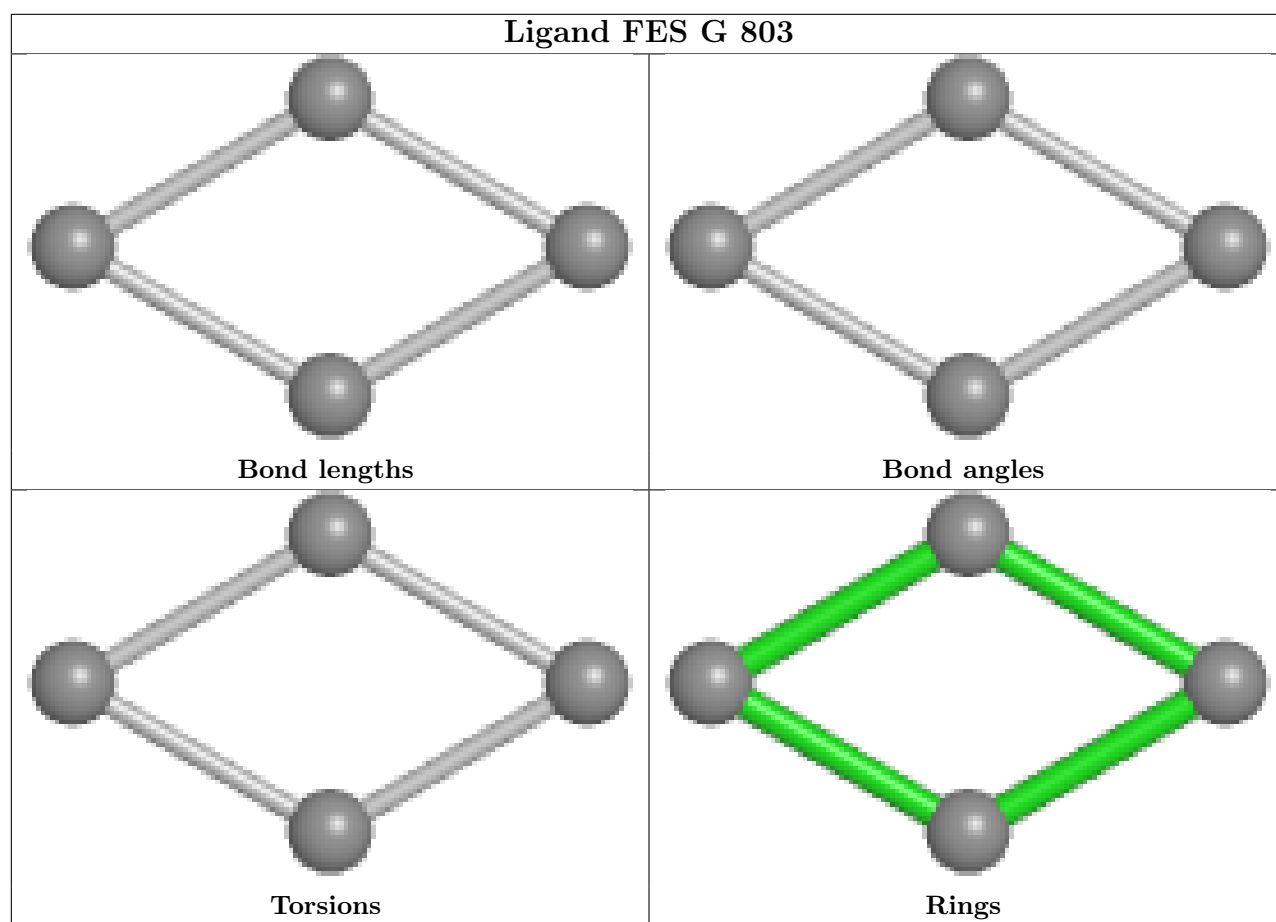
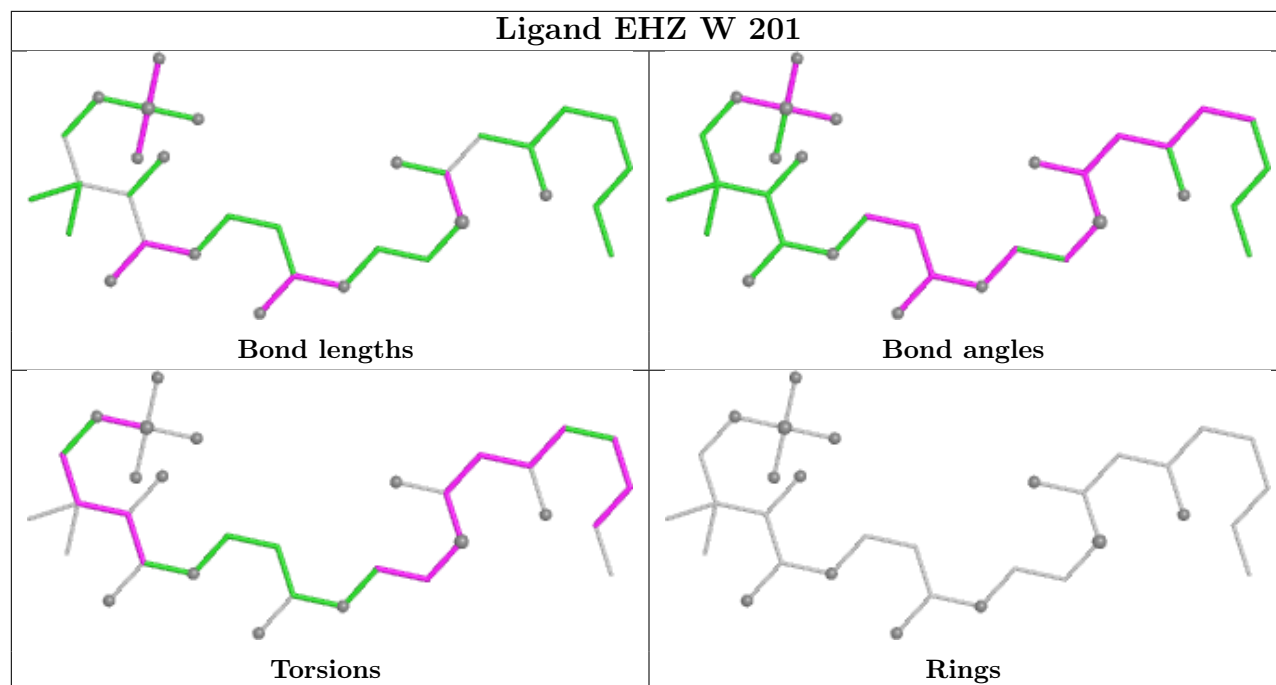


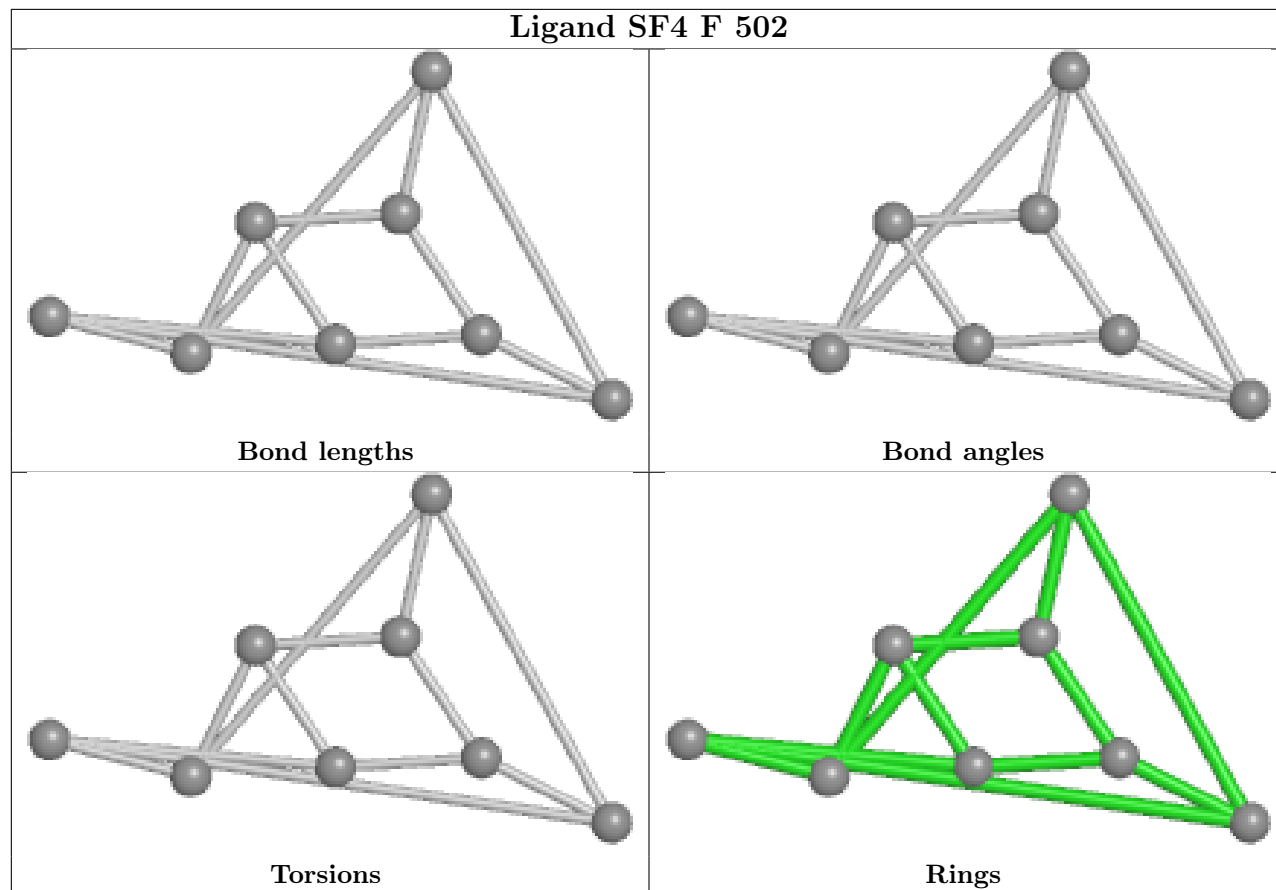
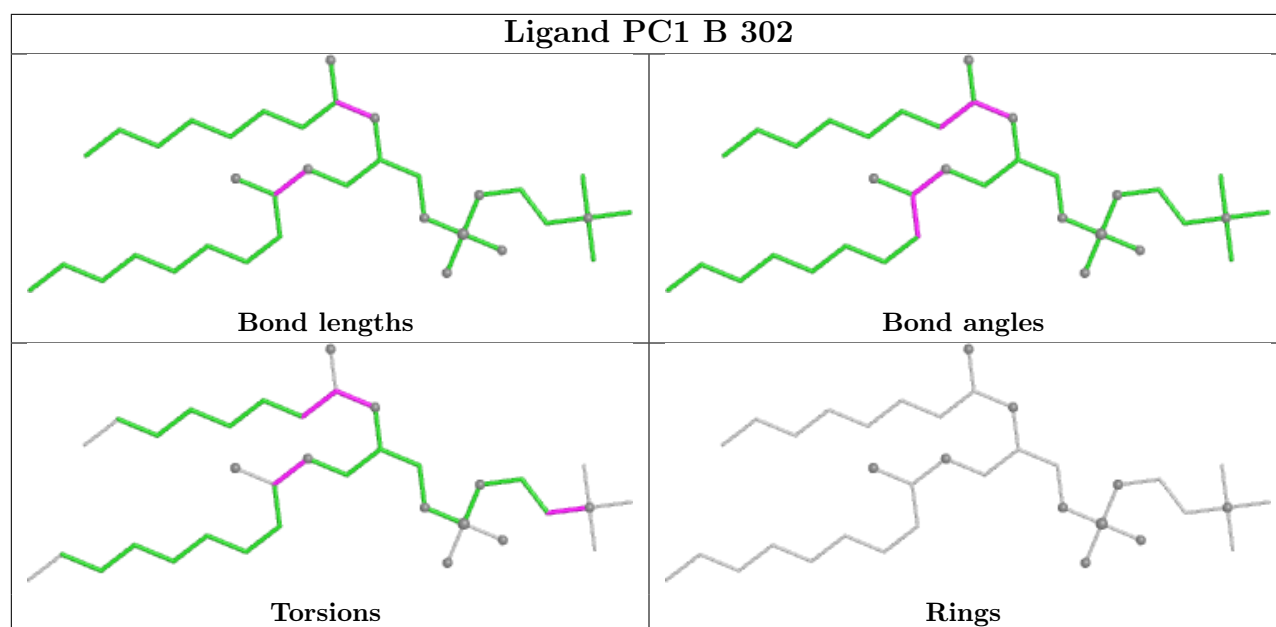
Ligand SF4 G 802

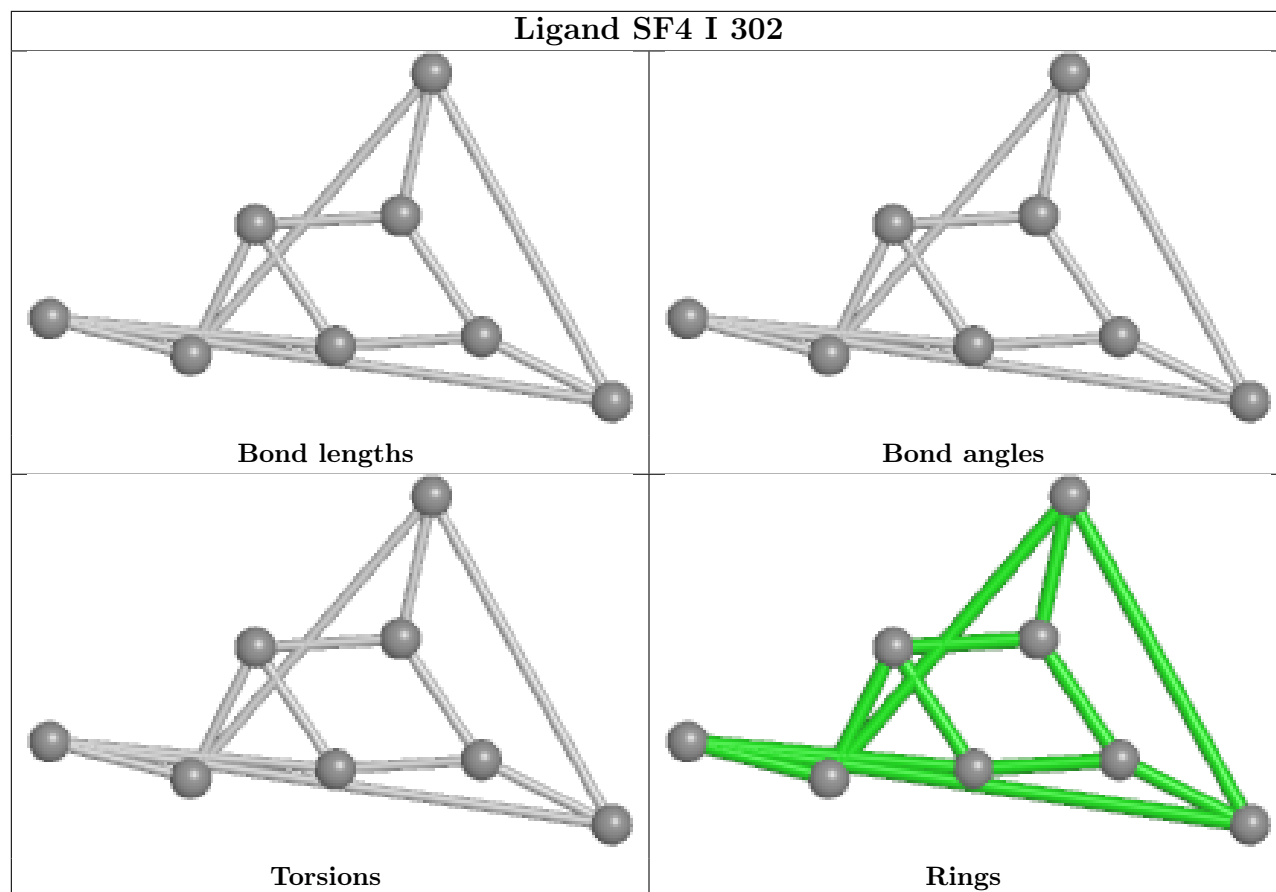


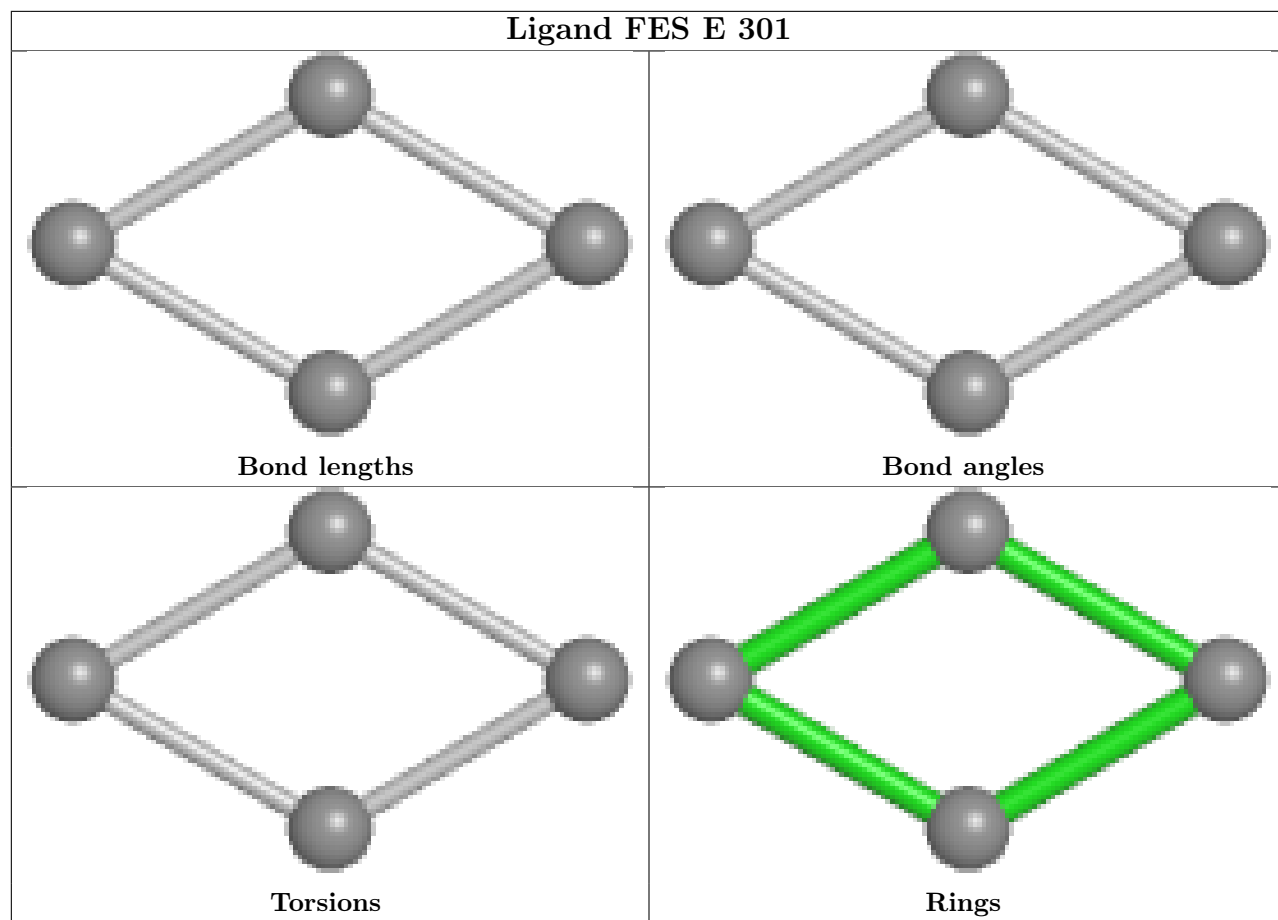


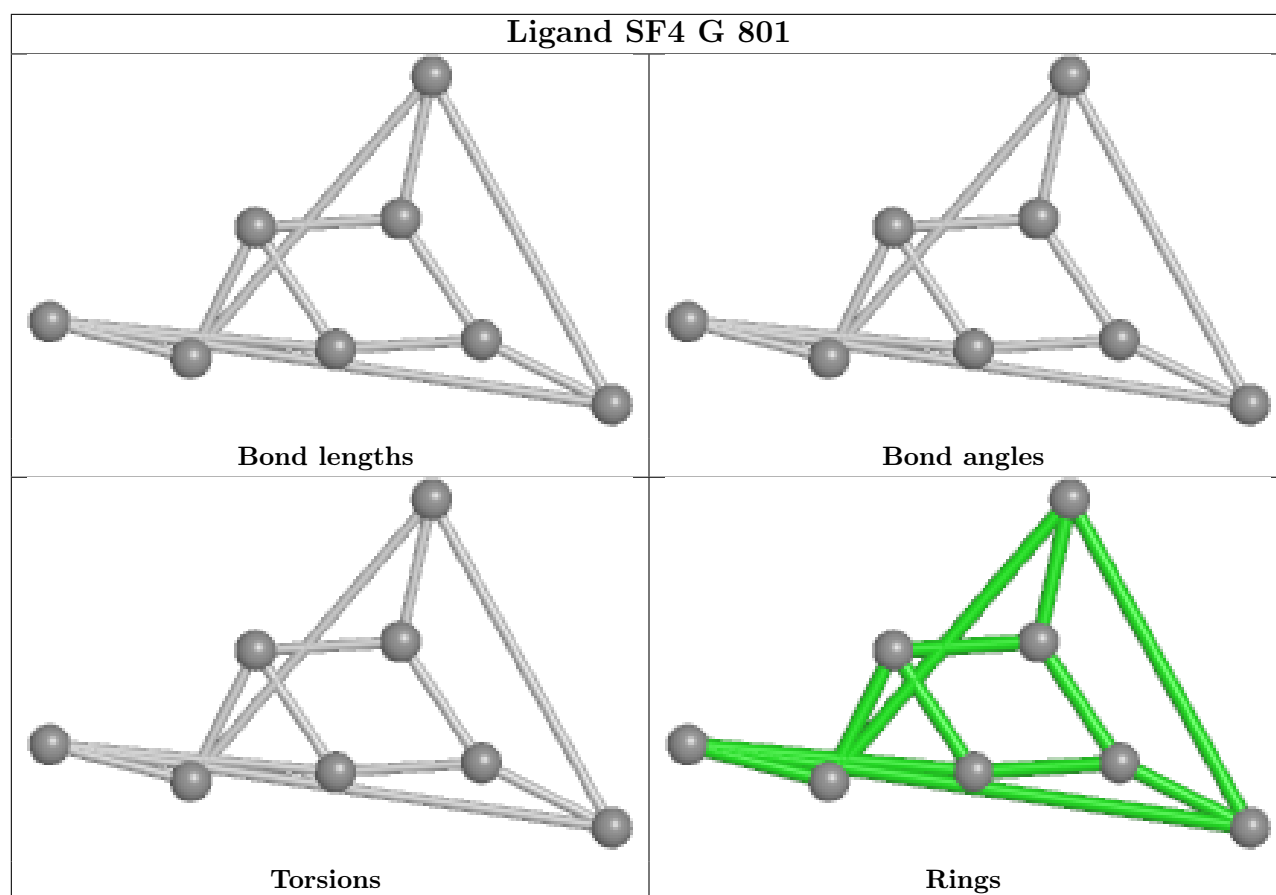












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

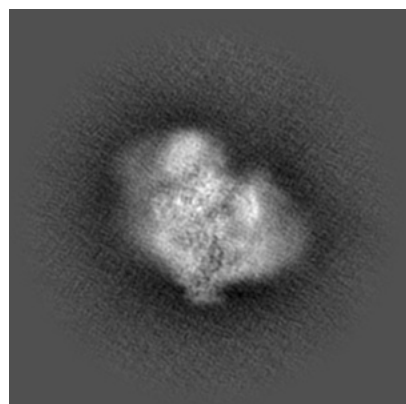
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38514. These allow visual inspection of the internal detail of the map and identification of artifacts.

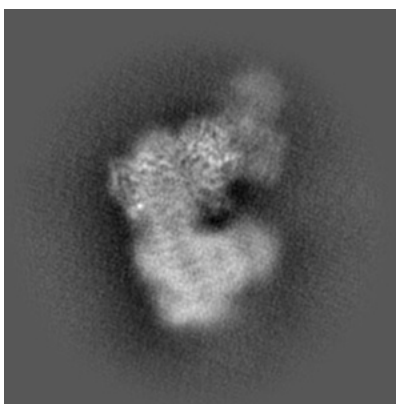
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

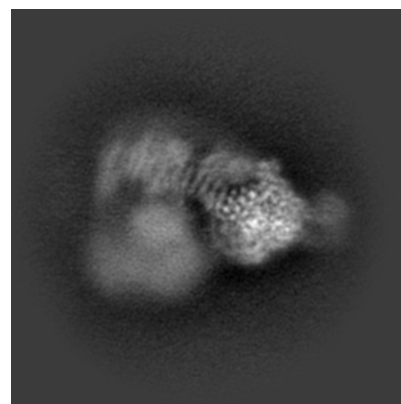
6.1.1 Primary map



X

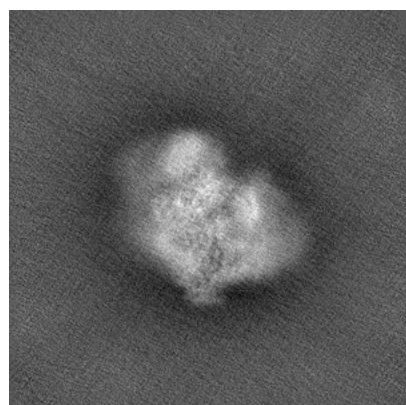


Y

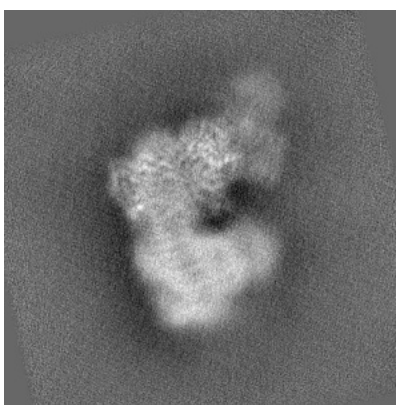


Z

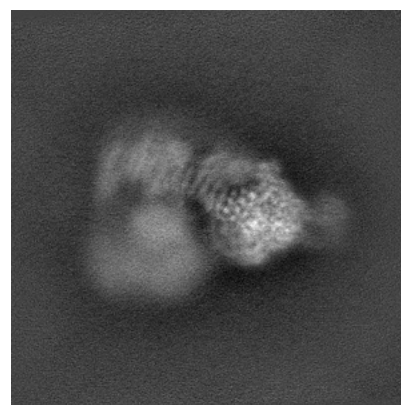
6.1.2 Raw map



X



Y

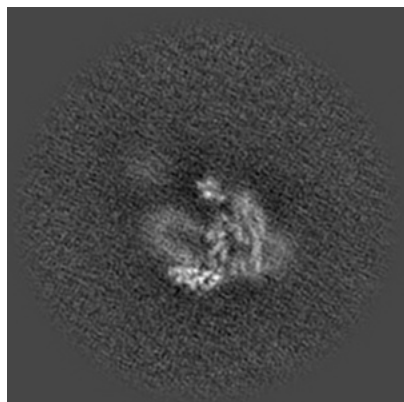


Z

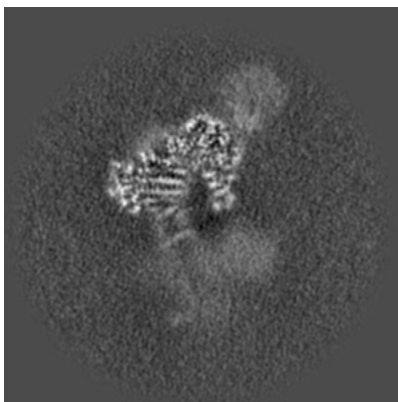
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

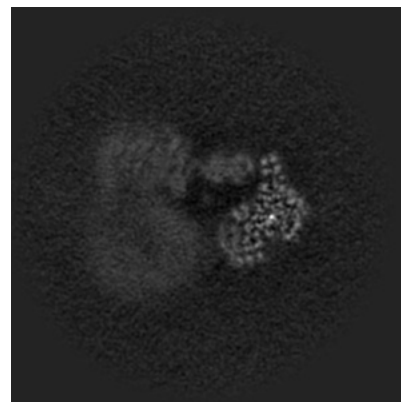
6.2.1 Primary map



X Index: 192

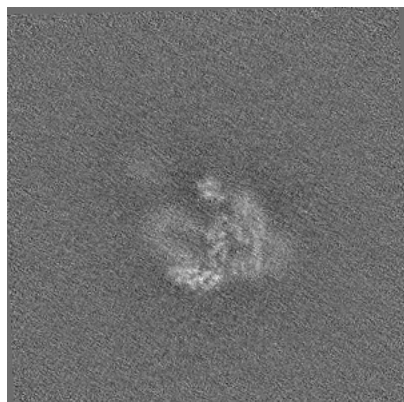


Y Index: 192

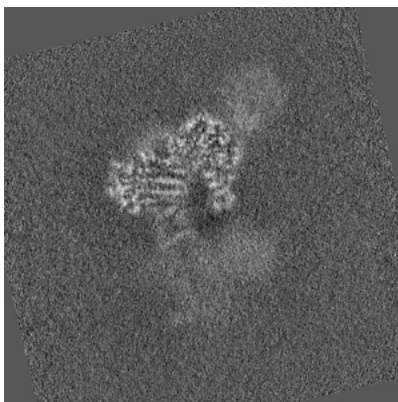


Z Index: 192

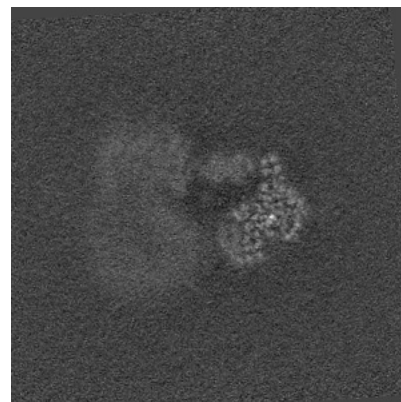
6.2.2 Raw map



X Index: 192



Y Index: 192

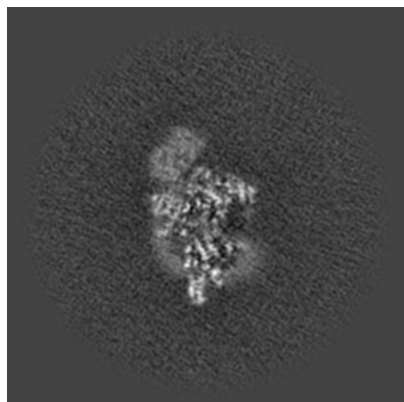


Z Index: 192

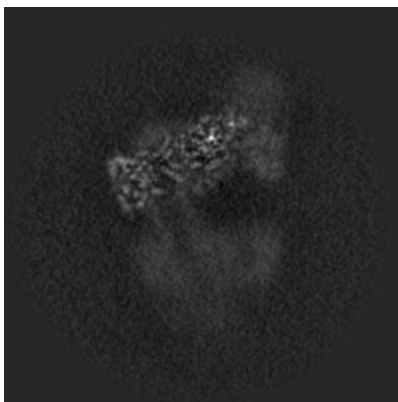
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

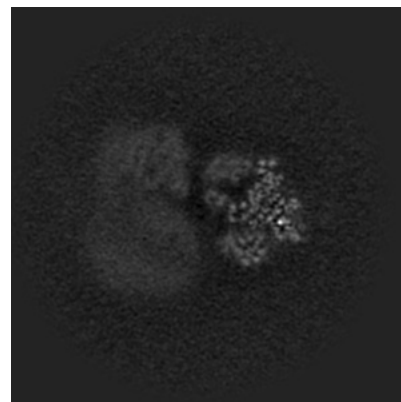
6.3.1 Primary map



X Index: 237

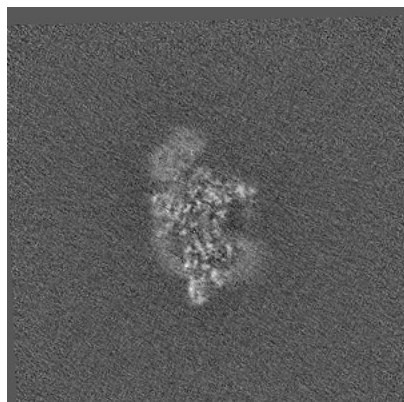


Y Index: 177

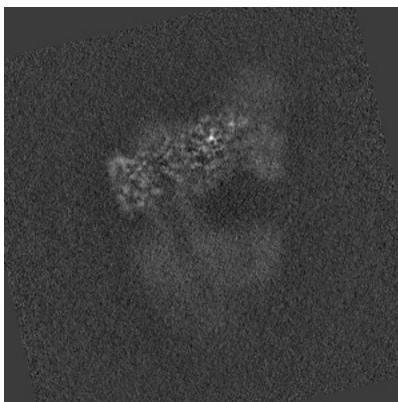


Z Index: 199

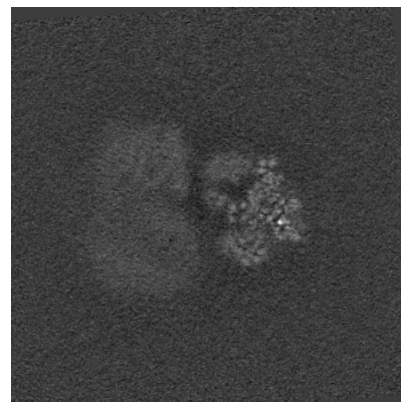
6.3.2 Raw map



X Index: 236



Y Index: 177

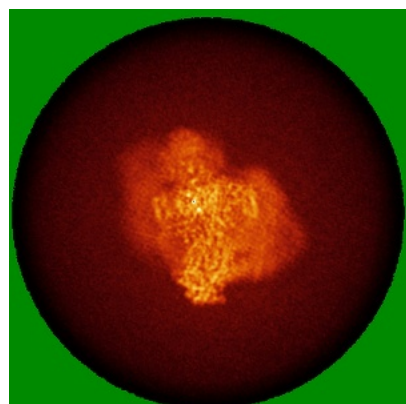


Z Index: 199

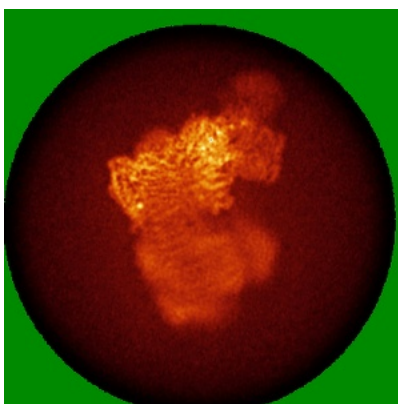
The images above show the largest variance slices of the map in three orthogonal directions.

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

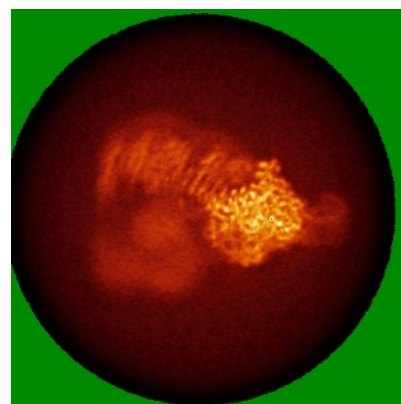
6.4.1 Primary map



X

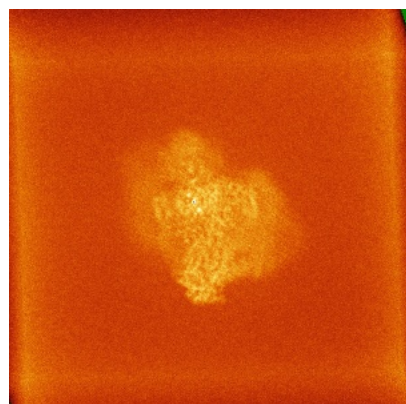


Y

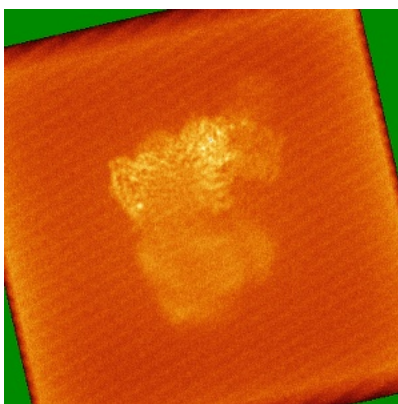


Z

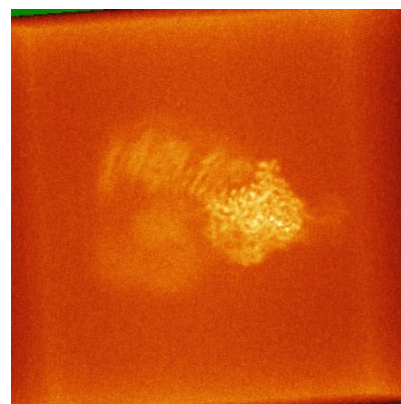
6.4.2 Raw map



X



Y



Z

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

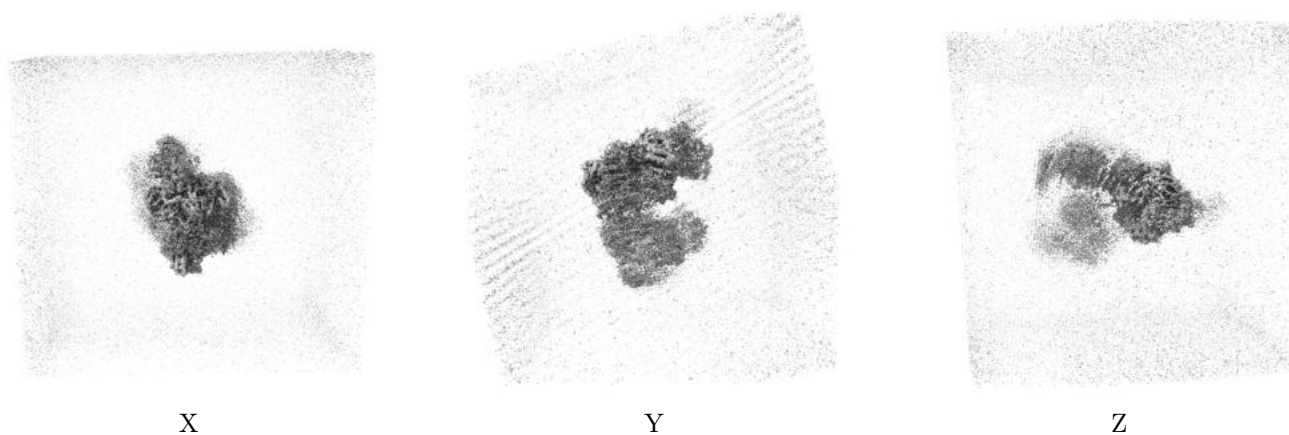
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

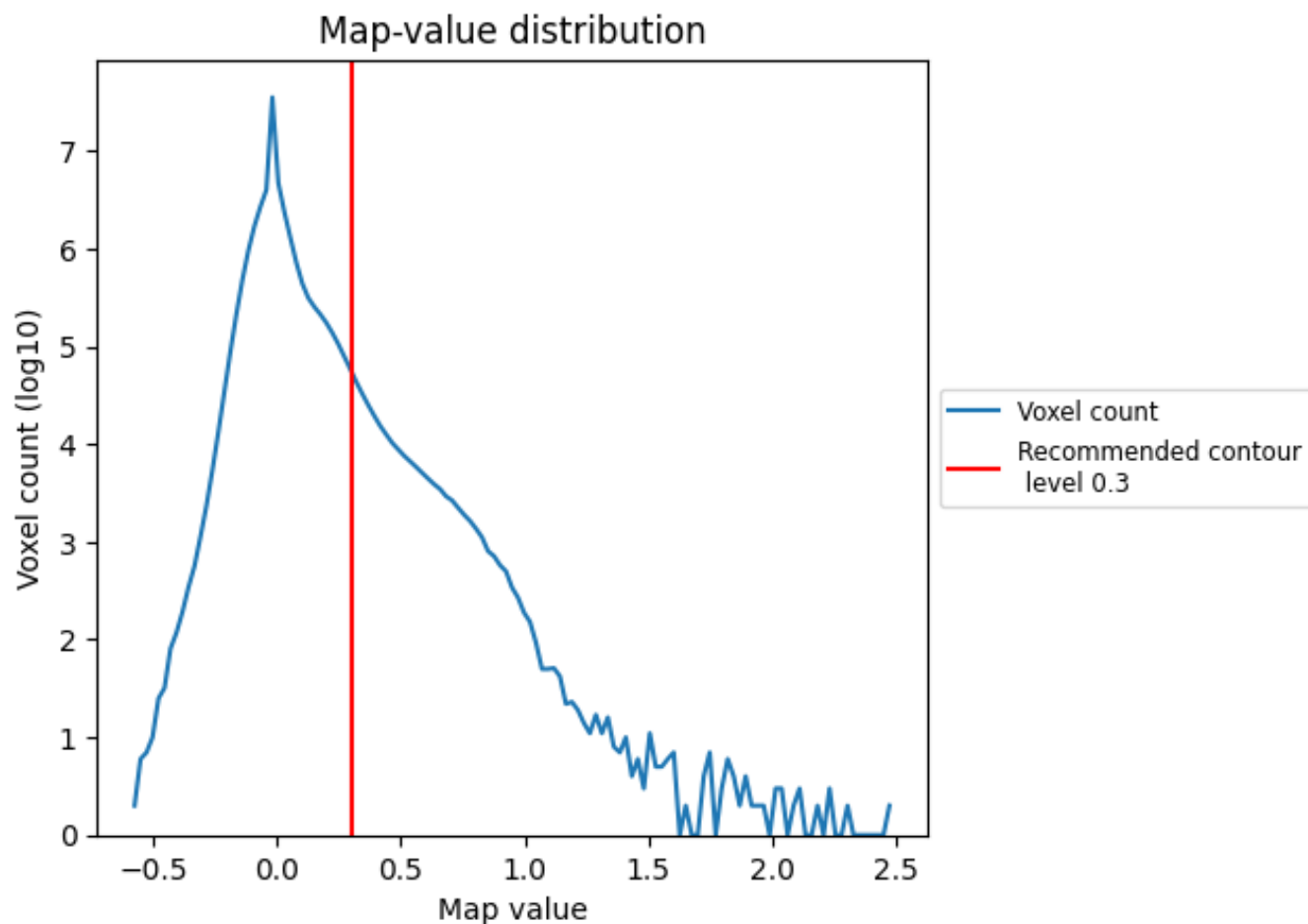
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

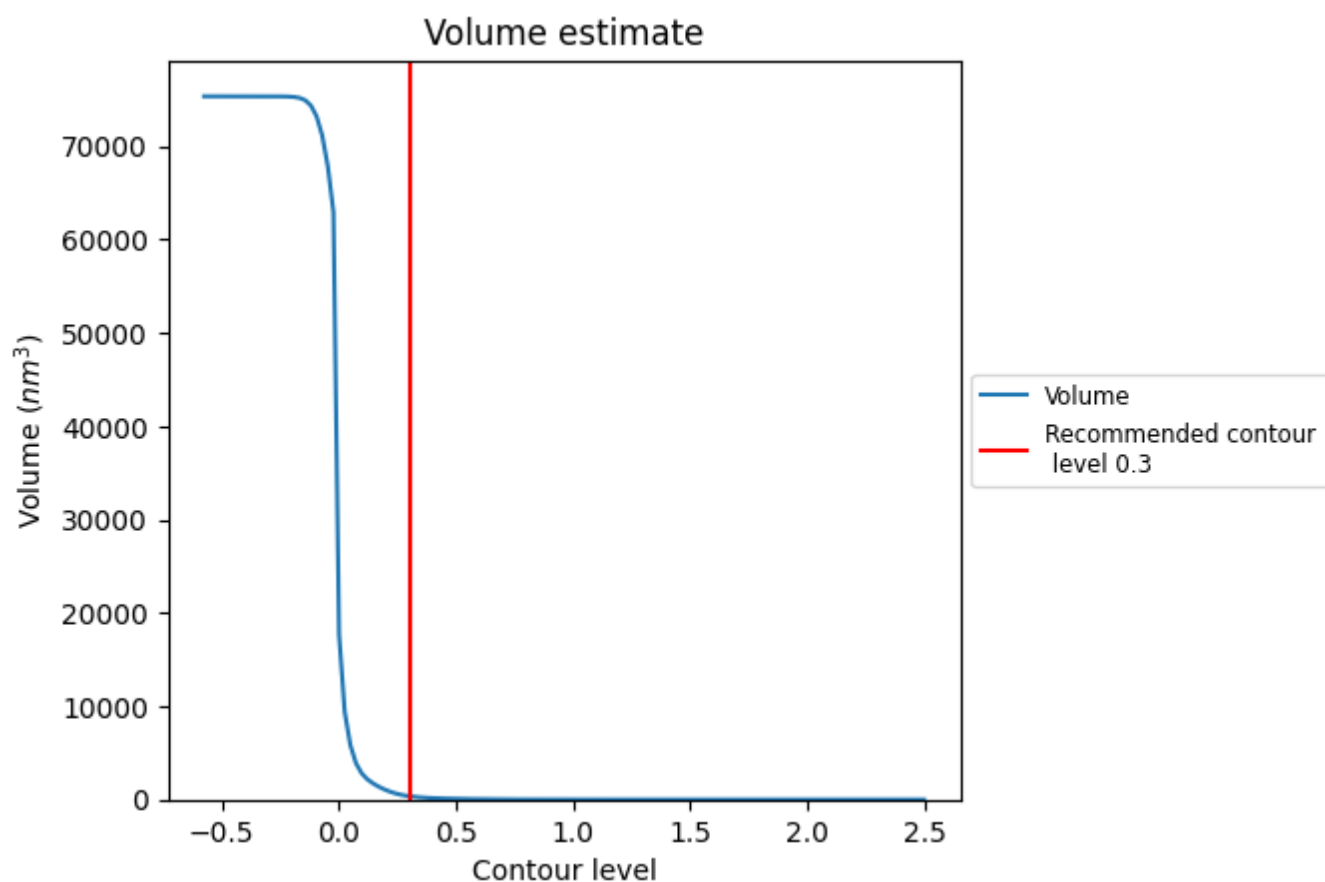
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

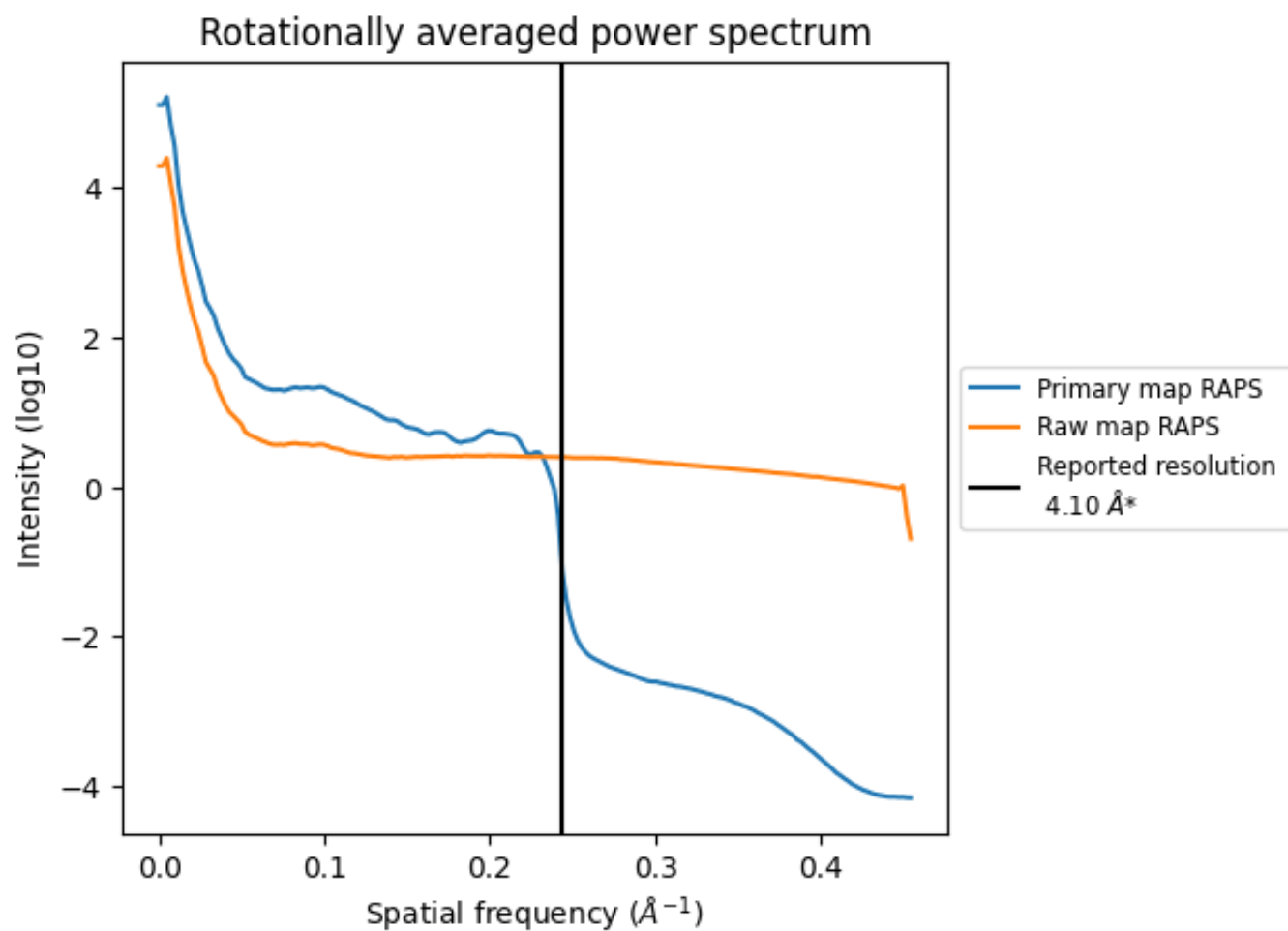
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 361 nm³; this corresponds to an approximate mass of 326 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 ⓘ

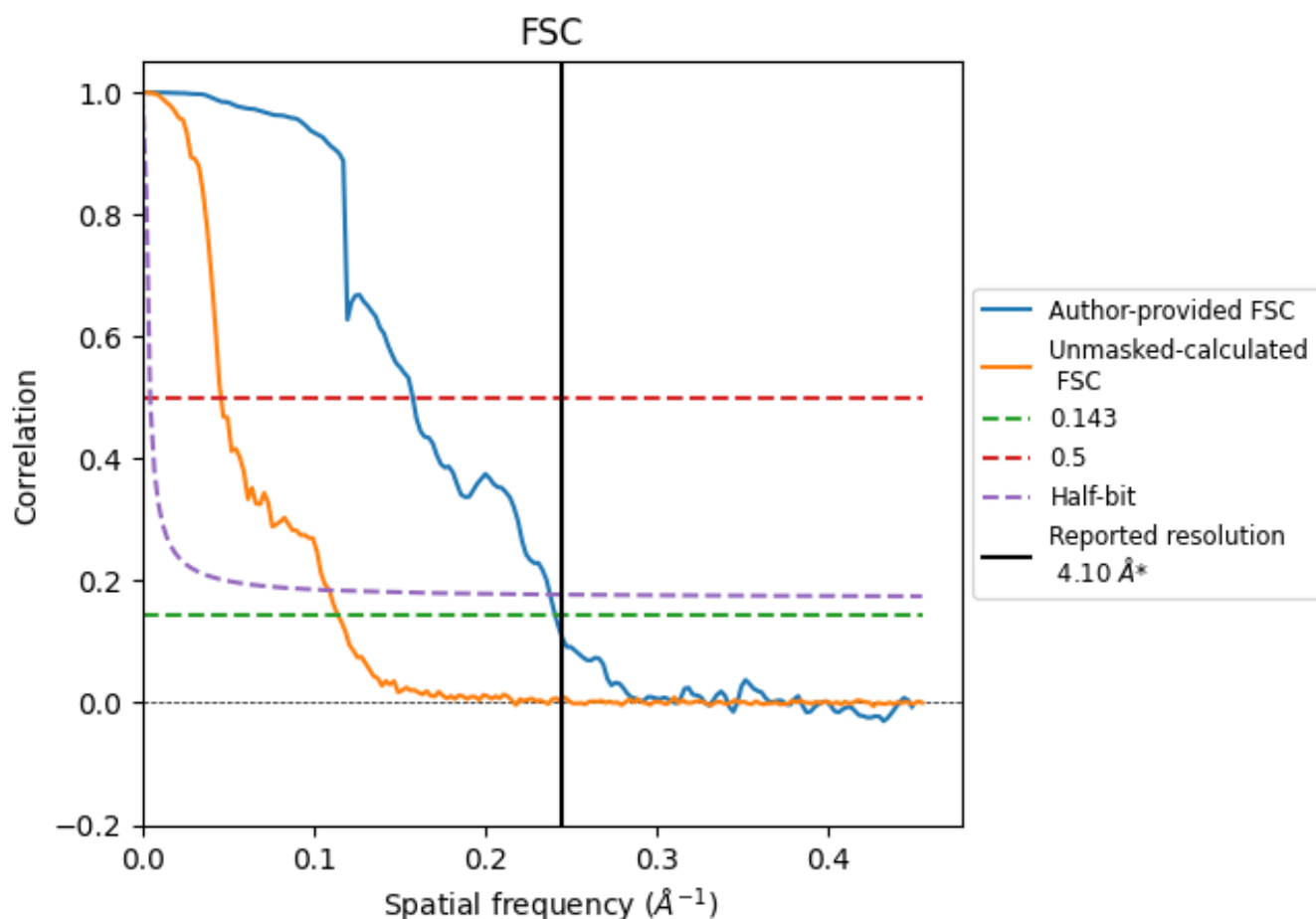


*Reported resolution corresponds to spatial frequency of 0.244 $\text{\AA}^{-1}$

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 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

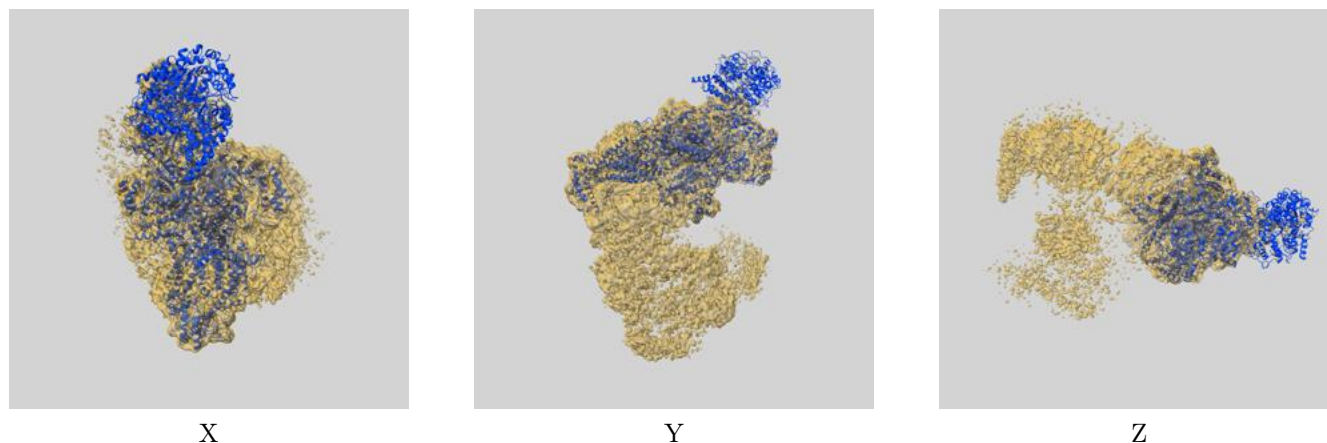
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.15	6.34	4.21
Unmasked-calculated*	8.76	21.79	9.17

*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 8.76 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

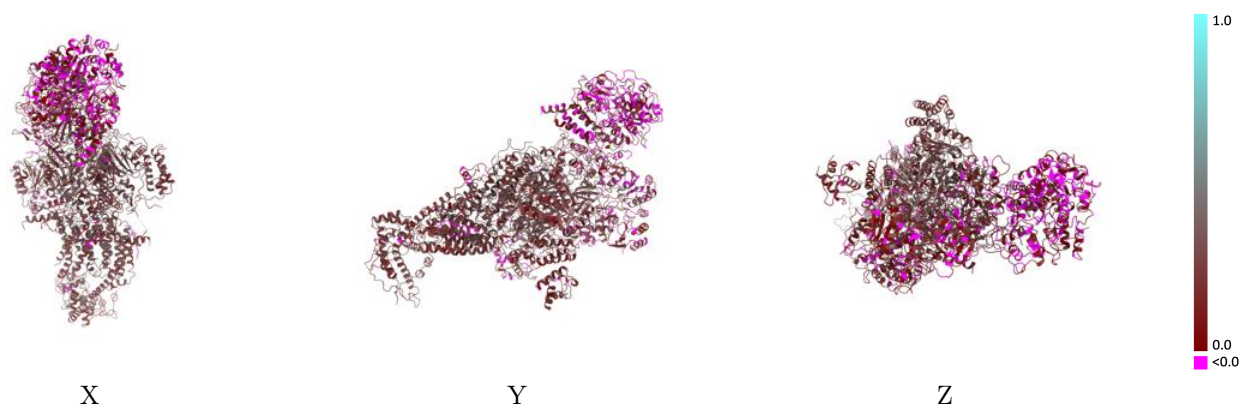
This section contains information regarding the fit between EMDB map EMD-38514 and PDB model 8XNT. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



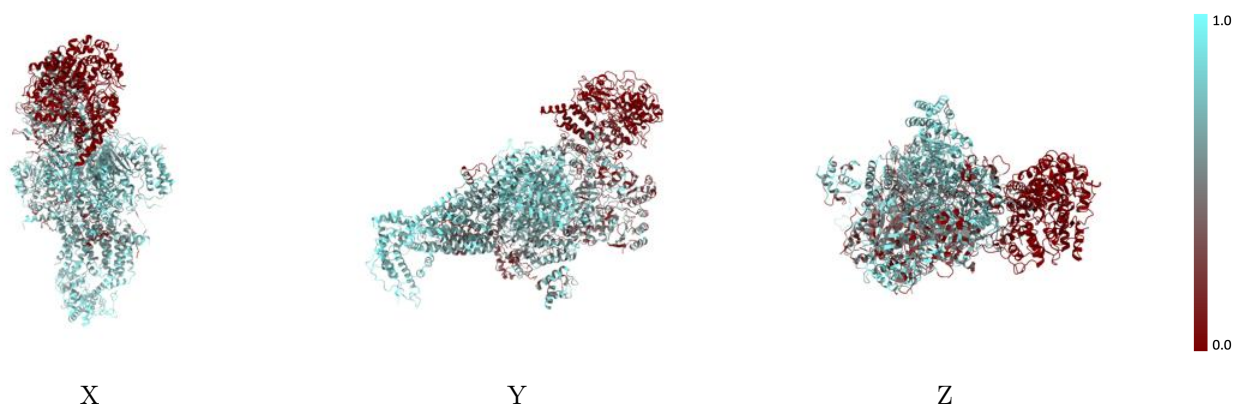
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



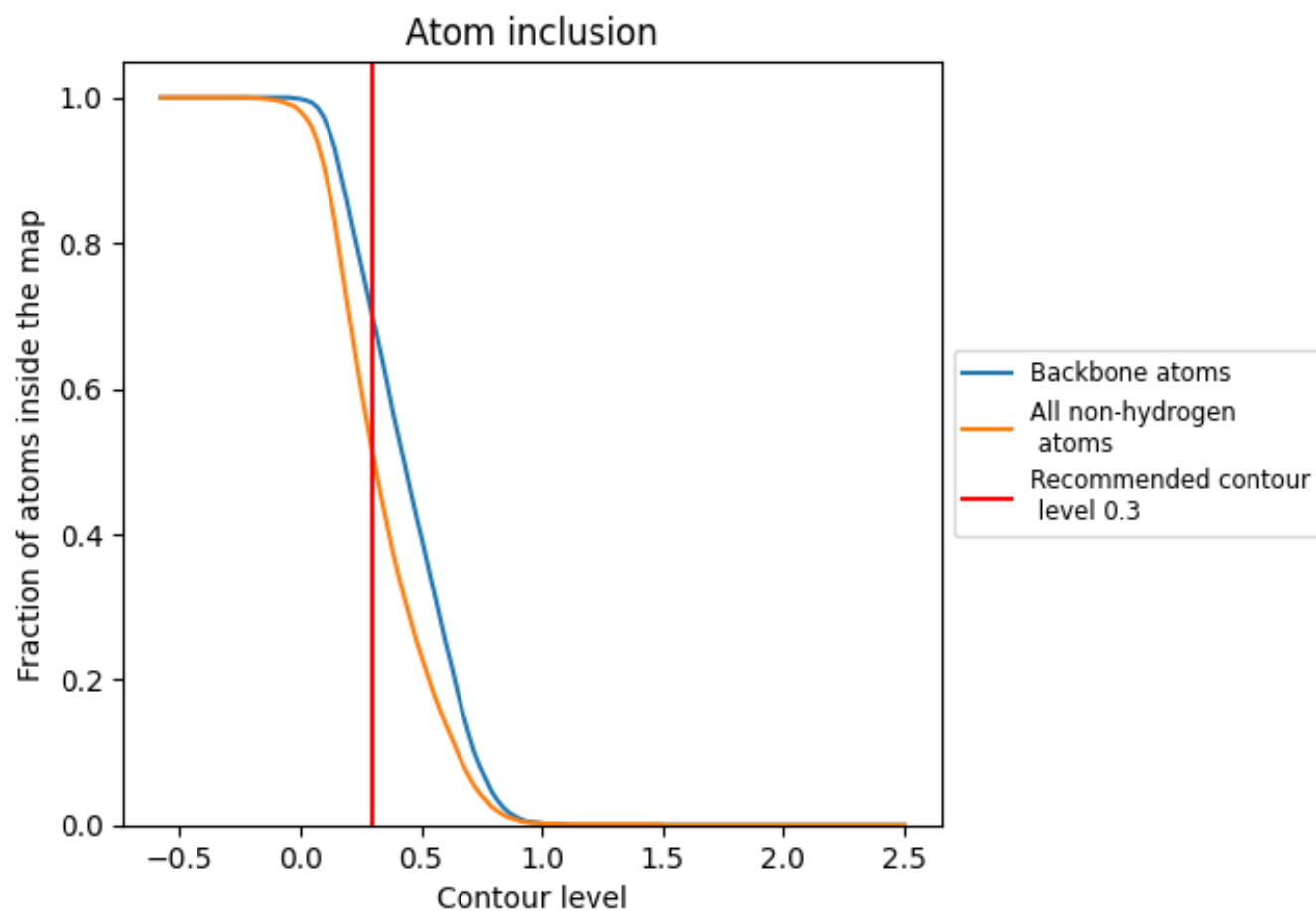
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 70% of all backbone atoms, 51% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5110	 0.2000
A	 0.5880	 0.2580
B	 0.7130	 0.3070
C	 0.6820	 0.2810
D	 0.7120	 0.2920
E	 0.0190	 0.0600
F	 0.0450	 0.0430
G	 0.4460	 0.1560
H	 0.6430	 0.2810
I	 0.7460	 0.2870
P	 0.5320	 0.1790
Q	 0.3430	 0.1900
R	 0.4140	 0.1810
S	 0.4380	 0.1070
T	 0.5790	 0.1680
V	 0.7420	 0.2520
W	 0.5710	 0.2030
X	 0.7930	 0.2540
Z	 0.7640	 0.2690
a	 0.7310	 0.2560
b	 0.7240	 0.2450
q	 0.2040	 0.1990
r	 0.3870	 0.1680
s	 0.0000	 0.0640

