



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:42 AM UTC

PDB ID : 8XNQ / pdb_00008xnq
EMDB ID : EMD-38511
Title : Respiratory complex Peripheral Arm of CI, open form A, focus-refined map of type IA, Wild type mouse under Cold Acclimation
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-12-30
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

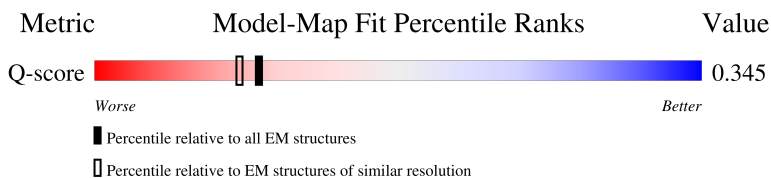
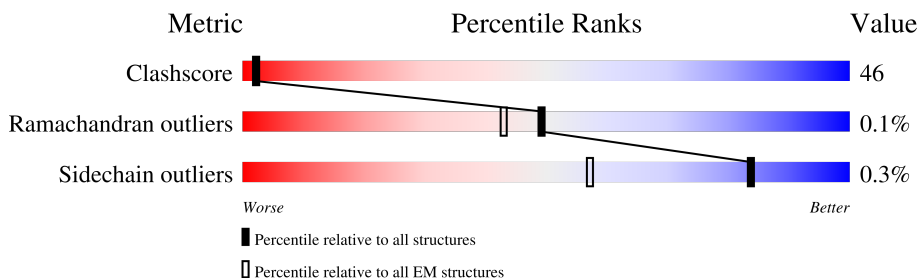
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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

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

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	FES	E	301	-	-	X	-
28	FES	G	803	-	-	X	-
34	CDL	q	201	-	-	X	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 33919 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	92	Total	C	N	O	S	0	0
			754	523	107	119	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	314	Total	C	N	O	S	0	0
			2510	1687	380	421	22		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	66	Total	C	N	O	S	0	0
			539	351	96	88	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	80	Total	C	N	O	S	0	0
			628	414	99	111	4		

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

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

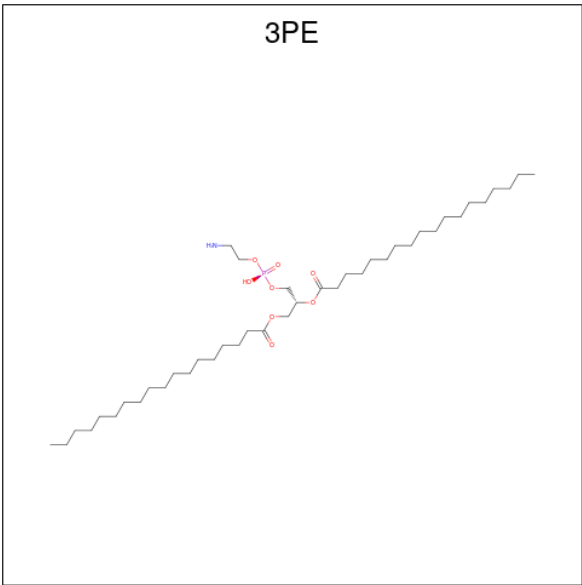
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	51	Total	C	N	O	S	0	0
			418	266	78	73	1		

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

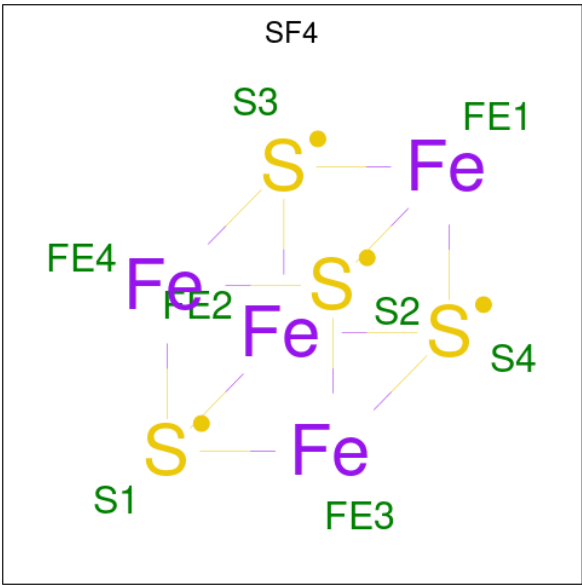
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	13	Total	C	N	O	0	0
			107	69	15	23		

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



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
24	b	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



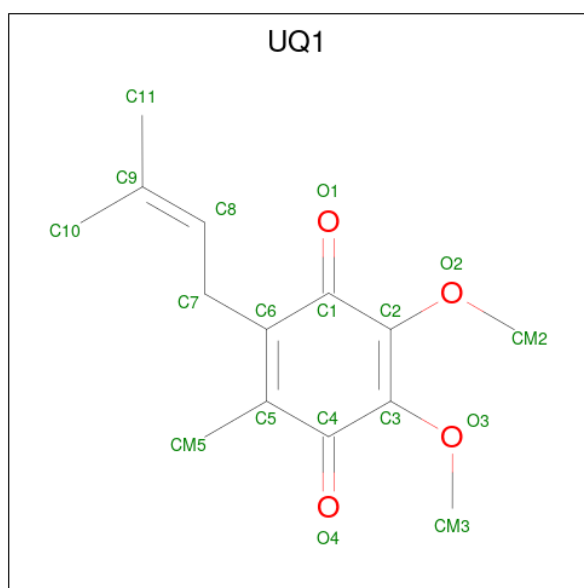
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	Fe	S	0
			8	4	4	

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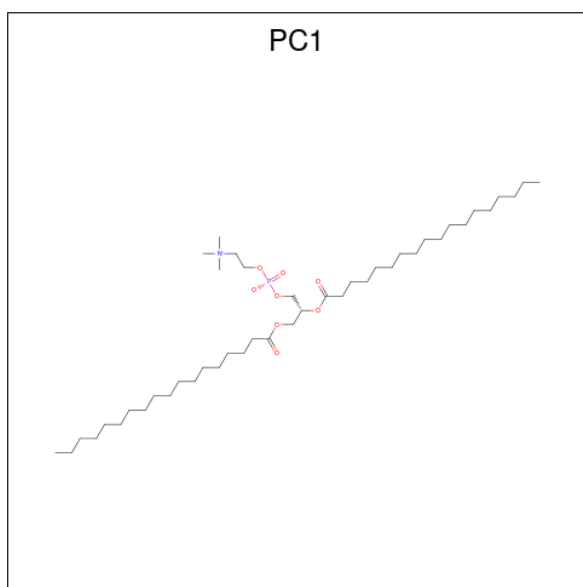
Mol	Chain	Residues	Atoms			AltConf
25	F	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



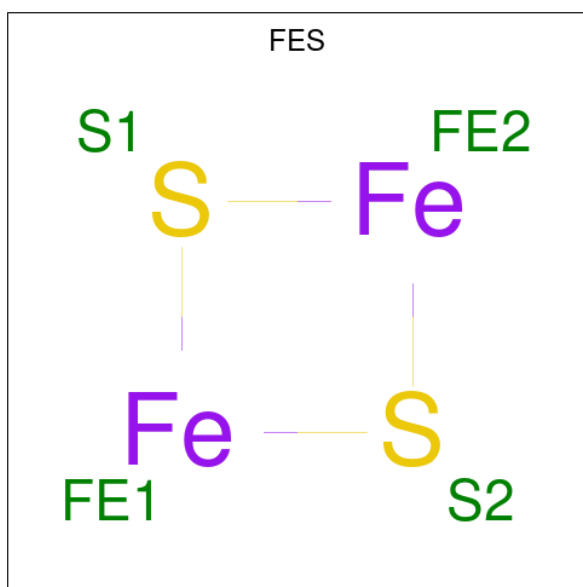
Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total	C	O	0
			18	14	4	

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



Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
27	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
27	I	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 28 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



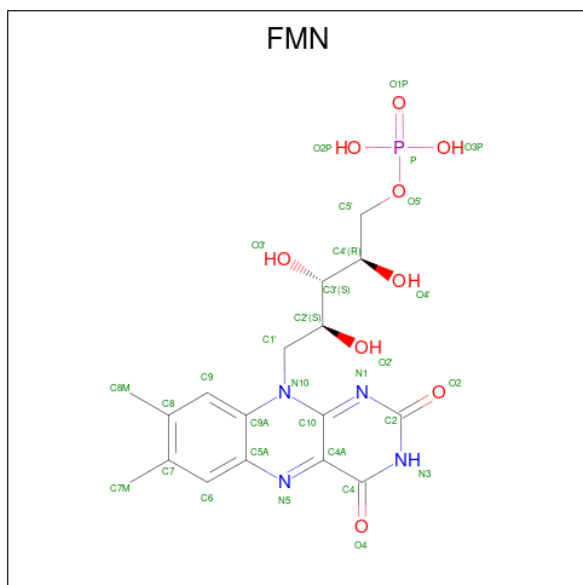
Mol	Chain	Residues	Atoms			AltConf
28	E	1	Total	Fe	S	0
			4	2	2	

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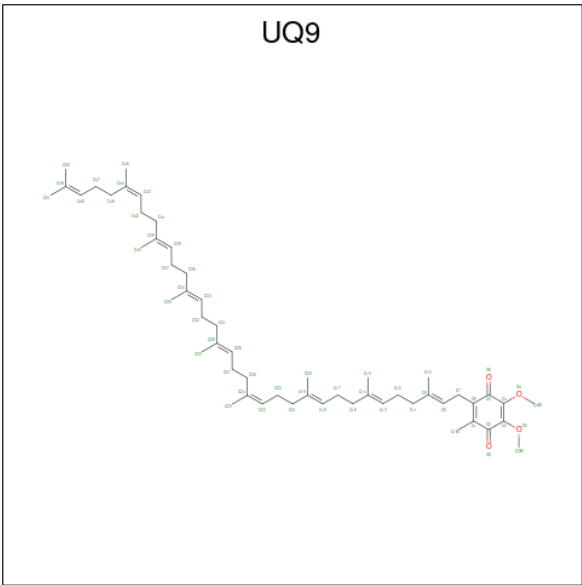
Mol	Chain	Residues	Atoms			AltConf
28	G	1	Total	Fe	S	0
			4	2	2	

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



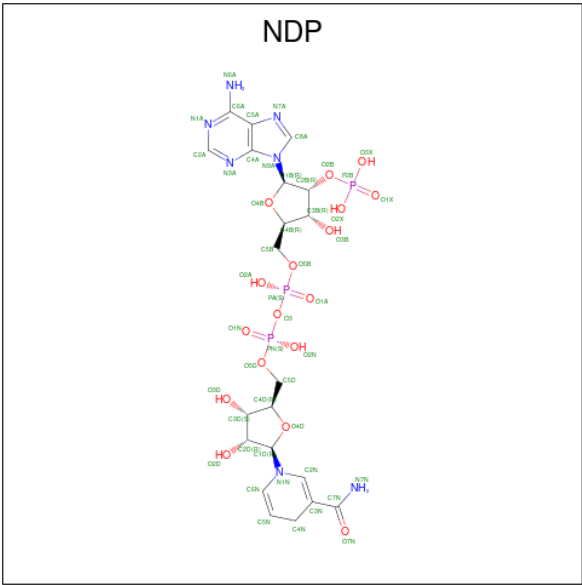
Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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



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

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

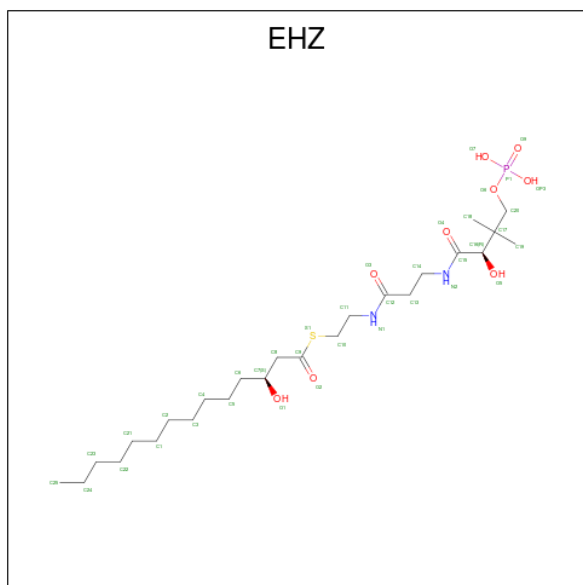


Mol	Chain	Residues	Atoms					AltConf
31	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

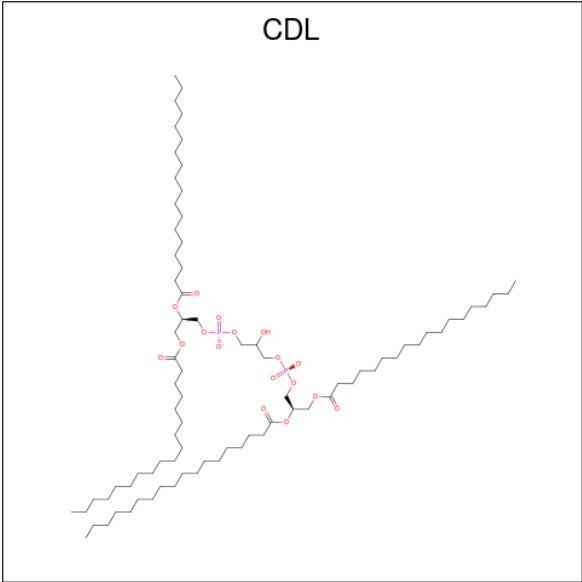
Mol	Chain	Residues	Atoms		AltConf
32	R	1	Total	Zn	0
			1	1	

- Molecule 33 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).

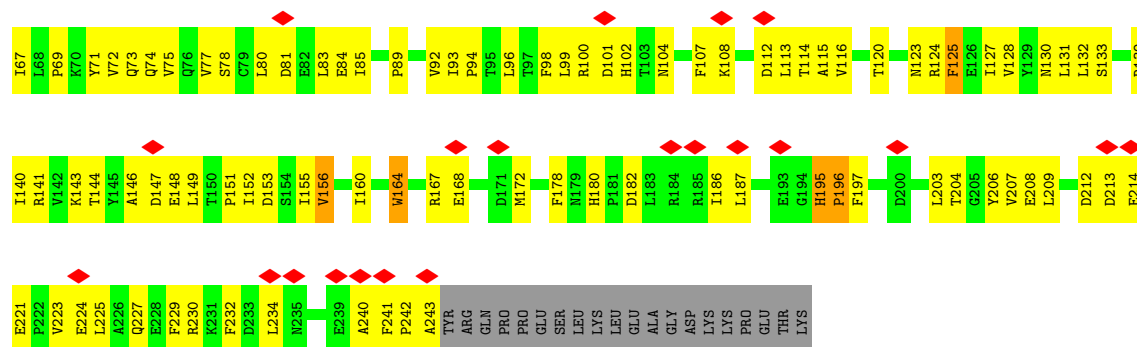


Mol	Chain	Residues	Atoms						AltConf
33	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

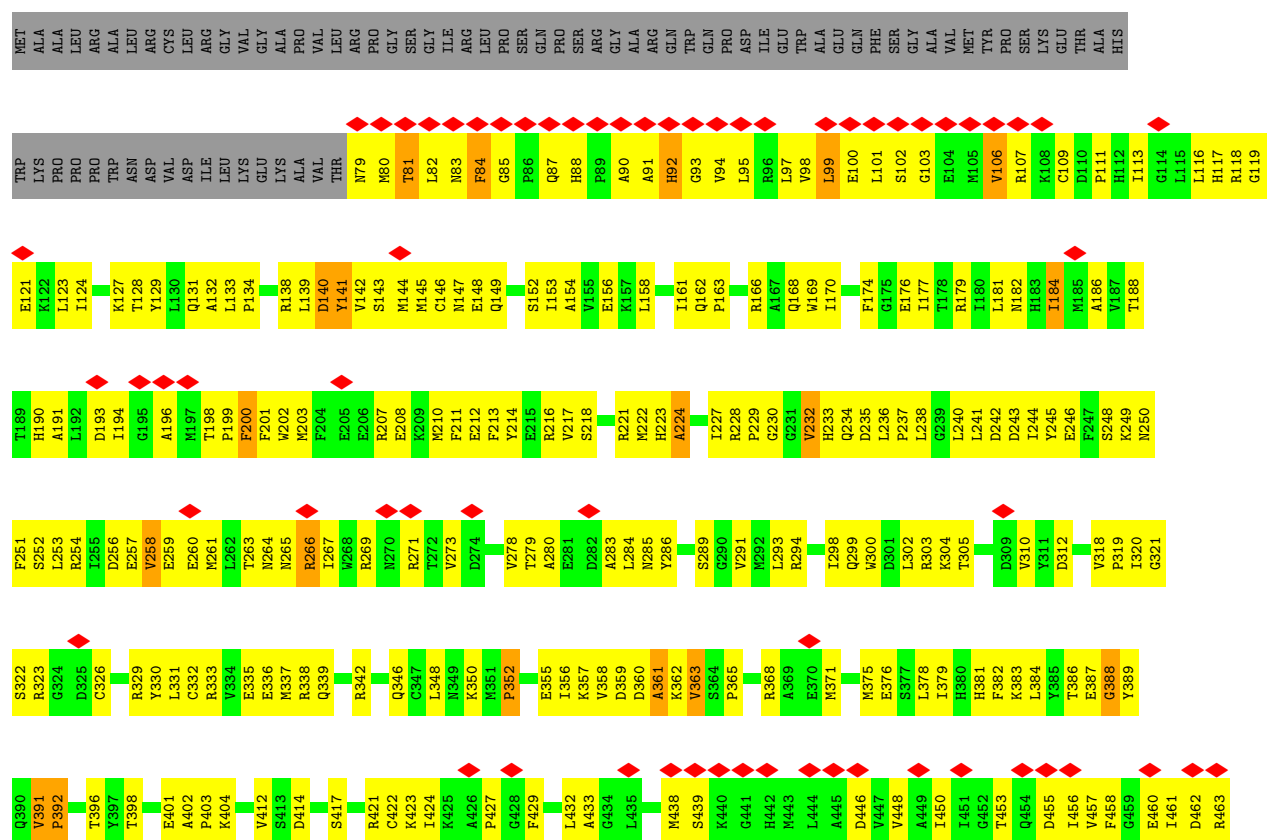
- Molecule 34 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



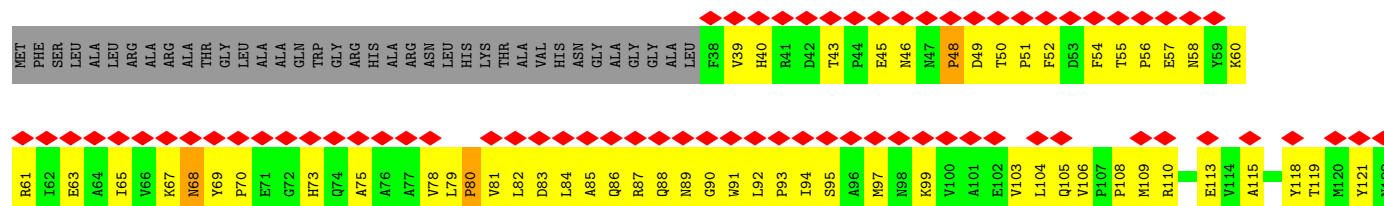
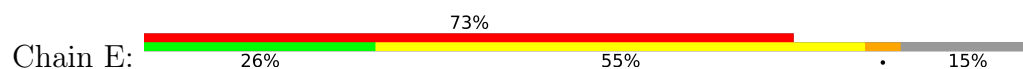
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
34	q	1	57	38	17	2	0

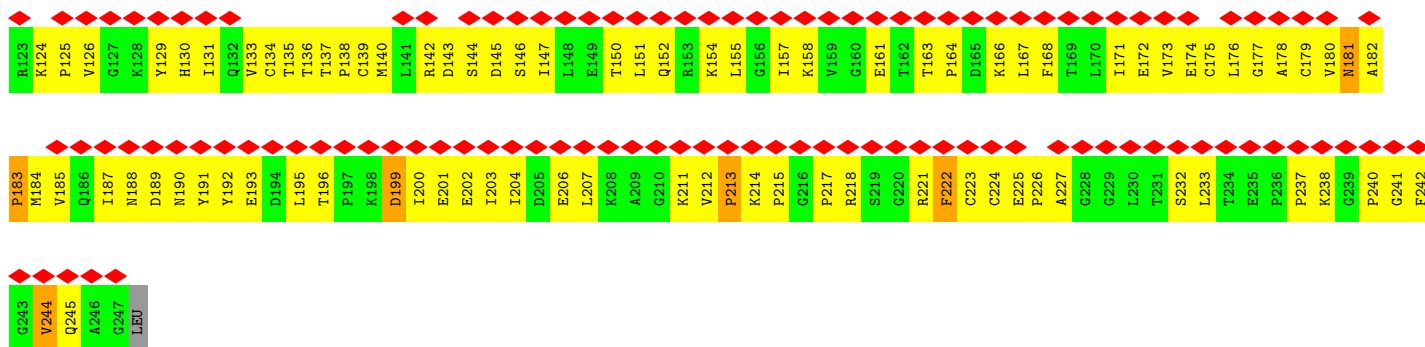


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

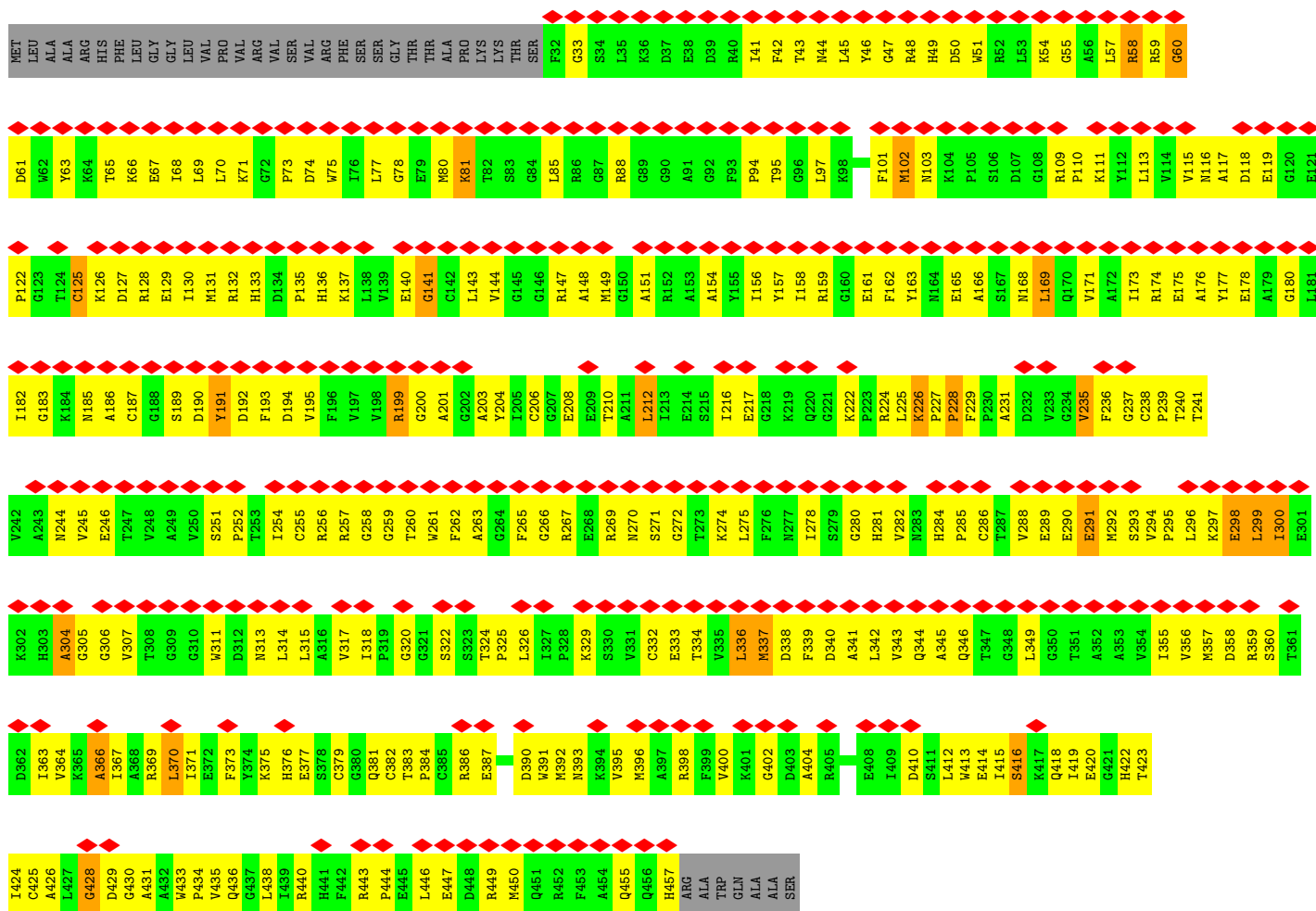


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

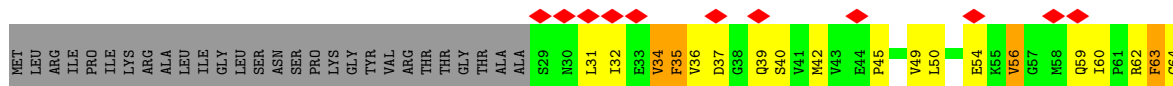


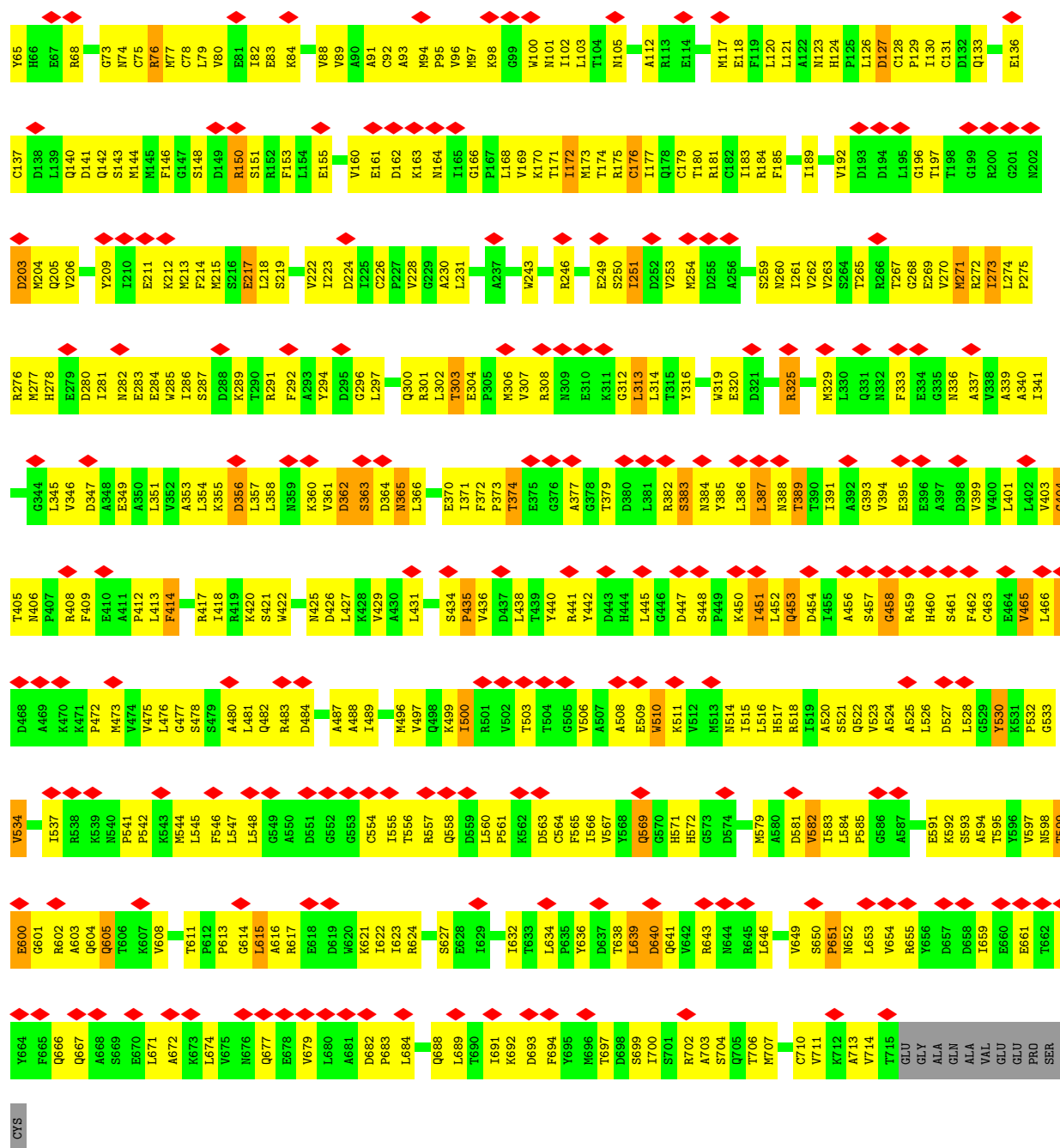


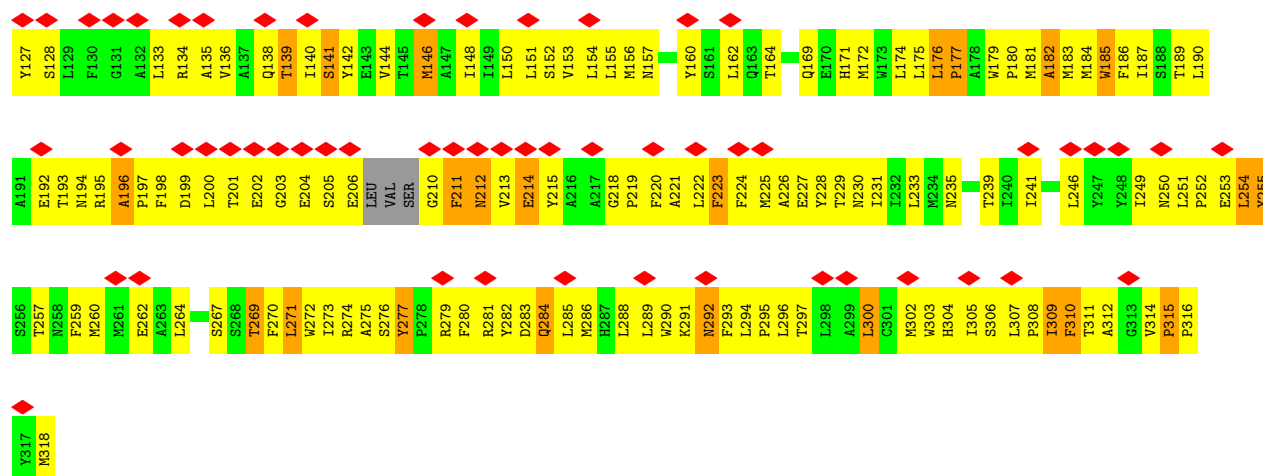
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



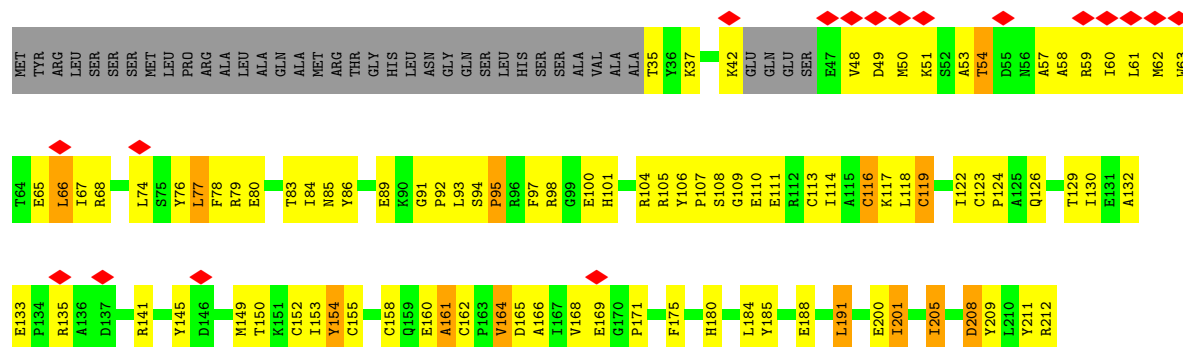
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



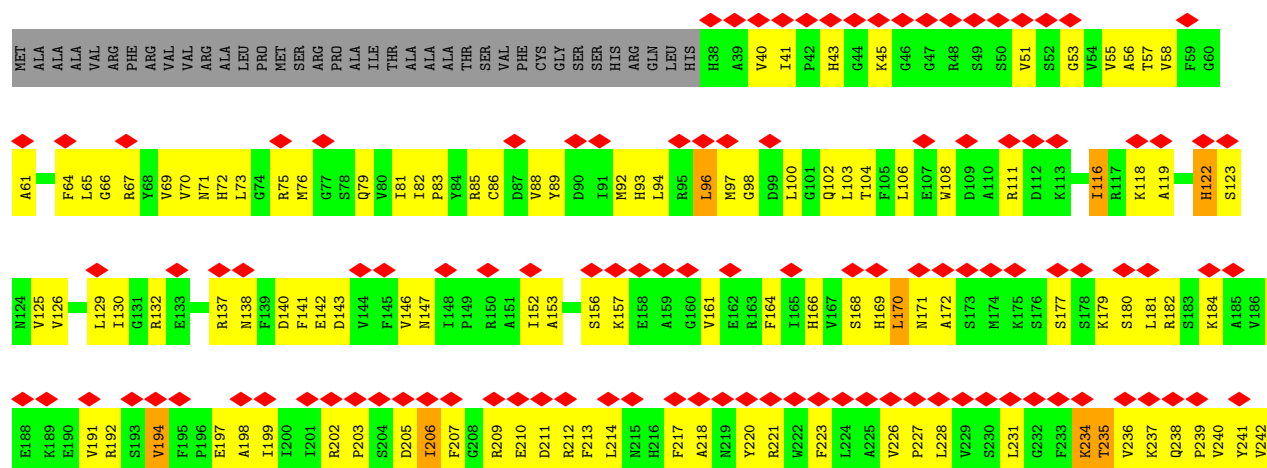




- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

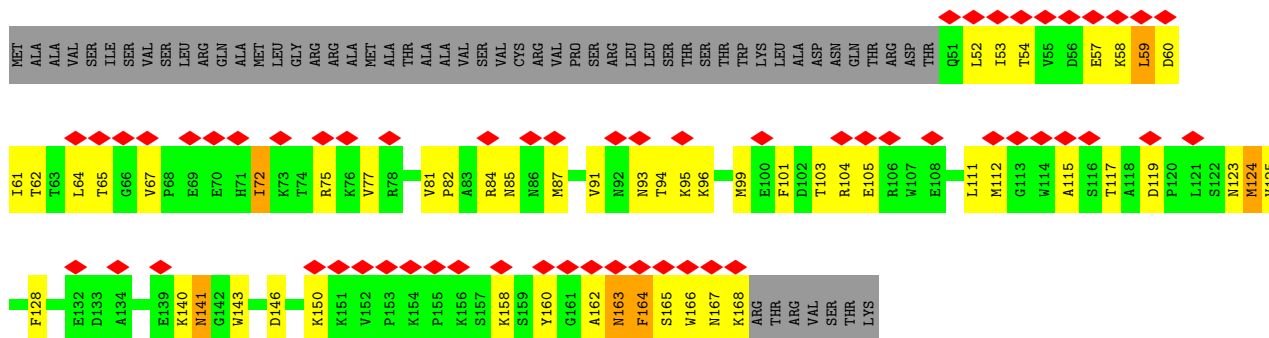


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

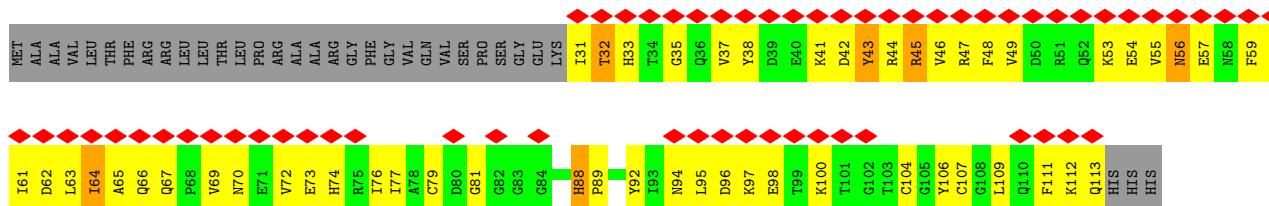
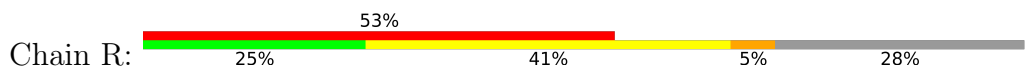




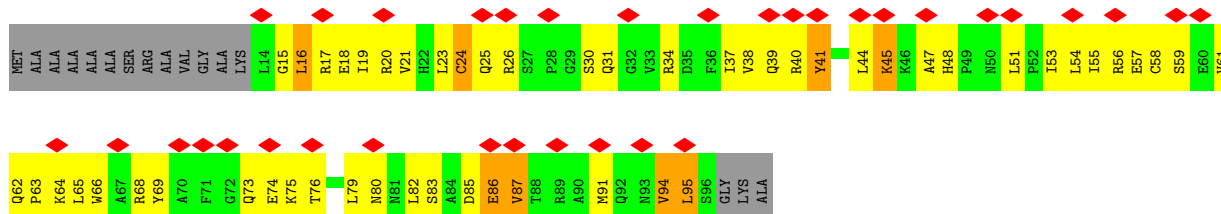
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



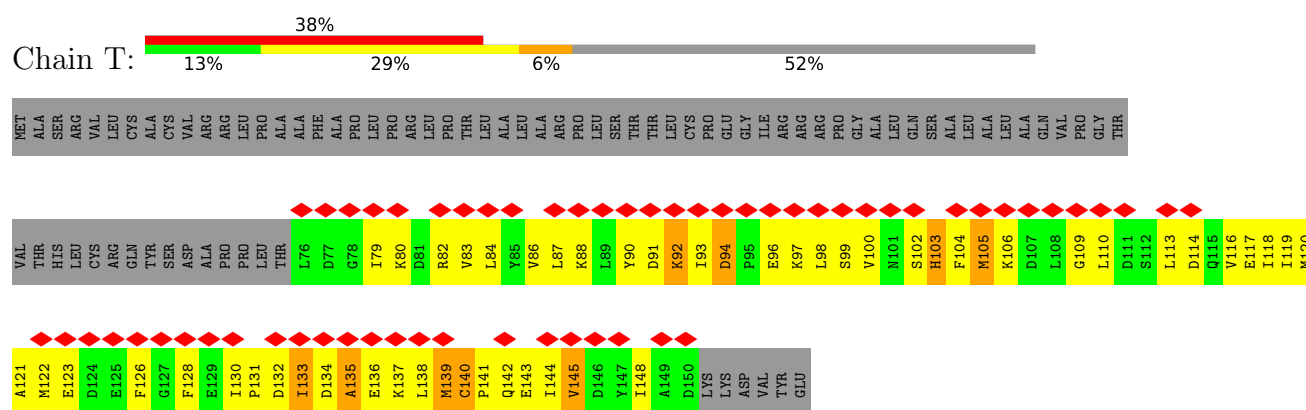
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



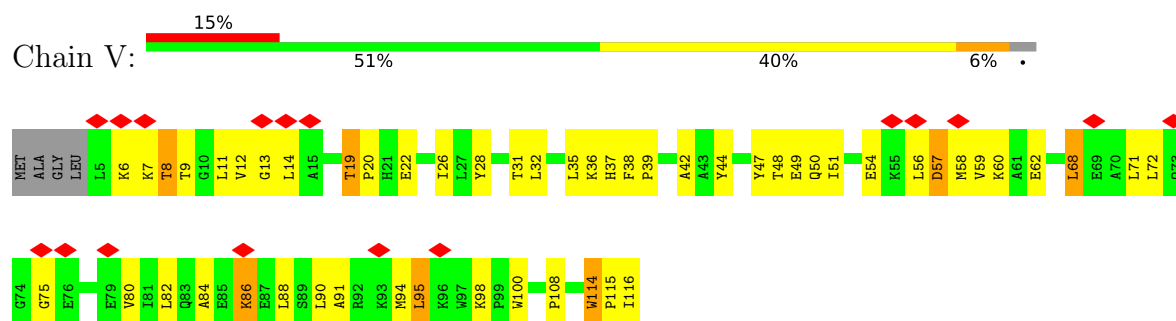
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



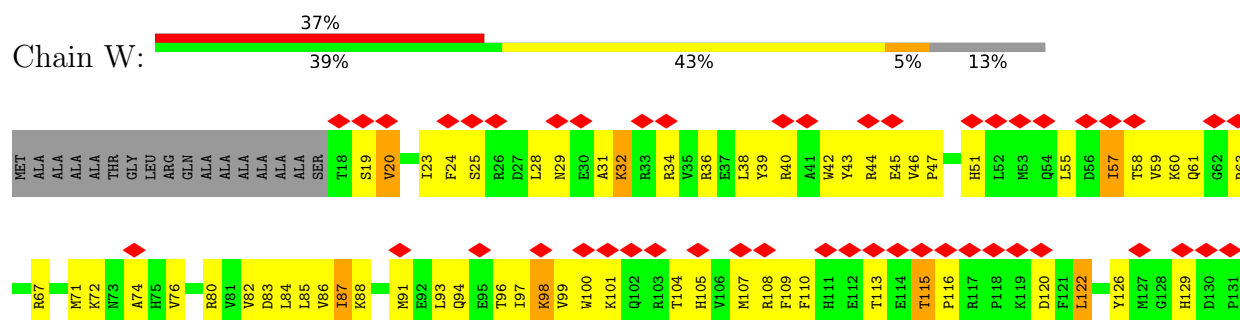
- Molecule 14: Acyl carrier protein, mitochondrial



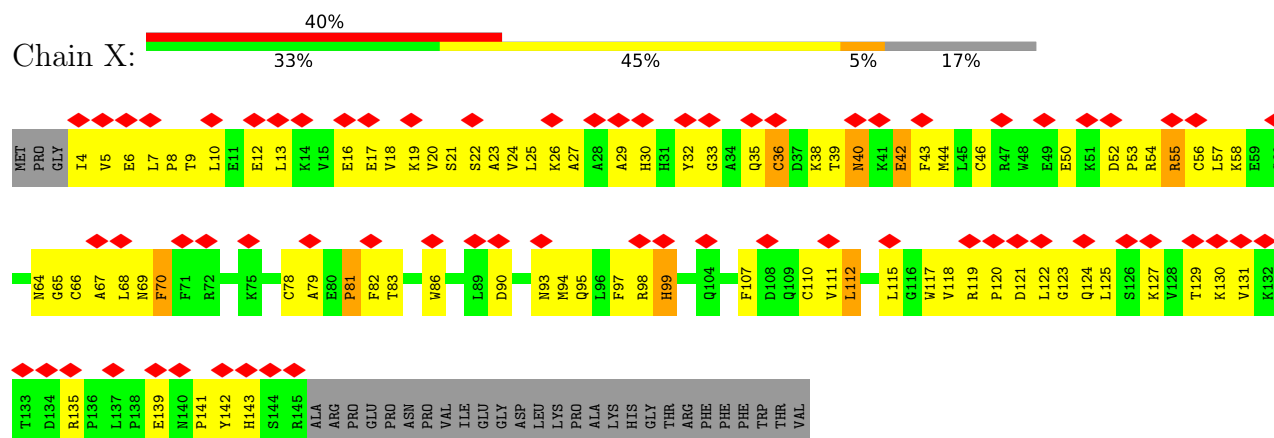
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



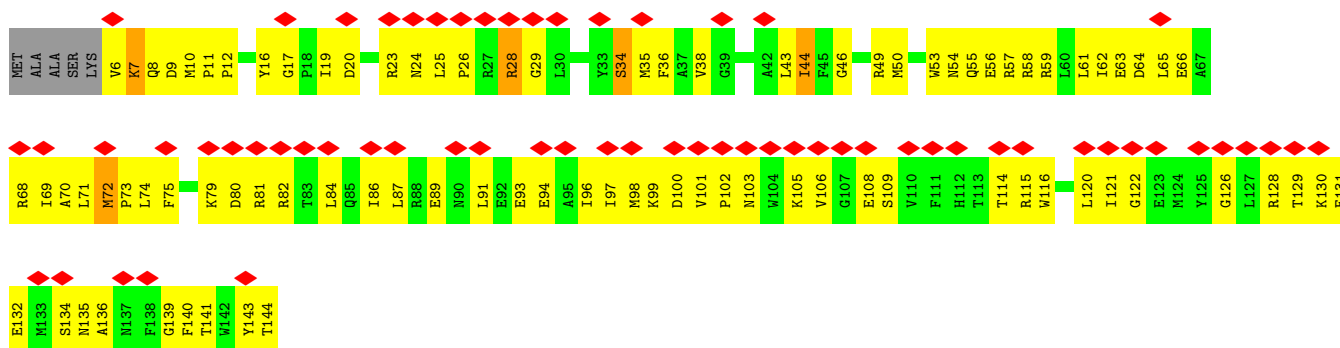
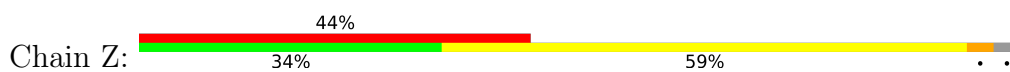
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



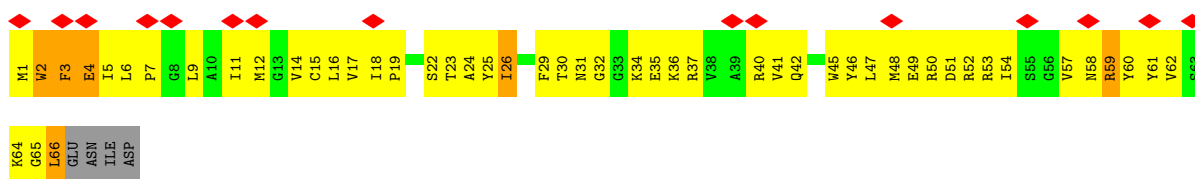
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



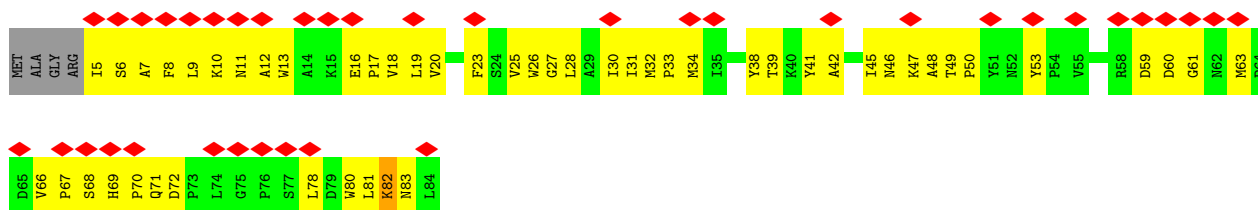
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



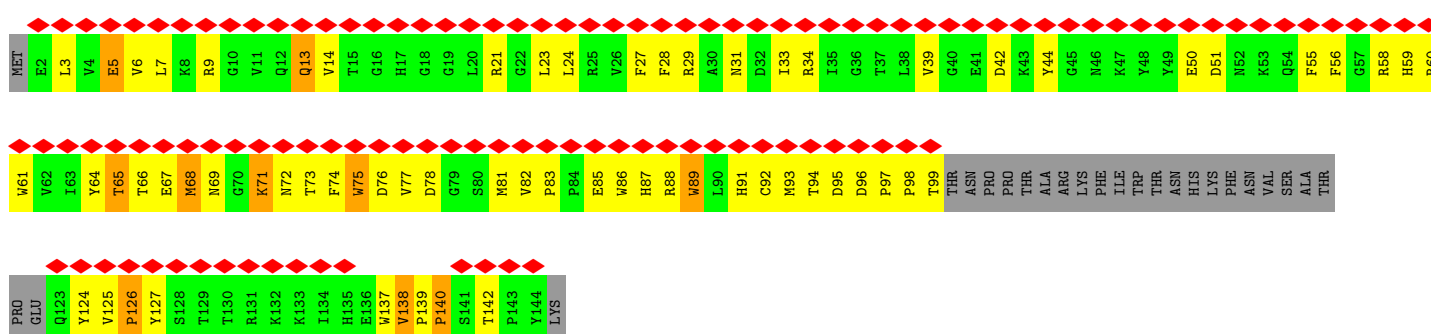
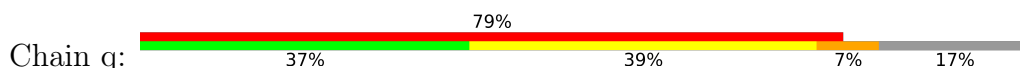
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



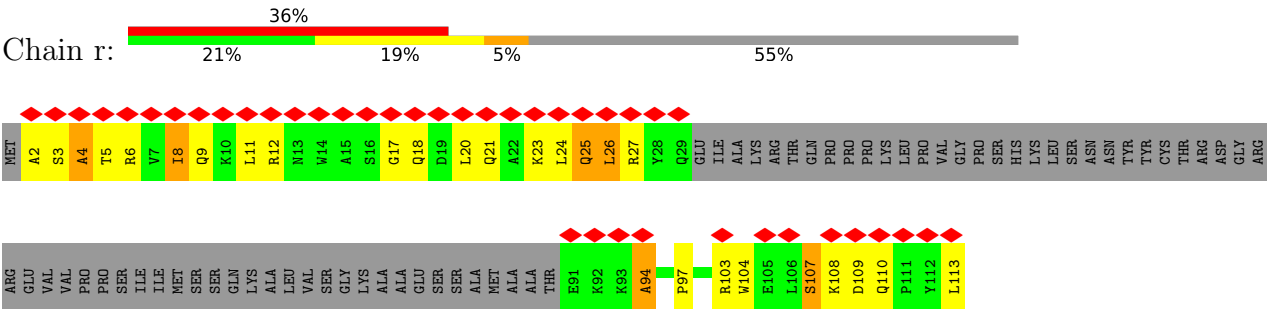
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



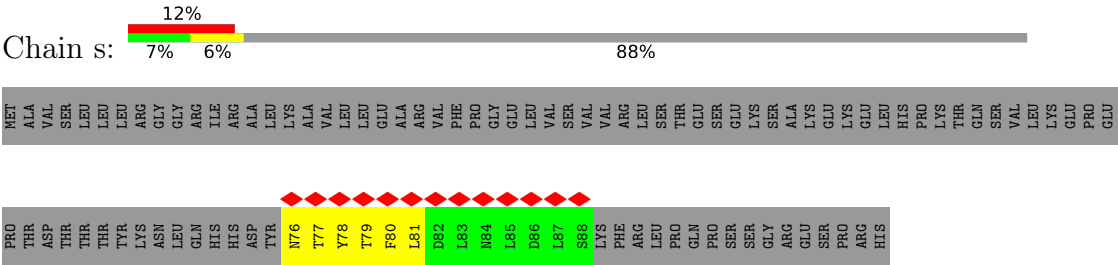
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31517	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.506	Depositor
Minimum map value	-1.026	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.55	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EHZ, FES, PC1, UQ9, UQ1, FMN, 3PE, NDP, CDL, 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	0.83	0/774	1.33	11/1056 (1.0%)
2	B	0.96	1/1289 (0.1%)	1.35	12/1744 (0.7%)
3	C	0.87	1/1687 (0.1%)	1.31	14/2297 (0.6%)
4	D	0.96	5/3162 (0.2%)	1.35	29/4276 (0.7%)
5	E	0.81	2/1675 (0.1%)	1.25	14/2282 (0.6%)
6	F	0.88	1/3363 (0.0%)	1.44	54/4543 (1.2%)
7	G	0.89	6/5374 (0.1%)	1.59	104/7281 (1.4%)
8	H	0.93	3/2585 (0.1%)	1.51	57/3529 (1.6%)
9	I	0.90	0/1427	1.54	18/1927 (0.9%)
10	P	0.79	1/2804 (0.0%)	1.26	34/3802 (0.9%)
11	Q	0.87	1/980 (0.1%)	1.29	12/1324 (0.9%)
12	R	0.63	0/671	1.19	9/903 (1.0%)
13	S	0.93	1/678 (0.1%)	1.65	17/915 (1.9%)
14	T	0.91	0/613	1.51	9/826 (1.1%)
15	V	0.87	0/937	1.47	14/1270 (1.1%)
16	W	0.80	0/993	1.32	15/1335 (1.1%)
17	X	0.84	1/1191 (0.1%)	1.45	21/1605 (1.3%)
18	Z	0.76	0/1183	1.11	7/1597 (0.4%)
19	a	0.85	1/552 (0.2%)	1.26	5/743 (0.7%)
20	b	0.70	0/651	0.91	1/895 (0.1%)
21	q	0.96	1/1037 (0.1%)	1.44	15/1408 (1.1%)
22	r	0.98	1/426 (0.2%)	1.57	9/573 (1.6%)
23	s	0.75	0/108	1.08	0/147
All	All	0.87	26/34160 (0.1%)	1.41	481/46278 (1.0%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	235	VAL	N-CA	-9.29	1.34	1.46
11	Q	53	ILE	C-O	7.75	1.33	1.24
7	G	203	ASP	CA-C	6.72	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	106	VAL	C-N	-6.54	1.24	1.33
7	G	600	GLU	CA-C	6.47	1.61	1.52
4	D	266	ARG	C-O	-6.28	1.16	1.24
2	B	110	PRO	C-O	-6.25	1.16	1.24
7	G	127	ASP	CA-C	6.25	1.62	1.52
7	G	76	ARG	CA-C	6.22	1.61	1.53
17	X	54	ARG	CA-C	5.96	1.60	1.52
5	E	93	PRO	N-CD	-5.92	1.39	1.47
7	G	361	VAL	CA-C	5.91	1.60	1.52
8	H	60	PRO	N-CD	5.78	1.55	1.47
22	r	25	GLN	CA-C	5.76	1.60	1.52
5	E	80	PRO	N-CD	5.68	1.55	1.47
4	D	392	PRO	C-O	-5.60	1.20	1.24
13	S	95	LEU	CA-C	5.53	1.59	1.52
4	D	107	ARG	C-N	5.50	1.40	1.33
7	G	683	PRO	N-CD	-5.43	1.40	1.47
21	q	126	PRO	N-CD	5.40	1.55	1.47
8	H	211	PHE	CA-C	5.36	1.59	1.52
10	P	235	THR	CA-C	5.27	1.59	1.53
4	D	266	ARG	CA-C	-5.25	1.45	1.52
3	C	61	GLY	C-N	-5.07	1.27	1.33
19	a	59	ARG	C-N	-5.03	1.27	1.33
8	H	310	PHE	CA-C	5.02	1.59	1.52

All (481) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	174	THR	N-CA-C	-16.80	89.11	114.64
7	G	251	ILE	N-CA-C	13.33	126.83	108.17
7	G	77	MET	N-CA-C	-13.06	97.31	113.38
9	I	164	VAL	N-CA-C	-12.87	100.09	112.83
7	G	500	ILE	N-CA-C	-12.52	98.76	110.53
6	F	171	VAL	N-CA-C	-11.85	99.39	110.53
7	G	204	MET	N-CA-C	-11.67	91.40	109.25
6	F	449	ARG	N-CA-C	-11.57	98.74	111.36
11	Q	60	ASP	N-CA-C	-11.33	90.32	109.24
7	G	599	THR	N-CA-C	11.31	126.19	112.38
13	S	39	GLN	N-CA-C	11.15	125.41	111.69
15	V	57	ASP	N-CA-C	-11.08	99.21	111.07
16	W	87	ILE	N-CA-C	-11.03	99.83	110.42
8	H	259	PHE	N-CA-C	-10.99	99.38	111.36
1	A	54	LYS	N-CA-C	-10.98	98.18	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	70	PHE	N-CA-C	-10.62	99.71	111.07
4	D	142	VAL	N-CA-C	-10.55	99.50	111.00
14	T	139	MET	N-CA-C	-10.44	97.39	113.89
9	I	77	LEU	N-CA-C	-10.43	99.72	111.71
5	E	68	ASN	N-CA-C	-10.36	99.99	111.07
8	H	284	GLN	N-CA-C	-10.36	99.99	111.07
2	B	195	PRO	N-CA-C	-10.35	98.08	110.70
16	W	59	VAL	N-CA-C	-10.32	100.51	110.42
19	a	4	GLU	N-CA-C	10.27	124.91	112.38
7	G	280	ASP	N-CA-C	10.26	122.47	111.28
4	D	140	ASP	CB-CA-C	-10.25	97.99	111.42
10	P	366	ILE	N-CA-C	10.24	121.06	110.62
4	D	337	MET	N-CA-C	-10.22	100.14	111.07
7	G	414	PHE	N-CA-C	-10.08	101.48	113.88
9	I	161	ALA	N-CA-C	10.06	122.25	111.28
14	T	135	ALA	N-CA-C	-10.03	100.35	111.28
7	G	325	ARG	N-CA-C	-9.89	100.19	110.97
9	I	166	ALA	N-CA-C	-9.86	100.79	113.12
6	F	178	GLU	N-CA-C	-9.86	99.28	111.11
6	F	141	GLY	N-CA-C	-9.80	101.14	112.50
6	F	103	ASN	N-CA-C	-9.78	101.04	113.16
7	G	654	VAL	N-CA-C	9.75	123.28	111.09
6	F	144	VAL	N-CA-C	-9.75	101.37	110.53
7	G	35	PHE	N-CA-C	9.69	124.37	108.96
6	F	418	GLN	N-CA-C	-9.60	100.77	111.14
7	G	337	ALA	N-CA-C	-9.58	100.80	114.12
8	H	52	ALA	N-CA-C	-9.49	100.92	111.07
19	a	2	TRP	N-CA-C	-9.49	101.63	113.01
4	D	427	PRO	N-CA-C	-9.48	95.62	110.50
7	G	692	LYS	N-CA-C	-9.36	100.44	112.23
14	T	133	ILE	N-CA-C	9.36	119.90	110.82
7	G	694	PHE	N-CA-C	9.34	121.46	111.28
10	P	367	GLU	N-CA-C	9.28	122.58	111.82
7	G	640	ASP	N-CA-C	-9.23	101.30	111.36
10	P	157	LYS	N-CA-C	-9.15	101.38	111.36
7	G	389	THR	N-CA-C	-9.15	96.24	109.96
5	E	85	ALA	N-CA-C	-9.13	101.41	111.36
17	X	55	ARG	N-CA-C	9.00	129.97	110.80
7	G	133	GLN	N-CA-CB	8.78	121.51	110.45
7	G	365	ASN	N-CA-C	-8.73	102.18	112.92
9	I	154	TYR	N-CA-CB	-8.70	99.18	111.62
8	H	60	PRO	N-CA-CB	8.70	108.56	102.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	212	LYS	N-CA-C	-8.69	94.74	108.90
10	P	96	LEU	N-CA-C	8.65	121.65	111.71
8	H	212	ASN	N-CA-C	-8.63	101.87	114.39
16	W	20	VAL	N-CA-C	8.63	120.70	108.36
12	R	57	GLU	N-CA-C	-8.51	98.26	110.59
13	S	86	GLU	N-CA-C	-8.51	102.09	111.36
10	P	373	LYS	N-CA-C	8.49	121.90	110.35
17	X	99	HIS	N-CA-C	-8.46	102.14	111.36
13	S	18	GLU	N-CA-C	8.45	123.18	109.40
16	W	100	TRP	N-CA-C	-8.42	99.92	112.04
11	Q	54	THR	N-CA-C	8.36	123.33	109.46
3	C	108	LYS	N-CA-C	8.36	120.01	111.07
7	G	452	LEU	N-CA-C	-8.35	102.17	111.28
16	W	57	ILE	N-CA-C	8.35	122.03	109.17
8	H	141	SER	N-CA-C	-8.32	102.16	111.07
7	G	558	GLN	N-CA-C	-8.25	102.24	111.07
8	H	311	THR	N-CA-C	-8.25	102.52	112.59
1	A	55	PHE	N-CA-C	-8.25	102.24	111.07
8	H	196	ALA	N-CA-C	8.24	128.02	109.81
7	G	691	ILE	N-CA-C	8.18	123.66	111.89
3	C	196	PRO	N-CA-C	8.16	124.88	113.53
15	V	86	LYS	N-CA-C	-8.16	102.33	111.14
16	W	96	THR	N-CA-C	-8.15	102.33	111.14
6	F	298	GLU	N-CA-C	8.13	120.14	111.28
7	G	484	ASP	N-CA-C	8.13	121.06	111.71
2	B	110	PRO	N-CA-C	8.12	124.61	113.65
6	F	191	TYR	N-CA-C	8.08	121.64	110.24
17	X	43	PHE	N-CA-C	-8.06	102.43	111.14
7	G	500	ILE	N-CA-CB	8.04	120.86	110.57
7	G	534	VAL	N-CA-C	-8.02	104.78	111.91
1	A	64	LEU	N-CA-C	-8.01	102.50	111.07
1	A	9	ILE	N-CA-C	-8.00	102.46	110.62
9	I	201	ILE	N-CA-C	-7.98	102.66	110.72
13	S	76	THR	N-CA-C	7.98	121.90	108.90
17	X	46	CYS	N-CA-C	-7.97	102.67	111.36
16	W	98	LYS	N-CA-C	-7.96	101.61	113.72
10	P	206	ILE	N-CA-C	7.95	120.96	108.87
8	H	271	LEU	N-CA-C	-7.94	102.56	111.14
17	X	112	LEU	N-CA-C	-7.94	102.57	111.14
21	q	67	GLU	CB-CA-C	-7.92	99.62	112.06
8	H	311	THR	N-CA-CB	7.91	123.58	110.92
7	G	651	PRO	CB-CA-C	-7.91	98.50	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	6	LYS	N-CA-C	-7.91	100.09	110.53
7	G	270	VAL	N-CA-CB	-7.88	100.62	110.31
17	X	55	ARG	N-CA-CB	-7.88	97.18	110.49
9	I	160	GLU	N-CA-C	7.82	124.19	111.37
7	G	389	THR	N-CA-CB	7.80	121.47	109.85
10	P	235	THR	CB-CA-C	-7.78	100.09	112.07
9	I	74	LEU	N-CA-C	-7.76	102.82	111.28
1	A	53	MET	N-CA-C	-7.76	103.96	113.19
17	X	58	LYS	N-CA-C	-7.75	102.78	111.07
4	D	361	ALA	N-CA-C	-7.73	102.94	112.38
2	B	153	PRO	CB-CA-C	-7.67	98.91	111.56
8	H	253	GLU	N-CA-C	7.66	121.89	112.54
6	F	171	VAL	N-CA-CB	7.66	120.37	110.57
21	q	44	TYR	N-CA-C	-7.65	98.96	110.28
7	G	56	VAL	N-CA-C	-7.64	103.01	110.72
7	G	569	GLN	N-CA-C	7.63	122.04	108.24
6	F	58	ARG	N-CA-C	-7.61	103.06	111.36
21	q	89	TRP	N-CA-C	-7.60	102.93	111.14
5	E	68	ASN	N-CA-CB	7.58	121.00	110.01
12	R	32	THR	N-CA-C	7.57	119.58	110.19
8	H	223	PHE	CB-CA-C	-7.56	99.01	110.88
9	I	119	CYS	N-CA-C	-7.53	103.15	111.36
12	R	74	HIS	N-CA-C	7.52	121.11	110.50
7	G	277	MET	N-CA-C	7.51	120.63	109.59
7	G	467	LYS	N-CA-C	-7.51	102.24	111.33
9	I	158	CYS	N-CA-C	-7.47	103.14	111.28
6	F	430	GLY	N-CA-C	7.42	121.64	112.73
7	G	303	THR	N-CA-C	7.42	123.05	113.18
7	G	510	TRP	N-CA-CB	7.42	120.90	109.85
4	D	99	LEU	N-CA-C	7.41	121.00	109.07
15	V	57	ASP	N-CA-CB	7.40	120.74	110.01
4	D	350	LYS	CB-CA-C	-7.35	101.04	111.85
2	B	183	ARG	N-CA-C	-7.35	104.56	113.97
21	q	24	LEU	N-CA-C	-7.30	103.32	111.28
8	H	309	ILE	N-CA-C	7.27	117.35	110.30
13	S	94	VAL	N-CA-C	7.26	117.39	110.42
7	G	384	ASN	N-CA-C	-7.26	103.40	111.82
3	C	195	HIS	CB-CA-C	7.25	117.35	110.17
14	T	105	MET	N-CA-C	7.25	119.26	111.36
7	G	497	VAL	N-CA-C	-7.24	103.23	110.62
8	H	139	THR	N-CA-CB	7.24	120.51	110.01
15	V	68	LEU	N-CA-C	-7.23	103.40	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	374	THR	CB-CA-C	-7.23	99.86	111.28
8	H	212	ASN	N-CA-CB	7.22	120.51	110.98
6	F	73	PRO	N-CA-C	-7.20	103.75	113.40
10	P	370	LYS	N-CA-C	7.20	119.25	109.24
8	H	50	ALA	N-CA-C	7.17	118.75	111.07
7	G	661	GLU	N-CA-C	7.17	118.79	110.97
7	G	465	VAL	N-CA-CB	7.17	118.47	110.51
7	G	217	GLU	N-CA-C	-7.15	101.61	110.41
6	F	81	LYS	N-CA-C	-7.13	103.59	111.36
8	H	214	GLU	N-CA-CB	-7.12	98.89	110.42
8	H	254	LEU	N-CA-C	-7.12	103.56	111.82
7	G	461	SER	N-CA-C	7.11	119.93	111.33
15	V	95	LEU	N-CA-C	-7.08	103.56	111.28
6	F	78	GLY	N-CA-C	-7.08	104.24	112.73
11	Q	162	ALA	N-CA-C	7.07	118.98	111.28
7	G	148	SER	N-CA-C	7.05	120.89	109.40
7	G	294	TYR	N-CA-C	-7.00	104.54	113.23
6	F	246	GLU	N-CA-C	-6.98	103.67	111.28
7	G	150	ARG	N-CA-C	6.98	119.53	109.14
8	H	176	LEU	CA-C-N	-6.98	113.61	120.52
8	H	176	LEU	C-N-CA	-6.98	113.61	120.52
21	q	77	VAL	N-CA-C	-6.98	99.72	109.21
6	F	455	GLN	N-CA-C	6.97	118.53	111.07
2	B	166	ASN	N-CA-C	-6.97	103.38	110.97
6	F	169	LEU	N-CA-C	6.96	118.87	111.28
7	G	582	VAL	N-CA-C	6.96	118.51	108.48
8	H	292	ASN	N-CA-C	6.96	118.94	111.36
6	F	418	GLN	N-CA-CB	6.96	120.16	110.07
6	F	428	GLY	N-CA-C	-6.95	103.87	112.77
5	E	152	GLN	N-CA-C	-6.95	103.64	111.07
6	F	103	ASN	N-CA-CB	6.93	121.05	110.44
10	P	235	THR	CA-C-O	6.93	128.12	121.67
3	C	69	PRO	N-CA-C	-6.93	104.30	113.65
7	G	300	GLN	N-CA-CB	6.92	122.53	112.08
18	Z	34	SER	N-CA-C	-6.91	103.67	111.07
8	H	300	LEU	N-CA-C	-6.90	104.12	112.54
6	F	148	ALA	N-CA-C	-6.89	103.85	111.36
7	G	362	ASP	N-CA-C	6.87	125.44	110.80
14	T	145	VAL	N-CA-C	-6.87	103.78	110.72
16	W	87	ILE	N-CA-CB	6.86	118.58	110.55
18	Z	28	ARG	N-CA-C	6.86	119.70	108.52
12	R	56	ASN	N-CA-C	6.83	120.03	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	244	ASN	N-CA-C	-6.82	100.88	110.50
7	G	133	GLN	N-CA-C	-6.78	101.25	110.68
7	G	268	GLY	N-CA-C	6.78	124.73	115.30
8	H	305	ILE	N-CA-C	-6.78	103.43	113.39
1	A	112	GLU	N-CA-C	-6.77	102.33	111.87
7	G	434	SER	N-CA-C	-6.74	100.99	110.29
15	V	8	THR	N-CA-C	6.71	119.06	108.79
7	G	601	GLY	N-CA-C	6.70	124.94	115.30
9	I	208	ASP	N-CA-C	6.70	121.61	113.17
16	W	105	HIS	N-CA-C	-6.69	104.93	113.23
22	r	11	LEU	N-CA-C	-6.69	104.06	111.36
5	E	199	ASP	N-CA-C	-6.69	103.68	110.97
17	X	97	PHE	N-CA-C	6.67	118.62	111.36
8	H	8	THR	N-CA-C	-6.66	101.29	110.35
15	V	114	TRP	N-CA-CB	6.66	120.22	110.30
7	G	640	ASP	N-CA-CB	6.65	120.01	110.16
17	X	129	THR	N-CA-C	6.65	120.87	110.17
10	P	116	ILE	N-CA-C	-6.64	104.01	110.72
15	V	86	LYS	N-CA-CB	6.64	119.70	110.07
3	C	125	PHE	N-CA-CB	-6.63	100.63	110.17
6	F	344	GLN	N-CA-C	-6.62	103.99	111.07
7	G	287	SER	N-CA-C	6.61	119.26	110.53
4	D	184	ILE	N-CA-C	-6.61	103.88	110.62
6	F	228	PRO	N-CA-C	-6.60	98.88	112.47
6	F	336	LEU	N-CA-CB	-6.59	100.95	111.43
8	H	182	ALA	N-CA-C	-6.59	104.02	111.07
13	S	40	ARG	N-CA-C	6.57	122.81	113.02
8	H	93	HIS	CB-CA-C	6.55	117.73	108.76
11	Q	141	ASN	N-CA-CB	6.54	120.74	110.46
7	G	435	PRO	N-CA-C	-6.53	100.24	110.50
8	H	223	PHE	N-CA-C	-6.52	104.09	111.07
17	X	81	PRO	N-CA-C	-6.51	104.17	113.47
7	G	605	GLN	N-CA-C	6.50	119.11	108.52
13	S	16	LEU	N-CA-C	-6.49	98.33	108.90
8	H	267	SER	N-CA-C	-6.48	104.30	111.36
6	F	178	GLU	N-CA-CB	6.46	119.57	109.94
4	D	388	GLY	N-CA-C	6.46	119.55	110.38
22	r	24	LEU	N-CA-C	6.46	119.60	110.50
12	R	81	GLY	N-CA-C	-6.45	106.83	115.21
21	q	75	TRP	N-CA-C	6.45	121.41	112.45
15	V	49	GLU	N-CA-C	-6.44	104.26	111.28
7	G	250	SER	N-CA-C	6.44	116.77	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	98	ARG	N-CA-C	6.43	120.39	112.54
8	H	255	TYR	N-CA-CB	6.41	119.31	110.01
8	H	177	PRO	N-CA-C	-6.41	101.58	111.13
7	G	273	ILE	N-CA-C	-6.41	98.29	107.77
3	C	125	PHE	N-CA-C	6.40	119.52	110.50
4	D	140	ASP	N-CA-C	-6.40	96.54	107.23
6	F	125	CYS	N-CA-C	-6.39	105.47	113.20
12	R	43	TYR	N-CA-C	-6.39	99.83	109.79
8	H	271	LEU	N-CA-CB	6.38	119.32	110.07
11	Q	59	LEU	N-CA-C	-6.36	100.75	110.30
9	I	66	LEU	N-CA-C	-6.36	104.43	111.36
9	I	205	ILE	N-CA-C	-6.36	104.30	110.72
6	F	370	LEU	N-CA-C	-6.35	104.43	111.36
7	G	95	PRO	N-CA-C	-6.35	101.21	110.80
6	F	144	VAL	N-CA-CB	6.35	118.69	110.57
4	D	141	TYR	N-CA-C	6.33	121.01	113.16
21	q	28	PHE	N-CA-C	6.32	117.83	111.07
22	r	8	ILE	N-CA-C	-6.31	104.34	110.72
15	V	91	ALA	N-CA-C	-6.31	104.40	111.28
1	A	101	GLY	N-CA-C	-6.29	105.20	112.50
15	V	71	LEU	N-CA-C	6.29	118.13	111.28
19	a	26	ILE	N-CA-C	-6.28	104.53	113.07
7	G	176	CYS	N-CA-C	6.28	119.59	110.42
7	G	356	ASP	N-CA-CB	6.28	119.35	110.12
7	G	383	SER	N-CA-C	-6.27	106.85	114.75
6	F	255	CYS	N-CA-C	-6.26	104.53	111.36
17	X	99	HIS	N-CA-CB	6.26	119.43	110.16
6	F	101	PHE	N-CA-C	6.25	118.90	111.33
6	F	415	ILE	N-CA-C	-6.25	104.41	110.72
8	H	269	THR	N-CA-C	6.24	118.08	111.28
5	E	50	THR	N-CA-CB	6.22	121.44	110.37
21	q	69	ASN	N-CA-CB	6.21	121.35	111.66
2	B	113	ASP	N-CA-CB	6.21	119.47	109.28
8	H	52	ALA	N-CA-CB	6.20	119.00	110.01
6	F	212	LEU	N-CA-C	-6.20	104.52	111.28
7	G	420	LYS	N-CA-C	6.20	118.83	111.33
11	Q	141	ASN	N-CA-C	-6.20	105.72	113.28
10	P	118	LYS	N-CA-C	6.18	118.99	111.82
6	F	192	ASP	N-CA-C	6.18	119.02	109.07
7	G	451	ILE	N-CA-C	-6.17	104.97	113.00
10	P	368	GLU	N-CA-CB	6.17	119.81	110.30
17	X	36	CYS	CB-CA-C	-6.17	97.30	110.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	291	VAL	N-CA-C	-6.17	103.37	111.09
22	r	26	LEU	N-CA-CB	-6.16	101.17	110.35
7	G	418	ILE	N-CA-C	-6.13	103.45	112.04
13	S	40	ARG	N-CA-CB	-6.13	101.09	111.27
7	G	508	ALA	N-CA-C	6.11	117.94	111.28
8	H	276	SER	N-CA-C	6.10	118.90	111.82
8	H	185	TRP	N-CA-C	-6.08	104.00	112.45
13	S	87	VAL	N-CA-C	-6.08	104.42	110.62
7	G	325	ARG	N-CA-CB	6.07	118.78	109.91
7	G	353	ALA	N-CA-C	-6.03	104.63	112.23
13	S	61	VAL	N-CA-C	-6.03	99.56	107.88
8	H	7	LEU	N-CA-C	-6.02	104.34	111.03
8	H	24	GLU	N-CA-C	-6.02	104.08	112.45
17	X	40	ASN	N-CA-C	-5.99	104.66	111.07
22	r	108	LYS	N-CA-C	5.99	117.88	111.36
7	G	638	THR	N-CA-C	-5.97	100.22	109.24
2	B	196	PRO	N-CA-C	-5.95	101.86	111.03
7	G	387	LEU	CB-CA-C	-5.95	101.68	111.68
6	F	291	GLU	N-CA-C	5.95	118.22	110.43
4	D	352	PRO	N-CA-C	5.94	117.94	110.70
8	H	103	LEU	N-CA-C	-5.93	104.89	111.36
21	q	5	GLU	N-CA-C	-5.93	104.90	111.36
9	I	116	CYS	N-CA-C	-5.92	105.55	112.89
4	D	84	PHE	N-CA-C	-5.91	98.21	110.80
13	S	30	SER	N-CA-C	-5.91	106.11	113.38
4	D	92	HIS	N-CA-C	-5.90	98.64	108.32
14	T	94	ASP	N-CA-CB	-5.90	105.11	111.66
18	Z	44	ILE	N-CA-C	-5.89	104.76	110.42
8	H	315	PRO	O-C-N	5.87	123.91	121.15
3	C	71	TYR	N-CA-C	5.87	120.25	113.38
7	G	480	ALA	N-CA-C	-5.86	104.97	111.36
4	D	258	VAL	N-CA-C	-5.86	103.94	110.62
1	A	58	VAL	CB-CA-C	-5.85	104.22	111.70
7	G	289	LYS	N-CA-C	5.84	117.64	111.28
3	C	209	LEU	N-CA-CB	-5.83	100.68	110.83
21	q	65	THR	N-CA-C	5.83	119.18	110.14
10	P	157	LYS	N-CA-CB	5.82	118.77	110.16
6	F	226	LYS	CA-C-N	-5.81	114.40	120.38
6	F	226	LYS	C-N-CA	-5.81	114.40	120.38
7	G	672	ALA	N-CA-C	-5.81	104.95	111.28
10	P	367	GLU	CB-CA-C	-5.81	99.52	110.67
10	P	122	HIS	N-CA-C	5.81	120.06	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	86	GLU	N-CA-CB	5.80	118.75	110.16
15	V	19	THR	N-CA-CB	5.79	120.68	110.37
8	H	116	ILE	N-CA-C	-5.79	104.86	110.42
7	G	639	LEU	N-CA-C	5.78	118.52	111.82
6	F	102	MET	CB-CA-C	-5.78	101.41	110.94
7	G	34	VAL	N-CA-C	5.78	116.20	108.11
12	R	45	ARG	N-CA-C	-5.78	104.95	113.61
10	P	234	LYS	CB-CA-C	-5.77	103.38	111.80
2	B	135	GLY	CA-C-O	-5.76	117.97	122.52
6	F	299	LEU	N-CA-C	5.76	118.50	111.82
4	D	414	ASP	N-CA-C	-5.74	101.46	110.36
10	P	272	LEU	N-CA-C	-5.74	101.79	110.28
11	Q	164	PHE	N-CA-CB	5.73	119.71	110.42
8	H	252	PRO	N-CA-CB	-5.72	98.02	103.51
6	F	41	ILE	N-CA-C	5.72	115.80	110.42
13	S	73	GLN	N-CA-C	-5.72	100.38	109.59
8	H	211	PHE	CA-C-O	5.72	126.87	119.95
21	q	140	PRO	N-CA-C	-5.72	102.16	110.80
6	F	393	ASN	N-CA-C	-5.71	104.96	111.07
1	A	55	PHE	N-CA-CB	5.71	118.29	110.01
17	X	79	ALA	N-CA-C	5.71	117.18	111.07
5	E	119	THR	N-CA-C	-5.71	105.81	112.89
10	P	119	ALA	N-CA-C	-5.70	104.98	111.14
6	F	457	HIS	N-CA-CB	-5.69	100.82	110.50
18	Z	72	MET	CA-C-N	-5.69	113.32	119.24
18	Z	72	MET	C-N-CA	-5.69	113.32	119.24
8	H	126	LYS	N-CA-C	5.66	117.45	111.28
7	G	599	THR	CA-C-N	-5.66	114.11	122.83
7	G	599	THR	C-N-CA	-5.66	114.11	122.83
11	Q	124	MET	CA-C-N	-5.66	114.94	122.98
11	Q	124	MET	C-N-CA	-5.66	114.94	122.98
6	F	304	ALA	CB-CA-C	-5.65	110.04	116.54
2	B	112	TYR	N-CA-C	5.65	122.83	110.80
6	F	416	SER	N-CA-C	5.63	117.87	111.11
4	D	81	THR	CA-C-N	-5.63	112.96	120.90
4	D	81	THR	C-N-CA	-5.63	112.96	120.90
17	X	65	GLY	N-CA-C	-5.63	105.97	112.50
7	G	530	TYR	N-CA-C	-5.62	101.96	110.28
9	I	191	LEU	N-CA-C	-5.62	105.23	111.36
2	B	71	ALA	N-CA-CB	-5.62	101.27	110.14
7	G	59	GLN	N-CA-C	5.61	117.92	107.99
8	H	76	THR	N-CA-C	-5.59	104.56	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	56	CYS	N-CA-C	5.59	119.80	112.92
6	F	176	ALA	N-CA-C	5.58	118.09	111.33
7	G	615	LEU	N-CA-C	-5.57	106.25	113.16
6	F	294	VAL	CA-C-N	-5.57	114.03	119.76
6	F	294	VAL	C-N-CA	-5.57	114.03	119.76
21	q	142	THR	N-CA-CB	5.57	119.86	109.68
5	E	183	PRO	N-CA-C	-5.56	102.20	111.26
17	X	54	ARG	CB-CA-C	5.56	119.52	110.96
21	q	71	LYS	N-CA-C	5.56	120.05	113.16
21	q	68	MET	N-CA-C	5.55	119.31	112.54
2	B	201	LEU	N-CA-C	-5.54	105.14	111.07
14	T	135	ALA	N-CA-CB	5.54	118.26	110.12
7	G	127	ASP	CA-C-O	5.53	129.02	121.89
5	E	222	PHE	CB-CA-C	-5.51	100.66	109.75
10	P	130	ILE	N-CA-C	5.51	115.19	107.37
7	G	363	SER	N-CA-C	-5.51	100.20	109.07
3	C	71	TYR	CB-CA-C	-5.48	102.29	111.23
22	r	94	ALA	N-CA-C	-5.48	101.74	109.96
10	P	86	CYS	N-CA-C	-5.48	103.15	110.55
4	D	132	ALA	N-CA-C	-5.47	106.61	113.72
8	H	141	SER	N-CA-CB	5.47	117.94	110.01
6	F	118	ASP	N-CA-C	-5.46	102.19	110.28
7	G	313	LEU	N-CA-C	5.46	118.46	109.72
7	G	682	ASP	CA-C-N	-5.44	114.16	119.76
7	G	682	ASP	C-N-CA	-5.44	114.16	119.76
19	a	25	TYR	N-CA-C	-5.43	107.90	114.75
12	R	88	HIS	CB-CA-C	5.43	117.39	109.08
17	X	27	ALA	N-CA-C	-5.43	105.02	111.69
4	D	200	PHE	CA-CB-CG	5.42	119.22	113.80
5	E	48	PRO	N-CA-C	5.42	120.88	113.84
7	G	150	ARG	N-CA-CB	-5.42	102.84	111.62
7	G	404	GLY	N-CA-C	5.41	121.38	113.48
3	C	81	ASP	N-CA-C	-5.41	104.44	111.74
10	P	357	ARG	N-CA-C	5.40	117.50	110.43
6	F	199	ARG	N-CA-C	5.39	117.52	109.59
7	G	420	LYS	N-CA-CB	-5.39	101.97	110.06
4	D	391	VAL	CA-C-N	-5.39	115.78	119.66
4	D	391	VAL	C-N-CA	-5.39	115.78	119.66
14	T	92	LYS	N-CA-C	-5.38	106.30	112.92
13	S	41	TYR	N-CA-C	-5.38	105.50	111.36
10	P	374	THR	N-CA-C	5.38	117.49	108.73
8	H	94	PRO	N-CA-C	5.37	118.73	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	201	PHE	N-CA-C	-5.36	105.52	111.36
18	Z	55	GLN	N-CA-C	-5.36	105.44	111.28
10	P	339	GLY	N-CA-C	5.35	122.70	115.00
18	Z	50	MET	N-CA-C	-5.35	105.45	111.28
13	S	24	CYS	N-CA-C	-5.34	103.34	110.55
11	Q	164	PHE	N-CA-C	-5.33	106.75	113.20
11	Q	163	ASN	CB-CA-C	-5.33	99.35	109.95
16	W	32	LYS	N-CA-C	-5.32	104.89	111.33
7	G	510	TRP	N-CA-C	-5.32	101.99	109.96
7	G	356	ASP	N-CA-C	-5.31	105.49	111.28
8	H	252	PRO	CA-N-CD	5.30	119.42	112.00
5	E	222	PHE	N-CA-C	5.29	117.86	109.24
4	D	141	TYR	N-CA-CB	-5.29	102.35	110.44
10	P	137	ARG	N-CA-C	5.28	122.04	110.80
4	D	363	VAL	N-CA-C	5.27	116.34	111.81
11	Q	72	ILE	N-CA-C	-5.27	108.36	113.53
5	E	48	PRO	CB-CA-C	-5.27	104.37	111.85
7	G	435	PRO	CB-CA-C	-5.27	105.82	111.56
9	I	160	GLU	N-CA-CB	-5.26	100.78	109.72
7	G	362	ASP	CA-CB-CG	5.26	117.86	112.60
16	W	122	LEU	N-CA-C	-5.26	105.55	111.28
6	F	300	ILE	N-CA-CB	5.26	119.34	110.56
10	P	330	THR	N-CA-C	-5.25	106.77	114.39
8	H	46	LEU	N-CA-C	-5.25	106.65	113.16
9	I	54	THR	N-CA-C	-5.25	104.97	111.33
8	H	146	MET	N-CA-C	-5.25	105.45	111.07
10	P	260	GLY	N-CA-C	-5.25	108.38	115.36
7	G	277	MET	N-CA-CB	-5.23	101.66	109.71
7	G	600	GLU	CB-CA-C	-5.22	102.96	111.06
10	P	192	ARG	N-CA-C	-5.22	105.59	111.28
7	G	713	ALA	N-CA-C	-5.21	105.49	111.07
8	H	310	PHE	N-CA-C	5.21	119.26	113.01
16	W	120	ASP	N-CA-C	-5.21	102.58	110.28
13	S	85	ASP	N-CA-C	5.20	117.86	111.82
7	G	556	THR	N-CA-C	-5.19	101.52	109.41
3	C	164	TRP	N-CA-C	5.19	117.01	111.36
1	A	106	TRP	CB-CA-C	-5.18	102.40	110.94
10	P	194	VAL	N-CA-CB	5.18	118.35	110.58
22	r	107	SER	N-CA-C	-5.18	102.19	109.96
22	r	25	GLN	N-CA-C	5.17	118.84	112.54
10	P	198	ALA	N-CA-C	-5.16	100.10	108.52
19	a	3	PHE	CB-CA-C	-5.16	102.55	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	172	ILE	N-CA-C	-5.16	98.61	109.34
6	F	337	MET	CB-CA-C	-5.15	103.03	111.68
7	G	569	GLN	CB-CA-C	-5.15	104.22	112.05
8	H	277	TYR	N-CA-C	5.15	117.97	110.10
2	B	94	THR	N-CA-CB	-5.13	102.22	110.69
8	H	90	PRO	CA-C-O	-5.13	117.43	121.38
8	H	196	ALA	CA-C-N	-5.12	113.53	119.47
8	H	196	ALA	C-N-CA	-5.12	113.53	119.47
4	D	391	VAL	N-CA-C	5.12	113.78	109.02
15	V	84	ALA	N-CA-C	5.12	116.55	111.07
16	W	115	THR	CA-C-N	-5.12	113.44	119.84
16	W	115	THR	C-N-CA	-5.12	113.44	119.84
4	D	224	ALA	CA-C-O	-5.12	115.43	120.90
7	G	387	LEU	N-CA-C	-5.12	98.36	107.98
7	G	63	PHE	CA-C-O	-5.11	115.13	121.06
20	b	82	LYS	N-CA-C	-5.11	103.78	110.53
6	F	60	GLY	N-CA-C	-5.11	106.01	114.48
9	I	95	PRO	N-CA-C	5.11	121.21	113.81
17	X	42	GLU	N-CA-C	-5.10	105.80	111.36
10	P	356	HIS	N-CA-C	-5.09	105.86	111.71
4	D	106	VAL	O-C-N	-5.08	116.74	122.94
5	E	181	ASN	N-CA-C	-5.08	99.51	108.20
7	G	203	ASP	CA-C-O	5.08	127.22	121.32
7	G	458	GLY	N-CA-C	-5.08	108.31	115.32
13	S	45	LYS	N-CA-C	-5.08	105.83	111.36
3	C	208	GLU	CA-C-O	-5.07	115.68	121.40
3	C	156	VAL	N-CA-C	-5.06	104.19	111.17
16	W	91	MET	N-CA-C	-5.06	105.95	111.82
3	C	221	GLU	N-CA-C	-5.05	102.39	108.25
21	q	13	GLN	N-CA-C	-5.05	105.67	111.07
8	H	101	GLY	N-CA-C	5.04	118.34	112.50
7	G	453	GLN	N-CA-C	-5.04	105.87	111.36
8	H	254	LEU	N-CA-CB	5.04	118.08	110.28
10	P	376	ASN	CB-CA-C	-5.04	102.29	110.85
14	T	140	CYS	CB-CA-C	-5.03	104.11	109.85
12	R	65	ALA	N-CA-C	-5.03	105.92	111.71
10	P	170	LEU	N-CA-C	5.03	117.02	110.43
7	G	280	ASP	N-CA-CB	-5.03	102.73	110.12
7	G	393	GLY	N-CA-C	-5.03	107.82	115.66
22	r	4	ALA	N-CA-C	-5.03	105.89	112.23
8	H	214	GLU	N-CA-C	5.02	119.27	113.20
10	P	289	ILE	CA-C-N	-5.02	114.41	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	289	ILE	C-N-CA	-5.02	114.41	119.83
6	F	366	ALA	N-CA-C	-5.02	105.50	110.97
5	E	213	PRO	CB-CA-C	-5.01	106.33	112.89
1	A	54	LYS	N-CA-CB	5.00	117.65	110.20

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	754	0	814	108	0
2	B	1258	0	1270	162	0
3	C	1641	0	1596	136	0
4	D	3088	0	3059	333	0
5	E	1635	0	1626	190	0
6	F	3288	0	3243	349	0
7	G	5287	0	5323	553	0
8	H	2510	0	2593	422	0
9	I	1398	0	1359	158	0
10	P	2730	0	2747	235	0
11	Q	957	0	949	71	0
12	R	660	0	639	77	0
13	S	667	0	685	70	0
14	T	604	0	596	89	0
15	V	915	0	954	78	0
16	W	970	0	991	76	0
17	X	1164	0	1150	109	0
18	Z	1152	0	1148	156	0
19	a	539	0	556	114	0
20	b	628	0	628	82	0
21	q	1004	0	962	84	0
22	r	418	0	434	44	0
23	s	107	0	100	9	0
24	A	46	0	69	5	0
24	I	51	0	82	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	b	46	0	69	18	0
25	B	8	0	0	6	0
25	F	8	0	0	10	0
25	G	16	0	0	7	0
25	I	16	0	0	16	0
26	B	18	0	18	5	0
27	B	35	0	44	7	0
27	H	42	0	58	8	0
27	I	47	0	71	13	0
28	E	4	0	0	5	0
28	G	4	0	0	5	0
29	F	31	0	19	1	0
30	H	35	0	43	14	0
31	P	48	0	26	7	0
32	R	1	0	0	0	0
33	W	32	0	0	7	0
34	q	57	0	58	21	0
All	All	33919	0	33979	3138	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 46.

All (3138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.28
8:H:1:MET:HE3	19:a:29:PHE:CD2	1.67	1.28
8:H:1:MET:HE3	19:a:29:PHE:CE2	1.73	1.24
10:P:93:HIS:CD2	10:P:94:LEU:HD12	1.75	1.21
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.38	1.20
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.20
15:V:44:TYR:CE1	15:V:48:THR:HG21	1.77	1.19
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.18
8:H:251:LEU:HD12	8:H:251:LEU:O	1.42	1.17
2:B:120:VAL:HG21	30:H:401:UQ9:H1MA	1.21	1.17
13:S:51:LEU:HD13	13:S:95:LEU:HD21	1.23	1.17
10:P:156:SER:HB2	10:P:161:VAL:CG2	1.75	1.15
17:X:4:ILE:HG22	17:X:5:VAL:H	1.00	1.14
6:F:392:MET:CE	6:F:419:ILE:HD12	1.76	1.14
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.64	1.13
4:D:81:THR:HG22	4:D:100:GLU:HG2	1.23	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:382:CYS:SG	25:F:502:SF4:FE3	1.38	1.13
8:H:1:MET:CE	19:a:29:PHE:CE2	2.31	1.13
7:G:126:LEU:CD1	12:R:89:PRO:HB2	1.77	1.13
9:I:123:CYS:SG	25:I:303:SF4:FE1	1.40	1.12
6:F:392:MET:HE3	6:F:419:ILE:CD1	1.78	1.11
4:D:448:VAL:HG21	8:H:204:GLU:CD	1.76	1.11
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.27	1.10
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.10
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.10
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.10
10:P:40:VAL:HG22	12:R:43:TYR:CE2	1.86	1.10
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.09
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.09
6:F:379:CYS:SG	25:F:502:SF4:FE4	1.43	1.08
7:G:399:VAL:HG21	7:G:462:PHE:CZ	1.88	1.08
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.33	1.07
8:H:1:MET:HG3	19:a:30:THR:CG2	1.85	1.07
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.36	1.07
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.10	1.06
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.37	1.06
22:r:2:ALA:N	22:r:26:LEU:HD12	1.69	1.06
2:B:100:CYS:SG	25:B:301:SF4:FE4	1.48	1.05
4:D:99:LEU:HD13	4:D:101:LEU:HD13	1.38	1.05
9:I:152:CYS:SG	25:I:303:SF4:FE2	1.46	1.05
10:P:299:SER:HB3	10:P:316:LYS:HE3	1.37	1.05
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.05
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.05
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.05
15:V:44:TYR:CE1	15:V:48:THR:CG2	2.39	1.05
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.04
14:T:138:LEU:HD12	14:T:138:LEU:O	1.55	1.04
3:C:102:HIS:HE1	15:V:48:THR:HG22	1.20	1.04
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.04	1.04
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.04
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.92	1.04
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.23	1.04
6:F:266:GLY:CA	6:F:271:SER:HA	1.86	1.04
10:P:156:SER:HB2	10:P:161:VAL:HG22	1.34	1.04
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.36	1.03
9:I:208:ASP:O	9:I:208:ASP:OD1	1.76	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:4:ILE:CG2	17:X:5:VAL:H	1.71	1.03
2:B:82:ILE:HG23	8:H:57:MET:SD	1.99	1.03
8:H:142:TYR:CD1	8:H:289:LEU:HD12	1.94	1.02
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.02
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.95	1.01
6:F:199:ARG:HD3	23:s:80:PHE:CE2	1.95	1.01
5:E:179:CYS:SG	28:E:301:FES:FE2	1.50	1.01
21:q:66:THR:HG22	21:q:74:PHE:HB2	1.39	1.01
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.42	1.01
2:B:120:VAL:HG21	30:H:401:UQ9:C1M	1.89	1.00
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	1.00
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.87	1.00
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.42	1.00
6:F:300:ILE:HG23	6:F:305:GLY:O	1.59	1.00
9:I:155:CYS:SG	25:I:303:SF4:FE4	1.51	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	1.00
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	1.00
15:V:44:TYR:CZ	15:V:48:THR:HG21	1.97	1.00
2:B:96:GLY:HA3	26:B:302:UQ1:HM31	1.39	0.99
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	0.99
6:F:266:GLY:HA3	6:F:271:SER:CA	1.90	0.99
2:B:96:GLY:HA3	26:B:302:UQ1:CM3	1.92	0.99
7:G:579:MET:O	7:G:579:MET:HG3	1.58	0.99
8:H:1:MET:CE	19:a:29:PHE:HE2	1.71	0.99
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.98
17:X:4:ILE:HG22	17:X:5:VAL:N	1.69	0.98
4:D:88:HIS:HD2	4:D:90:ALA:HB3	1.28	0.98
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.98
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.98
4:D:249:LYS:CA	18:Z:19:ILE:HG23	1.93	0.98
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	0.98
3:C:168:GLU:CB	3:C:186:ILE:HD11	1.92	0.98
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.97
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.97
2:B:123:ALA:HB1	30:H:401:UQ9:H3MB	1.46	0.97
2:B:82:ILE:HG12	8:H:57:MET:CE	1.94	0.97
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.43	0.97
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.97
7:G:126:LEU:HD11	12:R:89:PRO:HB2	1.44	0.97
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:376:ASN:OD1	10:P:377:TYR:N	1.98	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.96
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.96
7:G:399:VAL:HG21	7:G:462:PHE:HZ	1.30	0.96
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.96
8:H:1:MET:HG3	19:a:30:THR:HG22	1.44	0.96
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.96
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.96
17:X:123:GLY:HA2	18:Z:66:GLU:OE2	1.66	0.96
7:G:92:CYS:SG	28:G:803:FES:S1	2.63	0.95
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.95
10:P:40:VAL:HG22	12:R:43:TYR:CD2	1.99	0.95
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.95
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.95
13:S:16:LEU:HD11	13:S:51:LEU:HD11	1.46	0.95
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.95
6:F:379:CYS:HG	25:F:502:SF4:FE4	0.74	0.94
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.94
13:S:19:ILE:HG13	13:S:95:LEU:HD11	1.49	0.94
5:E:179:CYS:HG	28:E:301:FES:FE2	0.65	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.94
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.94
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.94
9:I:113:CYS:SG	25:I:304:SF4:FE3	1.59	0.93
6:F:300:ILE:HG22	6:F:306:GLY:HA2	1.46	0.93
6:F:382:CYS:HG	25:F:502:SF4:FE3	0.64	0.93
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.93
9:I:152:CYS:HG	25:I:303:SF4:FE2	0.69	0.93
21:q:3:LEU:HD13	34:q:201:CDL:HB4	1.49	0.93
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.93
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.32	0.92
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.92
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.48	0.92
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.51	0.92
5:E:240:PRO:HA	6:F:60:GLY:HA3	1.49	0.92
7:G:399:VAL:CG2	7:G:462:PHE:HZ	1.82	0.92
10:P:93:HIS:CD2	10:P:94:LEU:CD1	2.52	0.91
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.91
21:q:85:GLU:HG2	21:q:98:PRO:HB3	1.53	0.91
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.01	0.91
8:H:172:MET:HE1	18:Z:46:GLY:HA3	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:232:VAL:HG12	4:D:356:ILE:HD13	1.53	0.91
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.53	0.91
8:H:134:ARG:NH2	8:H:205:SER:HB2	1.85	0.90
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.86	0.90
15:V:75:GLY:HA2	22:r:103:ARG:HD2	1.52	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.36	0.90
2:B:95:PHE:HZ	2:B:148:VAL:HB	1.35	0.90
7:G:179:CYS:HG	25:G:802:SF4:FE3	0.80	0.90
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.55	0.90
8:H:19:PHE:CE1	19:a:11:ILE:HD12	2.06	0.90
8:H:200:LEU:HD12	8:H:201:THR:N	1.86	0.90
2:B:120:VAL:CG2	30:H:401:UQ9:H1MA	2.00	0.90
7:G:226:CYS:HG	25:G:802:SF4:FE1	0.70	0.89
10:P:93:HIS:NE2	10:P:94:LEU:CD1	2.35	0.89
10:P:96:LEU:HD12	10:P:97:MET:N	1.88	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.72	0.89
6:F:266:GLY:HA3	6:F:271:SER:HA	0.94	0.89
7:G:176:CYS:HG	25:G:802:SF4:FE4	0.62	0.89
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.89
17:X:52:ASP:HA	18:Z:116:TRP:CD1	2.06	0.89
8:H:1:MET:HE3	19:a:29:PHE:HD2	1.36	0.89
8:H:1:MET:HB2	19:a:30:THR:HG21	1.54	0.89
21:q:76:ASP:OD1	21:q:76:ASP:O	1.90	0.89
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.36	0.88
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.88
8:H:12:PRO:O	19:a:15:CYS:HB3	1.74	0.88
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.88
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.88
9:I:61:LEU:HD21	20:b:17:PRO:O	1.74	0.88
13:S:16:LEU:HD22	13:S:19:ILE:HD11	1.53	0.88
2:B:81:LEU:HG	27:B:303:PC1:H261	1.52	0.88
7:G:97:MET:HB2	7:G:100:TRP:CD1	2.09	0.88
20:b:60:ASP:OD1	20:b:61:GLY:N	2.07	0.88
4:D:101:LEU:HD11	4:D:106:VAL:HG22	1.56	0.87
8:H:67:SER:HA	27:H:402:PC1:H121	1.53	0.87
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.87
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.08	0.87
22:r:2:ALA:N	22:r:26:LEU:CD1	2.37	0.87
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.55	0.87
3:C:168:GLU:HB2	3:C:186:ILE:CD1	2.04	0.86
6:F:425:CYS:HG	25:F:502:SF4:FE1	0.60	0.86
13:S:16:LEU:HD12	13:S:16:LEU:O	1.76	0.86
14:T:79:ILE:HB	14:T:145:VAL:HG13	1.55	0.86
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.90	0.86
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.86
10:P:132:ARG:HG2	31:P:401:NDP:H8A	1.56	0.86
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.86
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.76	0.86
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.86
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.86
8:H:199:ASP:O	8:H:279:ARG:HD2	1.74	0.86
7:G:78:CYS:SG	28:G:803:FES:FE2	1.68	0.85
9:I:162:CYS:SG	25:I:304:SF4:FE4	1.68	0.85
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.85
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.85
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.58	0.85
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.55	0.85
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.85
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.85
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.59	0.85
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.07	0.85
3:C:80:LEU:CD1	4:D:396:THR:HG22	2.07	0.85
18:Z:58:ARG:NH2	20:b:49:THR:HG21	1.92	0.85
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.56	0.85
8:H:1:MET:CB	19:a:30:THR:HG21	2.07	0.84
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.77	0.84
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.84
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.96	0.84
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.84
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.08	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
4:D:248:SER:OG	18:Z:19:ILE:HD13	1.76	0.84
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.42	0.84
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.84
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.84
17:X:130:LYS:HE3	20:b:67:PRO:HB3	1.56	0.84
15:V:56:LEU:HD12	15:V:57:ASP:N	1.92	0.84
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.84
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.84
20:b:23:PHE:HB3	24:b:201:3PE:H2D2	1.58	0.84
4:D:271:ARG:HD2	8:H:279:ARG:O	1.78	0.84
9:I:80:GLU:HG3	19:a:1:MET:SD	2.16	0.83
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.83
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.83
2:B:93:MET:HE1	2:B:148:VAL:HG11	1.59	0.83
4:D:99:LEU:HD12	4:D:99:LEU:O	1.78	0.83
3:C:102:HIS:CE1	15:V:48:THR:HG22	2.11	0.82
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
3:C:186:ILE:CD1	4:D:429:PHE:HZ	1.93	0.82
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.60	0.82
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.82
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.82
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.61	0.82
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.94	0.82
4:D:92:HIS:C	4:D:94:VAL:H	1.85	0.82
4:D:94:VAL:HG11	4:D:116:LEU:HB2	1.62	0.82
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.82
6:F:117:ALA:HB1	6:F:131:MET:SD	2.19	0.82
1:A:108:GLN:HG2	1:A:109:LYS:H	1.43	0.81
4:D:448:VAL:HG21	8:H:204:GLU:OE1	1.79	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.81
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.81
2:B:126:ARG:HD2	8:H:214:GLU:HA	1.60	0.81
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.81
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.81
8:H:1:MET:CG	19:a:30:THR:CG2	2.59	0.81
21:q:71:LYS:O	21:q:72:ASN:OD1	1.99	0.81
17:X:130:LYS:CE	20:b:67:PRO:HB3	2.11	0.81
7:G:78:CYS:HG	28:G:803:FES:FE2	0.51	0.80
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.80
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.62	0.80
7:G:73:GLY:HA2	28:G:803:FES:S1	2.21	0.80
8:H:181:MET:CE	8:H:304:HIS:ND1	2.45	0.80
9:I:123:CYS:HG	25:I:303:SF4:FE1	0.52	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:3:LEU:CD1	34:q:201:CDL:HB4	2.11	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.12	0.80
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.80
8:H:251:LEU:O	8:H:251:LEU:CD1	2.28	0.80
22:r:4:ALA:HB1	22:r:9:GLN:HB2	1.60	0.80
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.80
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.80
14:T:93:ILE:HG21	14:T:110:LEU:HD22	1.63	0.80
8:H:176:LEU:O	18:Z:43:LEU:HD23	1.82	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.79
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79
4:D:80:MET:O	4:D:100:GLU:HA	1.82	0.79
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.46	0.79
2:B:89:SER:O	8:H:54:LYS:HD3	1.82	0.79
17:X:53:PRO:HG2	18:Z:84:LEU:HD21	1.62	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.79
7:G:617:ARG:NH1	16:W:129:HIS:HA	1.97	0.79
8:H:19:PHE:CZ	19:a:11:ILE:HD12	2.18	0.79
10:P:40:VAL:CG2	12:R:43:TYR:CE2	2.66	0.79
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.61	0.79
13:S:20:ARG:HG3	13:S:54:LEU:HB2	1.65	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.79
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.79
9:I:162:CYS:HG	25:I:304:SF4:FE4	0.51	0.79
14:T:87:LEU:HD21	14:T:104:PHE:HZ	1.47	0.79
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.66	0.78
8:H:142:TYR:OH	8:H:288:LEU:HD22	1.82	0.78
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.24	0.78
8:H:17:MET:SD	8:H:229:THR:OG1	2.41	0.78
8:H:127:TYR:CE1	8:H:206:GLU:HB2	2.18	0.78
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.66	0.78
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.78
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.78
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:ARG:HD2	6:F:237:GLY:O	1.82	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
8:H:204:GLU:O	8:H:206:GLU:HG3	1.84	0.78
13:S:51:LEU:HD13	13:S:95:LEU:CD2	2.11	0.78
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.99	0.78
8:H:1:MET:HB3	19:a:26:ILE:CG2	2.13	0.78
10:P:142:GLU:O	10:P:146:VAL:HG12	1.84	0.78
4:D:92:HIS:HB2	4:D:458:PHE:CD2	2.20	0.77
14:T:87:LEU:HD22	14:T:104:PHE:CE1	2.19	0.77
20:b:66:VAL:HG13	20:b:72:ASP:HB2	1.65	0.77
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.19	0.77
1:A:25:PRO:HG3	8:H:60:PRO:HD3	1.66	0.77
19:a:34:LYS:HZ3	19:a:60:TYR:HB2	1.49	0.77
4:D:256:ASP:OD1	18:Z:23:ARG:HA	1.83	0.77
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.77
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.77
14:T:83:VAL:CG2	14:T:126:PHE:HZ	1.97	0.77
16:W:47:PRO:HG3	16:W:63:ARG:HH21	1.49	0.77
1:A:61:THR:CG2	8:H:290:TRP:CH2	2.67	0.77
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.77
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
17:X:20:VAL:HG22	17:X:24:VAL:HG21	1.66	0.77
2:B:89:SER:O	8:H:54:LYS:CD	2.32	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
8:H:23:VAL:HG11	19:a:9:LEU:HD21	1.65	0.77
9:I:113:CYS:HG	25:I:304:SF4:FE3	0.49	0.77
2:B:112:TYR:OH	9:I:91:GLY:CA	2.27	0.77
4:D:145:MET:O	4:D:148:GLU:HG2	1.84	0.77
1:A:112:GLU:O	1:A:112:GLU:CD	2.28	0.77
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.77
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.76
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.76
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.24	0.76
21:q:96:ASP:OD1	21:q:97:PRO:HD2	1.85	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.21	0.76
1:A:61:THR:HG21	8:H:290:TRP:CZ3	2.20	0.76
4:D:249:LYS:HA	18:Z:19:ILE:CG2	2.01	0.76
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.76
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.76
4:D:88:HIS:CD2	4:D:90:ALA:HB3	2.16	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.76
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.67	0.76
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.76
8:H:183:MET:HE2	27:I:302:PC1:H2A1	1.67	0.76
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.50	0.76
8:H:19:PHE:HB3	19:a:12:MET:HG3	1.66	0.76
8:H:91:MET:O	8:H:92:PRO:C	2.26	0.76
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.48	0.75
14:T:93:ILE:HG23	14:T:110:LEU:HD13	1.66	0.75
19:a:34:LYS:NZ	19:a:60:TYR:HB2	2.01	0.75
2:B:68:ARG:HD3	2:B:70:ARG:HG2	1.69	0.75
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.75
5:E:139:CYS:SG	28:E:301:FES:FE1	1.78	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.75
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.75
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.75
6:F:225:LEU:H	11:Q:160:TYR:HE2	1.31	0.75
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.67	0.75
17:X:53:PRO:HD3	18:Z:116:TRP:CD1	2.20	0.75
20:b:31:ILE:HA	20:b:34:MET:HE2	1.69	0.75
3:C:80:LEU:CD1	4:D:396:THR:CG2	2.63	0.75
21:q:55:PHE:CD1	22:r:26:LEU:HD22	2.21	0.75
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.67	0.75
5:E:183:PRO:HB2	5:E:195:LEU:H	1.50	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
10:P:336:GLU:HG3	10:P:342:PRO:HD3	1.67	0.75
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.75
11:Q:167:ASN:O	11:Q:168:LYS:CD	2.35	0.75
6:F:314:LEU:HB3	6:F:329:LYS:HD3	1.68	0.75
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.51	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.74
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.74
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.74
14:T:117:GLU:HA	14:T:120:MET:HE3	1.67	0.74
2:B:123:ALA:CB	30:H:401:UQ9:H3MB	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.68	0.74
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.27	0.74
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.70	0.74
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.74
8:H:19:PHE:CB	19:a:12:MET:HG3	2.16	0.74
8:H:201:THR:C	8:H:203:GLY:H	1.95	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
9:I:110:GLU:OE2	12:R:64:ILE:HB	1.88	0.74
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.87	0.74
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.70	0.74
5:E:43:THR:HG23	5:E:46:ASN:H	1.52	0.74
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.74
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.74
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.74
14:T:88:LYS:HG3	14:T:98:LEU:HD22	1.70	0.74
14:T:94:ASP:HB3	14:T:98:LEU:HB2	1.69	0.74
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.16	0.74
3:C:99:LEU:HD13	3:C:140:ILE:HD11	1.70	0.74
8:H:272:TRP:HH2	27:I:302:PC1:H381	1.52	0.74
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.03	0.74
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.69	0.74
13:S:51:LEU:CD1	13:S:95:LEU:HD21	2.12	0.74
14:T:103:HIS:CG	14:T:106:LYS:HD2	2.23	0.74
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.73
8:H:195:ARG:O	8:H:199:ASP:HB2	1.87	0.73
17:X:4:ILE:HG22	17:X:6:GLU:H	1.51	0.73
3:C:186:ILE:HD12	4:D:429:PHE:CZ	2.19	0.73
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.22	0.73
21:q:68:MET:SD	21:q:81:MET:HB3	2.28	0.73
1:A:61:THR:HG21	8:H:290:TRP:CH2	2.23	0.73
9:I:57:ALA:HB2	20:b:13:TRP:O	1.87	0.73
10:P:203:PRO:HG2	31:P:401:NDP:H6N	1.69	0.73
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.70	0.73
4:D:280:ALA:CB	15:V:11:LEU:HG	2.19	0.73
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.53	0.73
10:P:40:VAL:CG2	12:R:43:TYR:CD2	2.71	0.73
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.73
20:b:69:HIS:HD2	20:b:70:PRO:HD2	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ALA:O	1:A:25:PRO:HD3	1.88	0.73
5:E:192:TYR:CE1	5:E:215:PRO:HA	2.23	0.73
6:F:293:SER:HA	6:F:336:LEU:HD13	1.68	0.73
21:q:56:PHE:HA	21:q:59:HIS:CD2	2.24	0.73
2:B:89:SER:O	8:H:54:LYS:HE2	1.87	0.73
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.73
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.73
18:Z:98:MET:HE3	18:Z:101:VAL:HG21	1.70	0.73
21:q:13:GLN:HE22	34:q:201:CDL:HA32	1.53	0.73
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.71	0.73
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.73
7:G:176:CYS:SG	25:G:802:SF4:FE4	1.78	0.73
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.70	0.72
11:Q:167:ASN:O	11:Q:168:LYS:HD2	1.88	0.72
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.72
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.72
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.72
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.71	0.72
10:P:262:THR:H	10:P:332:LEU:HD12	1.54	0.72
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.72
7:G:75:CYS:SG	7:G:76:ARG:N	2.62	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.19	0.72
8:H:172:MET:SD	18:Z:46:GLY:HA2	2.28	0.72
2:B:95:PHE:HE1	2:B:131:MET:HE2	1.54	0.72
2:B:124:SER:H	30:H:401:UQ9:C3M	2.01	0.72
5:E:163:THR:CG2	5:E:168:PHE:HB2	2.19	0.72
6:F:236:PHE:HA	11:Q:166:TRP:CD1	2.25	0.72
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.52	0.72
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.72
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.72
16:W:110:PHE:HZ	33:W:201:EHZ:C2	2.00	0.72
19:a:2:TRP:CZ2	34:q:201:CDL:HB62	2.25	0.72
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.71	0.72
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.72	0.72
8:H:179:TRP:CD1	18:Z:43:LEU:HD21	2.24	0.72
7:G:126:LEU:HD13	12:R:89:PRO:HB2	1.68	0.71
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.71
21:q:56:PHE:HD1	21:q:59:HIS:HE2	1.35	0.71
8:H:292:ASN:O	20:b:18:VAL:HG11	1.88	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.71
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.73	0.71
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.71
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.71
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.25	0.71
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.71
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.71
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.71
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	0.71
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.72	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.71
27:I:302:PC1:H2D1	27:I:302:PC1:H291	1.73	0.71
3:C:102:HIS:HE1	15:V:48:THR:CG2	2.01	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.71
6:F:329:LYS:HA	6:F:332:CYS:SG	2.31	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.26	0.71
5:E:232:SER:HB3	6:F:288:VAL:HG23	1.71	0.71
8:H:187:ILE:HD12	24:I:301:3PE:H242	1.72	0.71
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.73	0.70
10:P:170:LEU:O	10:P:171:ASN:OD1	2.09	0.70
2:B:92:PRO:HD2	2:B:120:VAL:HG12	1.73	0.70
2:B:93:MET:HE1	2:B:148:VAL:CG1	2.21	0.70
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.70
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.55	0.70
7:G:127:ASP:HA	12:R:106:TYR:OH	1.90	0.70
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.57	0.70
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.71	0.70
7:G:64:CYS:SG	28:G:803:FES:FE1	1.83	0.70
8:H:113:VAL:HG22	8:H:136:VAL:HG23	1.72	0.70
8:H:134:ARG:NH2	8:H:200:LEU:HD13	2.06	0.70
8:H:312:ALA:HB2	20:b:38:TYR:HB3	1.73	0.70
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.70
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.70
2:B:136:THR:HG21	2:B:177:VAL:HG22	1.73	0.70
4:D:266:ARG:HB2	9:I:65:GLU:OE2	1.91	0.70
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:48:HIS:ND1	13:S:95:LEU:HD23	2.05	0.70
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.72	0.70
9:I:155:CYS:HG	25:I:303:SF4:FE4	1.08	0.70
16:W:42:TRP:CD2	16:W:93:LEU:HD12	2.26	0.70
16:W:110:PHE:CZ	33:W:201:EHZ:C2	2.75	0.70
4:D:92:HIS:O	4:D:94:VAL:N	2.24	0.70
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.70
15:V:56:LEU:HD12	15:V:56:LEU:C	2.16	0.70
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.70
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.70
12:R:67:GLN:HG2	12:R:109:LEU:CD2	2.21	0.70
17:X:29:ALA:HA	18:Z:71:LEU:HD21	1.72	0.70
4:D:99:LEU:HD13	4:D:101:LEU:CD1	2.20	0.70
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.69
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.69
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.73	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.74	0.69
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.69
16:W:58:THR:HB	16:W:61:GLN:CB	2.22	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.69
4:D:248:SER:OG	18:Z:19:ILE:CD1	2.39	0.69
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.69
6:F:300:ILE:HG22	6:F:306:GLY:CA	2.22	0.69
9:I:200:GLU:OE2	21:q:93:MET:SD	2.51	0.69
10:P:191:VAL:HA	10:P:194:VAL:HG22	1.73	0.69
14:T:100:VAL:HB	14:T:142:GLN:HB2	1.74	0.69
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.69
3:C:84:GLU:HG2	3:C:141:ARG:HH11	1.56	0.69
4:D:235:ASP:OD1	4:D:236:LEU:N	2.25	0.69
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
5:E:190:ASN:HB3	5:E:192:TYR:CE2	2.28	0.69
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.74	0.69
9:I:93:LEU:O	21:q:93:MET:HG2	1.93	0.69
14:T:87:LEU:HD22	14:T:104:PHE:HE1	1.58	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.69
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.69
8:H:85:LEU:HD21	8:H:108:THR:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.75	0.69
3:C:186:ILE:HB	4:D:113:ILE:HD11	1.75	0.68
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.68
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.68
13:S:19:ILE:HG13	13:S:95:LEU:CD1	2.22	0.68
4:D:99:LEU:CD1	4:D:101:LEU:HD13	2.19	0.68
8:H:33:LEU:HD23	22:r:25:GLN:HG2	1.76	0.68
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.68
34:q:201:CDL:H341	34:q:201:CDL:H171	1.74	0.68
22:r:20:LEU:C	22:r:20:LEU:HD12	2.18	0.68
2:B:95:PHE:HZ	2:B:148:VAL:CB	2.05	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
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.68
10:P:171:ASN:OD1	10:P:171:ASN:O	2.11	0.68
13:S:16:LEU:HB3	13:S:69:TYR:HD1	1.58	0.68
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.76	0.68
15:V:116:ILE:HG23	15:V:116:ILE:O	1.92	0.68
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.68
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.68
8:H:15:ILE:CG2	19:a:15:CYS:SG	2.81	0.68
14:T:138:LEU:HD13	14:T:144:ILE:CG1	2.23	0.68
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.68
6:F:126:LYS:O	6:F:129:GLU:HG2	1.93	0.68
8:H:1:MET:HE2	19:a:29:PHE:HE2	1.55	0.68
13:S:23:LEU:HD12	13:S:23:LEU:O	1.93	0.68
16:W:84:LEU:HD21	16:W:88:LYS:HE3	1.74	0.68
17:X:64:ASN:O	17:X:68:LEU:HG	1.94	0.68
1:A:61:THR:HG22	8:H:290:TRP:CH2	2.29	0.68
8:H:283:ASP:OD1	8:H:284:GLN:N	2.26	0.68
4:D:248:SER:CB	18:Z:19:ILE:HD13	2.24	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.68
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.68
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.24	0.68
1:A:112:GLU:O	1:A:112:GLU:OE1	2.12	0.67
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.58	0.67
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.67
17:X:52:ASP:HB3	18:Z:116:TRP:CB	2.24	0.67
2:B:121:PHE:CD2	2:B:122:ARG:HD2	2.30	0.67
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:78:CYS:SG	17:X:111:VAL:HG13	2.34	0.67
23:s:78:TYR:HA	23:s:81:LEU:HD12	1.76	0.67
2:B:89:SER:O	8:H:54:LYS:CE	2.42	0.67
5:E:240:PRO:HG3	6:F:57:LEU:O	1.94	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
9:I:188:GLU:OE2	12:R:56:ASN:HB2	1.94	0.67
5:E:78:VAL:HG12	5:E:104:LEU:HD13	1.76	0.67
10:P:197:GLU:HB3	10:P:259:VAL:CG2	2.24	0.67
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.77	0.67
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.30	0.67
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.75	0.67
7:G:226:CYS:SG	25:G:802:SF4:FE1	1.82	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.27	0.67
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.67
10:P:302:GLY:HA2	10:P:314:THR:HG23	1.77	0.67
18:Z:121:ILE:HD11	18:Z:136:ALA:HB1	1.77	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.67
8:H:134:ARG:HH22	8:H:205:SER:HB2	1.60	0.67
10:P:94:LEU:HA	10:P:97:MET:HE3	1.77	0.67
10:P:320:GLU:O	10:P:324:ILE:HG12	1.95	0.67
18:Z:121:ILE:HD11	18:Z:136:ALA:CB	2.24	0.67
4:D:253:LEU:HB2	22:r:23:LYS:CD	2.25	0.66
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.66
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.66
10:P:180:SER:O	10:P:184:LYS:HG3	1.95	0.66
15:V:44:TYR:CE1	15:V:48:THR:HG23	2.30	0.66
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.66
2:B:82:ILE:HA	8:H:57:MET:HE1	1.77	0.66
6:F:300:ILE:HD11	6:F:356:VAL:HG21	1.78	0.66
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.24	0.66
9:I:35:THR:CG2	22:r:107:SER:HA	2.26	0.66
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.66
9:I:80:GLU:OE2	22:r:26:LEU:CD1	2.44	0.66
9:I:188:GLU:CD	12:R:56:ASN:HB2	2.19	0.66
14:T:83:VAL:HG22	14:T:126:PHE:CZ	2.31	0.66
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.66
1:A:54:LYS:O	1:A:58:VAL:HG23	1.95	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.66
6:F:300:ILE:CG2	6:F:307:VAL:N	2.58	0.66
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
9:I:67:ILE:HG13	27:I:302:PC1:H251	1.77	0.66
10:P:156:SER:CB	10:P:161:VAL:CG2	2.66	0.66
14:T:87:LEU:CD2	14:T:104:PHE:CZ	2.78	0.66
14:T:130:ILE:HG23	14:T:131:PRO:HD2	1.77	0.66
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.60	0.66
4:D:92:HIS:HB2	4:D:458:PHE:HD2	1.60	0.66
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.73	0.66
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.49	0.66
5:E:203:ILE:HG12	5:E:218:ARG:NH1	2.11	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.66
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.66
9:I:92:PRO:HA	21:q:91:HIS:O	1.96	0.66
10:P:199:ILE:HD11	10:P:258:ALA:O	1.96	0.66
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.78	0.66
1:A:61:THR:HG22	8:H:290:TRP:HH2	1.59	0.66
4:D:101:LEU:CD1	4:D:106:VAL:HA	2.26	0.66
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
8:H:249:ILE:HD13	17:X:99:HIS:CG	2.30	0.66
8:H:303:TRP:CZ3	20:b:28:LEU:HG	2.30	0.66
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.77	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.57	0.65
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.06	0.65
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.76	0.65
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.65
7:G:651:PRO:HG3	13:S:57:GLU:H	1.61	0.65
8:H:306:SER:HG	8:H:310:PHE:HE2	1.27	0.65
10:P:263:PHE:HD2	10:P:333:PRO:O	1.79	0.65
18:Z:98:MET:CE	18:Z:101:VAL:HG21	2.26	0.65
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.10	0.65
6:F:425:CYS:SG	25:F:502:SF4:FE1	1.78	0.65
8:H:310:PHE:HB3	20:b:33:PRO:HA	1.77	0.65
16:W:24:PHE:HB2	16:W:83:ASP:CG	2.20	0.65
6:F:300:ILE:HG21	6:F:307:VAL:N	2.11	0.65
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.78	0.65
10:P:236:VAL:CG1	10:P:270:ARG:HH21	2.10	0.65
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.65
16:W:115:THR:O	16:W:116:PRO:C	2.39	0.65
1:A:106:TRP:CZ2	8:H:291:LYS:HA	2.32	0.65
4:D:448:VAL:CG2	8:H:204:GLU:OE1	2.44	0.65
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.65
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.77	0.65
17:X:130:LYS:HG2	20:b:67:PRO:HA	1.77	0.65
19:a:32:GLY:HA3	19:a:60:TYR:CD1	2.32	0.65
2:B:146:ARG:O	2:B:147:LYS:C	2.39	0.65
4:D:144:MET:HE2	4:D:214:TYR:CE2	2.32	0.65
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.65
6:F:383:THR:N	6:F:384:PRO:HD2	2.10	0.65
8:H:1:MET:CG	19:a:30:THR:HG22	2.20	0.65
13:S:16:LEU:HB3	13:S:69:TYR:CD1	2.32	0.65
13:S:24:CYS:HA	13:S:58:CYS:O	1.96	0.65
17:X:53:PRO:HD3	18:Z:116:TRP:NE1	2.12	0.65
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.27	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.65
12:R:38:TYR:HB2	12:R:45:ARG:HD3	1.79	0.65
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.65
8:H:33:LEU:CD2	22:r:25:GLN:HG2	2.26	0.65
10:P:226:VAL:HG21	10:P:281:PHE:CZ	2.32	0.65
10:P:299:SER:CB	10:P:316:LYS:HE3	2.23	0.65
18:Z:62:ILE:HD12	20:b:81:LEU:HD22	1.79	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.65
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.64
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.62	0.64
4:D:92:HIS:C	4:D:94:VAL:N	2.52	0.64
6:F:110:PRO:O	6:F:238:CYS:HB3	1.96	0.64
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.79	0.64
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.64
11:Q:163:ASN:OD1	11:Q:164:PHE:N	2.30	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.64
8:H:19:PHE:CE2	19:a:11:ILE:HG21	2.31	0.64
8:H:42:PRO:HD2	8:H:45:ILE:HG12	1.78	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.32	0.64
14:T:87:LEU:HD21	14:T:104:PHE:CZ	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:GLU:CD	4:D:227:ILE:HB	2.22	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
10:P:156:SER:CB	10:P:161:VAL:HG22	2.20	0.64
14:T:118:ILE:HG23	14:T:122:MET:HE3	1.78	0.64
19:a:51:ASP:HA	19:a:54:ILE:HD12	1.78	0.64
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.62	0.64
13:S:16:LEU:HD12	13:S:16:LEU:C	2.22	0.64
14:T:83:VAL:HG23	14:T:126:PHE:HZ	1.62	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.61	0.64
18:Z:97:ILE:HG13	18:Z:98:MET:H	1.61	0.64
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.60	0.64
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.64
10:P:363:SER:HB3	16:W:51:HIS:CD2	2.32	0.64
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.64
3:C:99:LEU:HD13	3:C:140:ILE:CD1	2.27	0.64
4:D:375:MET:HE1	7:G:126:LEU:HA	1.80	0.64
5:E:163:THR:HG21	5:E:168:PHE:HB2	1.79	0.64
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.64
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.64
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.64
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.64
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.64
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.64
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.77	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.64
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.80	0.64
1:A:54:LYS:HD2	1:A:113:TRP:HB2	1.79	0.64
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.64
10:P:88:VAL:HG12	10:P:92:MET:HE2	1.79	0.64
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.64
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.64
18:Z:26:PRO:HG3	22:r:17:GLY:O	1.98	0.64
2:B:136:THR:CG2	2:B:177:VAL:HG22	2.28	0.64
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.64
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:169:HIS:H	10:P:184:LYS:HE3	1.61	0.64
10:P:333:PRO:HB2	10:P:337:ASP:HB2	1.80	0.64
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	0.63
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.63
14:T:79:ILE:CB	14:T:145:VAL:HG13	2.28	0.63
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.34	0.63
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.63
5:E:81:VAL:HB	5:E:104:LEU:HD11	1.79	0.63
12:R:98:GLU:CD	12:R:98:GLU:H	2.06	0.63
1:A:99:SER:HB3	24:b:201:3PE:H392	1.81	0.63
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
9:I:68:ARG:NH2	18:Z:26:PRO:O	2.32	0.63
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.63
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.63
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.63
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.28	0.63
17:X:7:LEU:HD13	18:Z:87:LEU:HB3	1.81	0.63
18:Z:58:ARG:NH2	20:b:49:THR:CG2	2.62	0.63
22:r:109:ASP:O	22:r:110:GLN:HG2	1.99	0.63
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.80	0.63
10:P:93:HIS:NE2	10:P:94:LEU:HD11	2.14	0.63
14:T:93:ILE:CG2	14:T:110:LEU:HD13	2.28	0.63
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.81	0.63
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.28	0.63
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.79	0.63
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.63
13:S:19:ILE:CG1	13:S:95:LEU:HD11	2.26	0.63
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.63
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.63
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.63
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.63
6:F:33:GLY:HA2	6:F:291:GLU:CB	2.16	0.63
13:S:15:GLY:HA3	13:S:17:ARG:HH22	1.62	0.63
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.62
1:A:49:LEU:HD21	4:D:80:MET:HG2	1.82	0.62
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.62
6:F:48:ARG:HH11	6:F:48:ARG:HA	1.64	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:28:ARG:HG3	18:Z:28:ARG:O	1.99	0.62
22:r:20:LEU:HD12	22:r:21:GLN:N	2.14	0.62
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.62
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.81	0.62
8:H:201:THR:C	8:H:203:GLY:N	2.55	0.62
10:P:240:VAL:HB	10:P:266:THR:O	1.99	0.62
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.62
21:q:137:TRP:CZ2	21:q:140:PRO:HD3	2.34	0.62
5:E:87:ARG:HD2	23:s:77:THR:HG22	1.79	0.62
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.78	0.62
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.28	0.62
17:X:53:PRO:O	17:X:57:LEU:HG	1.99	0.62
19:a:64:LYS:HG2	19:a:65:GLY:N	2.14	0.62
1:A:3:LEU:HD23	24:A:401:3PE:H251	1.80	0.62
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.77	0.62
8:H:42:PRO:HD2	8:H:45:ILE:CG1	2.30	0.62
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.34	0.62
4:D:235:ASP:OD2	18:Z:8:GLN:HG3	2.00	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.64	0.62
13:S:16:LEU:HA	13:S:69:TYR:HA	1.79	0.62
1:A:4:TYR:CE2	24:A:401:3PE:H231	2.34	0.62
2:B:124:SER:HB2	2:B:127:GLN:OE1	1.99	0.62
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.35	0.62
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.30	0.62
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.62
10:P:169:HIS:H	10:P:184:LYS:CE	2.13	0.62
14:T:83:VAL:CG2	14:T:126:PHE:CZ	2.83	0.62
16:W:83:ASP:O	16:W:86:VAL:HG22	1.99	0.62
14:T:103:HIS:ND1	14:T:140:CYS:SG	2.73	0.62
21:q:71:LYS:O	21:q:72:ASN:CG	2.43	0.62
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.62
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.99	0.62
21:q:34:ARG:NE	21:q:58:ARG:NH2	2.48	0.62
34:q:201:CDL:H1	22:r:3:SER:HB2	1.82	0.62
1:A:113:TRP:CE2	8:H:283:ASP:HB2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:226:LYS:O	6:F:227:PRO:C	2.42	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.82	0.62
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.62
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.29	0.62
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.62
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.15	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.29	0.61
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.81	0.61
5:E:182:ALA:O	5:E:183:PRO:C	2.43	0.61
7:G:82:ILE:CG2	7:G:100:TRP:HB3	2.30	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.30	0.61
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.81	0.61
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.61
16:W:24:PHE:HB2	16:W:83:ASP:HB3	1.82	0.61
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.82	0.61
6:F:426:ALA:HB3	29:F:501:FMN:HM81	1.81	0.61
8:H:172:MET:CE	18:Z:46:GLY:HA2	2.30	0.61
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.34	0.61
21:q:7:LEU:HD23	34:q:201:CDL:H311	1.82	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61
4:D:245:TYR:OH	18:Z:17:GLY:C	2.43	0.61
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.61
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.61
6:F:392:MET:HE1	6:F:419:ILE:HD12	1.80	0.61
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.61
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.30	0.61
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.49	0.61
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
3:C:100:ARG:HH12	15:V:86:LYS:NZ	1.99	0.61
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.83	0.61
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.66	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.35	0.61
10:P:179:LYS:HA	10:P:182:ARG:HG2	1.82	0.61
14:T:138:LEU:HD12	14:T:138:LEU:C	2.24	0.61
1:A:2:ASN:HB2	18:Z:143:TYR:HE1	1.66	0.61
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.61
5:E:240:PRO:CA	6:F:60:GLY:HA3	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.83	0.61
9:I:80:GLU:OE2	22:r:26:LEU:HD11	2.01	0.61
14:T:138:LEU:O	14:T:138:LEU:CD1	2.40	0.61
1:A:51:PHE:CD1	4:D:102:SER:HB2	2.36	0.61
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.26	0.61
3:C:98:PHE:CA	15:V:90:LEU:HD11	2.21	0.61
6:F:299:LEU:CD1	6:F:300:ILE:HG13	2.30	0.61
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.61
8:H:1:MET:CB	19:a:30:THR:CG2	2.78	0.61
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.31	0.61
21:q:6:VAL:HG13	34:q:201:CDL:HA21	1.82	0.61
21:q:74:PHE:CD2	21:q:75:TRP:CD1	2.89	0.61
5:E:39:VAL:HG11	7:G:163:LYS:NZ	2.16	0.61
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.61
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.33	0.61
16:W:25:SER:HB2	16:W:31:ALA:HB2	1.83	0.61
16:W:97:ILE:HG23	16:W:98:LYS:HG3	1.82	0.61
1:A:113:TRP:O	1:A:113:TRP:CD1	2.54	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.01	0.60
5:E:233:LEU:HD22	6:F:43:THR:HA	1.83	0.60
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.60
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.60
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.60
16:W:32:LYS:NZ	33:W:201:EHZ:C19	2.63	0.60
17:X:4:ILE:CG2	17:X:5:VAL:N	2.39	0.60
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.60
10:P:169:HIS:HD2	10:P:181:LEU:HD11	1.65	0.60
19:a:36:LYS:HA	19:a:59:ARG:HH21	1.65	0.60
20:b:8:PHE:C	20:b:9:LEU:HD12	2.25	0.60
4:D:88:HIS:CE1	4:D:95:LEU:HB3	2.36	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.83	0.60
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.66	0.60
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.01	0.60
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	0.60
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.60
10:P:66:GLY:O	10:P:67:ARG:C	2.42	0.60
11:Q:167:ASN:O	11:Q:168:LYS:CG	2.49	0.60
13:S:16:LEU:CB	13:S:69:TYR:HD1	2.15	0.60
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.60
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.60
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.82	0.60
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.60
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.60
8:H:183:MET:HE2	27:I:302:PC1:H271	1.83	0.60
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.60
10:P:132:ARG:HG2	31:P:401:NDP:C8A	2.29	0.60
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.37	0.60
13:S:31:GLN:HA	13:S:34:ARG:HE	1.64	0.60
17:X:20:VAL:HG12	17:X:25:LEU:HD21	1.84	0.60
17:X:52:ASP:HB3	18:Z:116:TRP:HB3	1.83	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.84	0.60
8:H:15:ILE:HG22	19:a:15:CYS:SG	2.41	0.60
21:q:85:GLU:HG2	21:q:98:PRO:CB	2.31	0.60
21:q:86:TRP:HA	21:q:98:PRO:HG2	1.84	0.60
22:r:12:ARG:HB3	22:r:20:LEU:HD21	1.84	0.60
1:A:54:LYS:HE3	1:A:55:PHE:CE1	2.37	0.60
3:C:186:ILE:HG13	3:C:187:LEU:HG	1.83	0.60
4:D:148:GLU:HG3	4:D:227:ILE:HB	1.82	0.60
4:D:338:ARG:CZ	18:Z:23:ARG:HB3	2.31	0.60
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	0.60
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.60
1:A:3:LEU:HA	8:H:96:ILE:CD1	2.32	0.60
2:B:100:CYS:SG	25:B:301:SF4:S2	2.99	0.60
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
14:T:103:HIS:HB2	14:T:106:LYS:HB2	1.83	0.60
18:Z:143:TYR:O	18:Z:144:THR:C	2.45	0.60
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.83	0.60
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.60
4:D:83:ASN:O	4:D:84:PHE:C	2.44	0.60
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.60
6:F:199:ARG:CD	23:s:80:PHE:CE2	2.80	0.60
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.66	0.60
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.60
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.60
17:X:143:HIS:CD2	18:Z:114:THR:OG1	2.54	0.60
21:q:96:ASP:OD1	21:q:97:PRO:CD	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:CYS:C	2:B:101:ALA:N	2.59	0.59
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.37	0.59
13:S:25:GLN:HG3	13:S:26:ARG:N	2.17	0.59
16:W:58:THR:HB	16:W:61:GLN:HB2	1.83	0.59
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.59
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.37	0.59
4:D:88:HIS:C	4:D:90:ALA:H	2.10	0.59
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.59
7:G:304:GLU:OE2	10:P:41:ILE:HG12	2.01	0.59
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.59
10:P:146:VAL:HG23	10:P:187:GLY:HA2	1.82	0.59
10:P:318:LYS:HG2	10:P:322:ILE:HD11	1.84	0.59
16:W:122:LEU:HD11	16:W:126:TYR:CZ	2.37	0.59
5:E:222:PHE:H	5:E:225:GLU:CD	2.10	0.59
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
24:A:401:3PE:H2E1	24:A:401:3PE:H2I2	1.84	0.59
2:B:144:ALA:O	2:B:145:LEU:C	2.45	0.59
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.83	0.59
3:C:224:GLU:OE2	10:P:45:LYS:HB3	2.02	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.10	0.59
9:I:63:TRP:CZ2	24:I:301:3PE:H331	2.37	0.59
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.84	0.59
17:X:16:GLU:CD	17:X:68:LEU:HD13	2.27	0.59
18:Z:61:LEU:HA	18:Z:64:ASP:OD2	2.03	0.59
19:a:64:LYS:HG2	19:a:65:GLY:H	1.67	0.59
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.84	0.59
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.59
8:H:171:HIS:HB3	18:Z:49:ARG:HD3	1.84	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.37	0.59
1:A:108:GLN:HG2	1:A:109:LYS:N	2.16	0.59
4:D:238:LEU:HA	18:Z:9:ASP:HB2	1.85	0.59
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.82	0.59
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.59
4:D:81:THR:O	4:D:82:LEU:C	2.45	0.59
5:E:237:PRO:HG3	6:F:49:HIS:CD2	2.38	0.59
8:H:19:PHE:CE2	19:a:11:ILE:CG2	2.86	0.59
17:X:7:LEU:CD1	18:Z:87:LEU:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.85	0.59
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.17	0.59
4:D:128:THR:H	4:D:131:GLN:NE2	2.00	0.59
5:E:233:LEU:HD11	6:F:289:GLU:OE2	2.02	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.59
8:H:127:TYR:HE1	8:H:206:GLU:HB2	1.64	0.59
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.62	0.59
10:P:57:THR:HG23	10:P:123:SER:CB	2.33	0.59
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.32	0.59
19:a:51:ASP:HA	19:a:54:ILE:HB	1.85	0.59
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.32	0.59
5:E:163:THR:HG23	5:E:168:PHE:HB2	1.84	0.59
6:F:297:LYS:HB2	6:F:333:GLU:CB	2.32	0.59
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.59
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.59
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.85	0.59
16:W:67:ARG:HD3	16:W:71:MET:HG2	1.85	0.59
4:D:248:SER:O	18:Z:19:ILE:CG2	2.51	0.59
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.59
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.59
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
10:P:96:LEU:HD12	10:P:96:LEU:C	2.28	0.59
18:Z:105:LYS:O	18:Z:106:VAL:C	2.46	0.59
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.37	0.58
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.84	0.58
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.58
1:A:68:GLU:CD	1:A:98:LEU:HG	2.28	0.58
3:C:130:ASN:HD21	3:C:141:ARG:HE	1.51	0.58
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.58
4:D:248:SER:O	18:Z:19:ILE:HG21	2.02	0.58
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.58
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.84	0.58
8:H:179:TRP:CD1	18:Z:43:LEU:CD2	2.86	0.58
16:W:104:THR:O	16:W:108:ARG:HG3	2.02	0.58
21:q:51:ASP:O	21:q:59:HIS:HB2	2.03	0.58
5:E:190:ASN:HB3	5:E:192:TYR:CD2	2.37	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.86	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
10:P:220:TYR:HA	10:P:223:PHE:HD2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.58
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.58
8:H:142:TYR:CG	8:H:289:LEU:HD12	2.38	0.58
16:W:42:TRP:CZ2	33:W:201:EHZ:O1	2.56	0.58
17:X:21:SER:HA	19:a:54:ILE:HD13	1.84	0.58
17:X:57:LEU:HD11	18:Z:84:LEU:CD1	2.33	0.58
18:Z:82:ARG:O	18:Z:86:ILE:HG13	2.03	0.58
18:Z:122:GLY:O	18:Z:126:GLY:N	2.36	0.58
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.58
4:D:266:ARG:CB	9:I:65:GLU:OE2	2.52	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.16	0.58
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.58
13:S:23:LEU:HD12	13:S:23:LEU:C	2.29	0.58
4:D:388:GLY:HA3	4:D:417:SER:OG	2.02	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.86	0.58
6:F:227:PRO:HB2	6:F:228:PRO:HD3	1.84	0.58
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.58
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.58
12:R:48:PHE:CD2	21:q:125:VAL:HG21	2.39	0.58
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.04	0.58
2:B:115:ASP:O	2:B:116:ARG:C	2.44	0.58
2:B:153:PRO:HB2	2:B:155:PRO:HD2	1.85	0.58
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.58
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.18	0.58
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.37	0.58
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.84	0.58
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.58
8:H:175:LEU:HD21	27:I:302:PC1:H2C1	1.84	0.58
10:P:81:ILE:CD1	12:R:46:VAL:HG11	2.34	0.58
10:P:156:SER:CB	10:P:161:VAL:HG21	2.30	0.58
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.86	0.58
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.02	0.58
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.85	0.58
4:D:338:ARG:HH12	18:Z:23:ARG:HA	1.69	0.58
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
10:P:57:THR:HG23	10:P:123:SER:HB2	1.86	0.58
17:X:53:PRO:CG	18:Z:84:LEU:HD21	2.32	0.58
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.32	0.58
6:F:217:GLU:CD	11:Q:166:TRP:HE1	2.10	0.58
6:F:382:CYS:SG	25:F:502:SF4:S1	3.02	0.58
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.58
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.58
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.39	0.58
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.58
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.86	0.58
13:S:16:LEU:O	13:S:16:LEU:CD1	2.52	0.58
1:A:112:GLU:O	1:A:113:TRP:C	2.47	0.57
4:D:338:ARG:NH2	18:Z:23:ARG:HB3	2.19	0.57
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.57
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.57
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.57
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.57
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.34	0.57
14:T:90:TYR:CE2	14:T:92:LYS:CB	2.87	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	2.36	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.86	0.57
16:W:25:SER:CB	16:W:31:ALA:HB2	2.35	0.57
2:B:110:PRO:HB3	8:H:33:LEU:O	2.04	0.57
8:H:85:LEU:CD2	8:H:108:THR:HB	2.34	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
7:G:171:THR:HG22	7:G:231:LEU:CB	2.34	0.57
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
8:H:99:ASN:OD1	19:a:40:ARG:HG3	2.04	0.57
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.57
10:P:245:VAL:O	10:P:249:ILE:HG13	2.04	0.57
4:D:79:ASN:O	4:D:100:GLU:HB3	2.05	0.57
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.57
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.57
7:G:275:PRO:HB3	7:G:286:ILE:HG23	1.85	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
14:T:90:TYR:CE2	14:T:92:LYS:HB3	2.39	0.57
2:B:92:PRO:HD3	2:B:119:VAL:HG13	1.87	0.57
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.57
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.57
7:G:655:ARG:HH12	13:S:59:SER:N	2.03	0.57
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.04	0.57
17:X:130:LYS:HG2	20:b:67:PRO:CA	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.85	0.57
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.87	0.57
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.57
8:H:5:ASN:HD21	19:a:23:THR:CG2	2.15	0.57
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.57
19:a:60:TYR:O	19:a:62:VAL:HG13	2.04	0.57
2:B:194:CYS:HB2	9:I:153:ILE:O	2.05	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:372:PHE:H	7:G:532:PRO:HB2	1.70	0.57
8:H:127:TYR:HE1	8:H:206:GLU:OE2	1.87	0.57
16:W:83:ASP:O	16:W:87:ILE:HG12	2.04	0.57
17:X:123:GLY:HA2	18:Z:66:GLU:CD	2.29	0.57
4:D:81:THR:HB	4:D:98:VAL:CG2	2.34	0.57
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.57
1:A:52:SER:C	1:A:54:LYS:H	2.11	0.57
4:D:87:GLN:O	4:D:88:HIS:C	2.46	0.57
18:Z:70:ALA:O	18:Z:73:PRO:HD2	2.04	0.57
27:B:303:PC1:H131	8:H:39:ILE:HD11	1.87	0.56
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.56
10:P:315:THR:HG22	10:P:317:ASP:H	1.69	0.56
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.56
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.70	0.56
8:H:9:LEU:HA	19:a:19:PRO:HB3	1.87	0.56
8:H:69:SER:HB3	27:H:402:PC1:H221	1.87	0.56
8:H:69:SER:C	8:H:71:PHE:H	2.12	0.56
21:q:14:VAL:HG13	21:q:23:LEU:CD2	2.35	0.56
21:q:65:THR:HG22	21:q:66:THR:N	2.20	0.56
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.71	0.56
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.05	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.86	0.56
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.56
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.56
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.40	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.56
8:H:69:SER:C	8:H:71:PHE:N	2.61	0.56
8:H:142:TYR:CE1	8:H:289:LEU:HD12	2.39	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:134:ASP:OD1	14:T:134:ASP:O	2.23	0.56
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.56
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.46	0.56
14:T:130:ILE:HD11	14:T:148:ILE:HD11	1.86	0.56
17:X:5:VAL:HG13	17:X:7:LEU:HG	1.87	0.56
2:B:81:LEU:HD22	27:B:303:PC1:H352	1.87	0.56
2:B:154:GLU:O	10:P:89:TYR:OH	2.20	0.56
2:B:173:TYR:O	3:C:203:LEU:HD22	2.05	0.56
4:D:82:LEU:HG	4:D:84:PHE:H	1.70	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
8:H:127:TYR:CE1	8:H:206:GLU:OE2	2.58	0.56
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.89	0.56
10:P:358:THR:HG22	10:P:359:TYR:CD1	2.41	0.56
12:R:62:ASP:O	12:R:66:GLN:HG3	2.06	0.56
17:X:29:ALA:HB2	18:Z:71:LEU:HD11	1.86	0.56
21:q:55:PHE:CG	22:r:26:LEU:HD22	2.40	0.56
2:B:171:TYR:CE1	4:D:120:THR:HG22	2.41	0.56
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.85	0.56
14:T:90:TYR:HE2	14:T:92:LYS:CB	2.19	0.56
2:B:122:ARG:HG3	26:B:302:UQ1:C8	2.35	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.56
4:D:81:THR:HA	4:D:99:LEU:O	2.06	0.56
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.80	0.56
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.87	0.56
1:A:1:MET:O	1:A:4:TYR:N	2.38	0.56
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.06	0.56
8:H:318:MET:HG2	19:a:40:ARG:NH2	2.21	0.56
10:P:64:PHE:HE1	10:P:209:ARG:O	1.88	0.56
10:P:323:HIS:ND1	10:P:323:HIS:O	2.39	0.56
11:Q:167:ASN:O	11:Q:168:LYS:HG2	2.05	0.56
21:q:3:LEU:HD13	34:q:201:CDL:OB7	2.06	0.56
2:B:136:THR:HG21	4:D:118:ARG:HG2	1.87	0.56
3:C:167:ARG:HB3	3:C:186:ILE:HG23	1.87	0.56
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.30	0.56
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.56
12:R:38:TYR:OH	21:q:127:TYR:HB2	2.06	0.56
16:W:32:LYS:HZ3	33:W:201:EHZ:C19	2.19	0.56
17:X:52:ASP:HB3	18:Z:116:TRP:HB2	1.87	0.56
17:X:124:GLN:C	17:X:125:LEU:HD12	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:36:LYS:HA	19:a:59:ARG:NH2	2.21	0.56
20:b:11:ASN:OD1	20:b:12:ALA:N	2.39	0.56
21:q:68:MET:HE1	21:q:81:MET:O	2.06	0.56
2:B:171:TYR:HE1	4:D:120:THR:HG22	1.70	0.56
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.88	0.56
17:X:44:MET:SD	18:Z:73:PRO:HA	2.46	0.56
18:Z:68:ARG:O	18:Z:69:ILE:C	2.49	0.56
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.55
5:E:139:CYS:CB	5:E:144:SER:HB3	2.35	0.55
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.86	0.55
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.55
7:G:126:LEU:HD11	12:R:89:PRO:CB	2.29	0.55
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.55
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.55
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.55
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.55
8:H:172:MET:CE	18:Z:46:GLY:CA	2.81	0.55
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.88	0.55
12:R:41:LYS:H	12:R:41:LYS:HD2	1.71	0.55
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.55
9:I:106:TYR:O	9:I:107:PRO:C	2.49	0.55
11:Q:165:SER:HB3	11:Q:168:LYS:O	2.06	0.55
16:W:24:PHE:HB2	16:W:83:ASP:CB	2.37	0.55
16:W:58:THR:HG22	16:W:60:LYS:N	2.21	0.55
18:Z:69:ILE:HD12	20:b:53:TYR:HA	1.88	0.55
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.87	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
10:P:104:THR:HG22	10:P:106:LEU:CD1	2.37	0.55
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.49	0.55
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.41	0.55
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.55
17:X:55:ARG:HB3	17:X:135:ARG:HH22	1.72	0.55
17:X:119:ARG:NH1	18:Z:63:GLU:OE1	2.39	0.55
1:A:22:PHE:O	1:A:25:PRO:HD2	2.05	0.55
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.31	0.55
3:C:100:ARG:HH12	15:V:86:LYS:HZ1	1.54	0.55
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.55
7:G:179:CYS:SG	25:G:802:SF4:FE3	1.88	0.55
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.83	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.55
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.55
1:A:106:TRP:HZ3	20:b:19:LEU:HD21	1.71	0.55
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.88	0.55
8:H:93:HIS:CE1	19:a:24:ALA:HA	2.42	0.55
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.55
10:P:376:ASN:OD1	10:P:376:ASN:C	2.50	0.55
18:Z:56:GLU:HA	18:Z:59:ARG:HH11	1.72	0.55
24:A:401:3PE:H322	24:A:401:3PE:H262	1.88	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
7:G:399:VAL:HG22	7:G:462:PHE:HZ	1.68	0.55
8:H:5:ASN:ND2	19:a:23:THR:HG23	2.16	0.55
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.55
8:H:134:ARG:NH2	8:H:200:LEU:CD1	2.70	0.55
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.55
10:P:237:LYS:HE3	10:P:322:ILE:O	2.07	0.55
5:E:178:ALA:HA	6:F:125:CYS:SG	2.46	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55
14:T:128:PHE:CE2	14:T:130:ILE:HG13	2.42	0.55
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.06	0.55
18:Z:62:ILE:HD12	20:b:81:LEU:CD2	2.36	0.55
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.55
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.88	0.55
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.36	0.55
6:F:382:CYS:SG	25:F:502:SF4:S4	3.05	0.55
6:F:382:CYS:C	6:F:384:PRO:HD2	2.32	0.55
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.55
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.55
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.55
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.71	0.55
2:B:123:ALA:HB2	30:H:401:UQ9:O2	2.07	0.55
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.07	0.55
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.55
6:F:67:GLU:O	6:F:71:LYS:HG2	2.06	0.55
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.37	0.55
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.55
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.55
10:P:71:ASN:HA	10:P:97:MET:SD	2.47	0.55
13:S:44:LEU:HD13	13:S:91:MET:HG2	1.88	0.55
1:A:52:SER:C	1:A:54:LYS:N	2.62	0.54
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.42	0.54
3:C:186:ILE:O	4:D:113:ILE:HG13	2.07	0.54
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
10:P:98:GLY:HA3	10:P:103:LEU:HG	1.87	0.54
13:S:16:LEU:HD11	13:S:51:LEU:CD1	2.29	0.54
1:A:54:LYS:CG	1:A:55:PHE:N	2.71	0.54
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.54
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.54
4:D:253:LEU:HD11	22:r:18:GLN:HG3	1.90	0.54
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.08	0.54
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.54
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.54
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
12:R:48:PHE:CD2	12:R:53:LYS:HB2	2.42	0.54
14:T:87:LEU:HD22	14:T:104:PHE:CZ	2.41	0.54
16:W:23:ILE:HG22	16:W:24:PHE:CD1	2.42	0.54
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.54
1:A:54:LYS:HG3	1:A:55:PHE:N	2.21	0.54
1:A:72:LEU:HB3	8:H:151:LEU:HD21	1.90	0.54
4:D:242:ASP:HA	18:Z:16:TYR:CE1	2.42	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
7:G:655:ARG:HH12	13:S:59:SER:H	1.55	0.54
8:H:19:PHE:CZ	19:a:11:ILE:CD1	2.89	0.54
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.54
8:H:133:LEU:O	8:H:136:VAL:HG12	2.08	0.54
10:P:357:ARG:HB2	10:P:362:LEU:HD23	1.88	0.54
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.72	0.54
14:T:97:LYS:HG3	14:T:97:LYS:O	2.08	0.54
18:Z:65:LEU:HB3	20:b:50:PRO:O	2.08	0.54
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.54
20:b:59:ASP:HA	20:b:63:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:MET:HE2	2:B:95:PHE:CE1	2.42	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.54
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.54
8:H:123:SER:HB3	8:H:214:GLU:HG3	1.88	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
10:P:370:LYS:HG3	10:P:370:LYS:O	2.08	0.54
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.54
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.54
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.89	0.54
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.54
5:E:131:ILE:HG13	5:E:187:ILE:HG12	1.89	0.54
5:E:187:ILE:O	5:E:188:ASN:C	2.48	0.54
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.22	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.37	0.54
10:P:236:VAL:HG13	10:P:270:ARG:HH21	1.71	0.54
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.73	0.54
14:T:118:ILE:HG23	14:T:122:MET:CE	2.37	0.54
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.35	0.54
21:q:64:TYR:CE2	21:q:82:VAL:HG13	2.42	0.54
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.43	0.54
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
27:H:402:PC1:H281	27:H:402:PC1:H3B1	1.90	0.54
10:P:300:TRP:O	10:P:304:LEU:HG	2.08	0.54
1:A:52:SER:HB3	1:A:54:LYS:HG2	1.88	0.54
1:A:95:VAL:HG11	8:H:302:MET:CG	2.38	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
4:D:81:THR:HG22	4:D:100:GLU:CG	2.17	0.54
4:D:92:HIS:HB2	4:D:458:PHE:CE2	2.43	0.54
5:E:139:CYS:C	5:E:144:SER:HB3	2.33	0.54
9:I:80:GLU:CB	22:r:26:LEU:HD11	2.38	0.54
17:X:90:ASP:OD2	19:a:62:VAL:HG11	2.07	0.54
21:q:95:ASP:OD1	21:q:96:ASP:N	2.41	0.54
2:B:116:ARG:O	8:H:39:ILE:HG22	2.08	0.54
6:F:80:MET:HE2	6:F:95:THR:HG21	1.90	0.54
6:F:199:ARG:HD3	23:s:80:PHE:CD2	2.41	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.73	0.54
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.54
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:123:CYS:SG	25:I:303:SF4:S3	3.06	0.54
11:Q:160:TYR:CZ	11:Q:164:PHE:HZ	2.26	0.54
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.54
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.54
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.90	0.54
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.48	0.54
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.54
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.38	0.54
10:P:207:PHE:CE1	10:P:214:LEU:HD22	2.43	0.54
18:Z:131:GLU:O	18:Z:132:GLU:C	2.48	0.54
19:a:3:PHE:HB3	34:q:201:CDL:H162	1.89	0.54
21:q:68:MET:SD	21:q:81:MET:CB	2.95	0.54
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.53
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.89	0.53
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.53
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.90	0.53
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.27	0.53
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.53
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.53
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.90	0.53
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.53
16:W:58:THR:HG22	16:W:60:LYS:H	1.72	0.53
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.21	0.53
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.89	0.53
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.38	0.53
8:H:19:PHE:HB2	19:a:12:MET:CG	2.37	0.53
10:P:58:VAL:O	10:P:83:PRO:HD2	2.09	0.53
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.44	0.53
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.90	0.53
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.23	0.53
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.53
8:H:19:PHE:CB	19:a:12:MET:CG	2.85	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
10:P:122:HIS:CB	12:R:46:VAL:HG22	2.39	0.53
1:A:1:MET:O	1:A:2:ASN:C	2.48	0.53
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.71	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.53
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.53
27:I:302:PC1:C22	18:Z:35:MET:HE2	2.39	0.53
27:I:302:PC1:H222	18:Z:35:MET:CE	2.38	0.53
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.53
1:A:105:GLU:HG2	1:A:111:LEU:HG	1.90	0.53
4:D:88:HIS:HE1	4:D:95:LEU:H	1.55	0.53
4:D:148:GLU:CG	4:D:227:ILE:HB	2.39	0.53
6:F:85:LEU:HD13	6:F:262:PHE:CE2	2.44	0.53
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.53
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.53
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.52	0.53
10:P:203:PRO:HG2	31:P:401:NDP:C6N	2.37	0.53
10:P:206:ILE:HG13	31:P:401:NDP:H42N	1.89	0.53
13:S:16:LEU:HD13	13:S:19:ILE:CD1	2.38	0.53
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.53
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.90	0.53
2:B:138:THR:HG21	4:D:116:LEU:HA	1.91	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.44	0.53
6:F:238:CYS:O	6:F:239:PRO:C	2.51	0.53
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.53
19:a:1:MET:HB2	19:a:3:PHE:CE2	2.43	0.53
1:A:54:LYS:HD2	1:A:113:TRP:CB	2.38	0.53
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.24	0.53
4:D:81:THR:HB	4:D:98:VAL:HG22	1.90	0.53
5:E:81:VAL:CB	5:E:104:LEU:HD11	2.38	0.53
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.91	0.53
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.53
6:F:300:ILE:CG2	6:F:305:GLY:O	2.45	0.53
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.53
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.53
9:I:109:GLY:O	12:R:63:LEU:HD12	2.08	0.53
14:T:87:LEU:HD23	14:T:122:MET:HE1	1.91	0.53
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.90	0.53
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.39	0.53
6:F:296:LEU:CD1	6:F:337:MET:HE3	2.34	0.53
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.53
10:P:85:ARG:HE	31:P:401:NDP:C2A	2.22	0.53
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.53
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:66:LEU:H	19:a:66:LEU:HD13	1.73	0.53
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.90	0.53
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.91	0.53
4:D:170:ILE:HG21	4:D:232:VAL:HG21	1.90	0.53
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.53
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.53
8:H:1:MET:HB3	19:a:26:ILE:HG23	1.90	0.53
10:P:262:THR:N	10:P:332:LEU:HD12	2.24	0.53
21:q:137:TRP:CH2	21:q:140:PRO:HD3	2.44	0.53
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.90	0.53
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.53
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.53
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.53
7:G:364:ASP:C	7:G:364:ASP:OD1	2.51	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
9:I:80:GLU:HB3	22:r:26:LEU:HD11	1.90	0.53
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.53
10:P:265:PHE:HD1	10:P:334:GLY:HA3	1.74	0.53
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.53
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.53
16:W:101:LYS:HZ1	16:W:109:PHE:HE2	1.57	0.53
17:X:35:GLN:HB2	17:X:70:PHE:CE1	2.44	0.53
2:B:170:TYR:OH	4:D:131:GLN:O	2.28	0.52
3:C:104:ASN:O	22:r:97:PRO:HD3	2.09	0.52
5:E:180:VAL:CG1	5:E:224:CYS:SG	2.96	0.52
5:E:226:PRO:HD3	6:F:46:TYR:CZ	2.44	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.52
7:G:35:PHE:HB2	7:G:101:ASN:HA	1.90	0.52
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.52
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.52
8:H:12:PRO:HB2	19:a:19:PRO:HG3	1.90	0.52
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.52
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.52
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.52
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.23	0.52
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.52
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.52
12:R:69:VAL:HG12	12:R:112:LYS:N	2.24	0.52
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:65:LEU:O	18:Z:69:ILE:HG12	2.09	0.52
21:q:56:PHE:HD1	21:q:59:HIS:NE2	2.06	0.52
2:B:194:CYS:O	25:B:301:SF4:S2	2.67	0.52
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.52
3:C:234:LEU:O	4:D:387:GLU:HG3	2.08	0.52
4:D:101:LEU:HD12	4:D:106:VAL:HA	1.91	0.52
4:D:198:THR:OG1	4:D:261:MET:HE1	2.10	0.52
7:G:36:VAL:O	7:G:39:GLN:HG2	2.07	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.25	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
10:P:283:MET:HE2	10:P:366:ILE:HG22	1.92	0.52
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.52
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.52
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.52
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.74	0.52
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.52
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.75	0.52
6:F:296:LEU:HD22	6:F:337:MET:CE	2.39	0.52
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.52
9:I:54:THR:HA	20:b:13:TRP:HE1	1.73	0.52
10:P:179:LYS:O	10:P:182:ARG:HG2	2.10	0.52
21:q:125:VAL:HG23	21:q:125:VAL:O	2.08	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.09	0.52
26:B:302:UQ1:HM21	4:D:91:ALA:O	2.09	0.52
5:E:134:CYS:SG	5:E:139:CYS:SG	3.06	0.52
6:F:227:PRO:HG3	7:G:94:MET:SD	2.50	0.52
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.52
7:G:35:PHE:CE1	7:G:40:SER:HB2	2.45	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
8:H:16:ALA:HB2	19:a:15:CYS:HB2	1.92	0.52
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.52
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.52
10:P:305:PHE:CG	10:P:314:THR:HG22	2.45	0.52
14:T:130:ILE:CG2	14:T:131:PRO:HD2	2.40	0.52
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.92	0.52
4:D:368:ARG:HA	4:D:371:MET:HG2	1.89	0.52
5:E:87:ARG:HD2	23:s:77:THR:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:80:GLU:OE2	22:r:26:LEU:HD13	2.08	0.52
10:P:153:ALA:CB	10:P:191:VAL:HG23	2.39	0.52
10:P:236:VAL:HG11	10:P:270:ARG:HH21	1.75	0.52
17:X:53:PRO:HD3	18:Z:116:TRP:CE2	2.45	0.52
18:Z:94:GLU:HA	18:Z:97:ILE:CG1	2.39	0.52
21:q:29:ARG:HD3	21:q:74:PHE:CE1	2.44	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.52
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.52
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.52
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.75	0.52
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.92	0.52
14:T:79:ILE:CG2	14:T:145:VAL:HG13	2.40	0.52
1:A:54:LYS:CD	1:A:113:TRP:HB2	2.39	0.52
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.52
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.52
6:F:259:GLY:O	6:F:263:ALA:N	2.40	0.52
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.52
8:H:134:ARG:CZ	8:H:200:LEU:HD13	2.39	0.52
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.52
12:R:98:GLU:HA	12:R:113:GLN:CD	2.34	0.52
18:Z:99:LYS:HG3	18:Z:100:ASP:N	2.25	0.52
20:b:66:VAL:HG11	20:b:70:PRO:HA	1.91	0.52
21:q:29:ARG:HD3	21:q:74:PHE:CD1	2.45	0.52
4:D:85:GLY:O	4:D:88:HIS:ND1	2.43	0.52
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	2.06	0.52
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.40	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
7:G:34:VAL:HG11	7:G:96:VAL:HG22	1.92	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
8:H:5:ASN:ND2	19:a:23:THR:HA	2.25	0.52
12:R:45:ARG:HD2	12:R:48:PHE:CD1	2.44	0.52
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.52
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.52
5:E:196:THR:O	5:E:200:ILE:HD12	2.10	0.52
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.52
7:G:399:VAL:CG2	7:G:462:PHE:CE1	2.87	0.52
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.91	0.52
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.52
16:W:94:GLN:HA	16:W:97:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TRP:CZ3	20:b:19:LEU:HD21	2.45	0.51
3:C:84:GLU:CG	3:C:141:ARG:HH11	2.23	0.51
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.51
6:F:299:LEU:HD12	6:F:300:ILE:HG13	1.91	0.51
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.51
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.51
18:Z:143:TYR:HE2	19:a:36:LYS:NZ	2.07	0.51
19:a:2:TRP:CZ2	34:q:201:CDL:CB6	2.93	0.51
2:B:123:ALA:HB1	30:H:401:UQ9:C3M	2.31	0.51
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.45	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.75	0.51
8:H:222:LEU:O	8:H:223:PHE:C	2.50	0.51
10:P:336:GLU:CG	10:P:342:PRO:HD3	2.38	0.51
14:T:100:VAL:O	14:T:141:PRO:HD2	2.10	0.51
20:b:7:ALA:C	20:b:9:LEU:N	2.68	0.51
20:b:20:VAL:HG22	24:b:201:3PE:H282	1.92	0.51
21:q:65:THR:CG2	21:q:66:THR:N	2.72	0.51
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.92	0.51
1:A:19:LEU:O	1:A:20:VAL:C	2.51	0.51
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
8:H:135:ALA:HB2	8:H:201:THR:OG1	2.10	0.51
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.98	0.51
9:I:155:CYS:SG	25:I:303:SF4:S2	3.08	0.51
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.91	0.51
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.34	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
7:G:639:LEU:HD23	7:G:639:LEU:C	2.36	0.51
8:H:1:MET:HB3	19:a:26:ILE:HG22	1.93	0.51
8:H:200:LEU:HD12	8:H:200:LEU:C	2.36	0.51
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.51
4:D:148:GLU:O	4:D:149:GLN:C	2.52	0.51
5:E:63:GLU:O	5:E:67:LYS:HD3	2.09	0.51
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.92	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
7:G:557:ARG:CG	7:G:579:MET:HE3	2.33	0.51
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.51
2:B:126:ARG:CD	8:H:214:GLU:HA	2.37	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.51
9:I:89:GLU:HG3	21:q:61:TRP:HB3	1.92	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
10:P:65:LEU:HD23	10:P:129:LEU:HD22	1.93	0.51
14:T:87:LEU:HD23	14:T:122:MET:CE	2.40	0.51
16:W:97:ILE:C	16:W:99:VAL:H	2.18	0.51
17:X:52:ASP:HA	18:Z:116:TRP:CG	2.45	0.51
17:X:52:ASP:CB	18:Z:116:TRP:CB	2.89	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.51
2:B:224:ARG:HG3	10:P:85:ARG:HH22	1.76	0.51
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.43	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.51
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.51
10:P:315:THR:HB	10:P:318:LYS:HB2	1.92	0.51
7:G:31:LEU:HB3	7:G:42:MET:HE2	1.93	0.51
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.51
7:G:541:PRO:HB2	7:G:561:PRO:HD3	1.93	0.51
8:H:20:LEU:HA	19:a:12:MET:SD	2.50	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
27:H:402:PC1:H151	10:P:359:TYR:CD1	2.46	0.51
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.46	0.51
10:P:234:LYS:HG2	10:P:234:LYS:O	2.10	0.51
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.51
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.93	0.51
16:W:71:MET:O	16:W:72:LYS:C	2.51	0.51
17:X:25:LEU:O	17:X:29:ALA:N	2.44	0.51
17:X:141:PRO:HG2	17:X:142:TYR:HD1	1.75	0.51
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.29	0.51
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:212:ASN:HA	8:H:215:TYR:HB2	1.93	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
13:S:16:LEU:HD21	13:S:95:LEU:CD1	2.41	0.51
13:S:54:LEU:HD22	13:S:56:ARG:NH1	2.25	0.51
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:22:SER:H	19:a:51:ASP:CG	2.18	0.51
17:X:130:LYS:CG	20:b:67:PRO:HA	2.39	0.51
18:Z:130:LYS:O	18:Z:131:GLU:C	2.52	0.51
2:B:87:ARG:HH11	27:B:303:PC1:P	2.34	0.51
4:D:271:ARG:CD	8:H:279:ARG:O	2.56	0.51
4:D:279:THR:HA	15:V:12:VAL:HG13	1.93	0.51
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.41	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:201:THR:O	8:H:203:GLY:N	2.44	0.51
8:H:249:ILE:HG21	17:X:99:HIS:CE1	2.45	0.51
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.51
10:P:197:GLU:HB3	10:P:259:VAL:HG23	1.93	0.51
10:P:209:ARG:N	10:P:352:VAL:HG22	2.26	0.51
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.51
18:Z:93:GLU:O	18:Z:97:ILE:HG12	2.11	0.51
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.26	0.51
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.46	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.50
6:F:42:PHE:CD1	6:F:137:LYS:HD2	2.46	0.50
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.50
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.12	0.50
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.50
14:T:105:MET:HB2	14:T:139:MET:SD	2.51	0.50
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.50
1:A:2:ASN:HB2	18:Z:143:TYR:CE1	2.46	0.50
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.93	0.50
1:A:108:GLN:CG	1:A:109:LYS:H	2.19	0.50
2:B:94:THR:CG2	2:B:104:MET:SD	3.00	0.50
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.46	0.50
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.50
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.50
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.46	0.50
15:V:44:TYR:CD1	15:V:48:THR:HG23	2.46	0.50
16:W:28:LEU:HG	16:W:32:LYS:HE2	1.93	0.50
17:X:142:TYR:HA	18:Z:115:ARG:HD3	1.92	0.50
1:A:109:LYS:O	1:A:109:LYS:HG2	2.12	0.50
2:B:95:PHE:CZ	2:B:148:VAL:HB	2.28	0.50
5:E:214:LYS:HG3	5:E:214:LYS:O	2.11	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
10:P:212:ARG:O	10:P:213:PHE:C	2.55	0.50
17:X:78:CYS:C	17:X:81:PRO:HD2	2.36	0.50
3:C:241:PHE:H	7:G:146:PHE:HE1	1.59	0.50
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.50
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.50
8:H:15:ILE:HG21	19:a:15:CYS:SG	2.51	0.50
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.50
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.50
27:I:302:PC1:H221	18:Z:35:MET:HE2	1.93	0.50
10:P:172:ALA:H	10:P:202:ARG:NH2	2.08	0.50
12:R:55:VAL:HG22	12:R:56:ASN:H	1.77	0.50
14:T:130:ILE:HG23	14:T:131:PRO:CD	2.40	0.50
17:X:38:LYS:HZ1	17:X:131:VAL:HA	1.76	0.50
18:Z:81:ARG:HG3	18:Z:82:ARG:N	2.25	0.50
1:A:21:ALA:HB2	8:H:218:GLY:HA3	1.91	0.50
2:B:99:CYS:O	2:B:101:ALA:N	2.44	0.50
4:D:146:CYS:SG	4:D:402:ALA:HA	2.52	0.50
4:D:304:LYS:HE2	9:I:35:THR:N	2.26	0.50
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.50
6:F:392:MET:CE	6:F:419:ILE:CD1	2.60	0.50
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.50
13:S:21:VAL:CG2	13:S:91:MET:HE1	2.41	0.50
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.46	0.50
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.50
17:X:124:GLN:O	20:b:70:PRO:HB2	2.10	0.50
19:a:60:TYR:CE1	19:a:61:TYR:CE2	2.99	0.50
4:D:338:ARG:NH1	18:Z:23:ARG:N	2.60	0.50
5:E:75:ALA:O	5:E:78:VAL:HG22	2.11	0.50
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.50
8:H:273:ILE:HD11	24:I:301:3PE:H2A1	1.93	0.50
8:H:280:PHE:HD2	8:H:284:GLN:CG	2.23	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50
10:P:207:PHE:HE1	10:P:214:LEU:HD22	1.76	0.50
11:Q:167:ASN:C	11:Q:168:LYS:HG2	2.36	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
2:B:116:ARG:NH2	2:B:117:PHE:CZ	2.79	0.50
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.50
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.50
6:F:185:ASN:HA	6:F:189:SER:O	2.12	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.50
8:H:30:TYR:OH	19:a:1:MET:O	2.29	0.50
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.77	0.50
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.50
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.50
10:P:305:PHE:HB2	10:P:314:THR:HG22	1.92	0.50
10:P:367:GLU:HG2	10:P:368:GLU:N	2.26	0.50
10:P:374:THR:HG23	10:P:374:THR:O	2.11	0.50
12:R:32:THR:HA	12:R:59:PHE:CZ	2.46	0.50
15:V:56:LEU:HA	15:V:59:VAL:HB	1.94	0.50
18:Z:102:PRO:O	18:Z:103:ASN:C	2.53	0.50
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.50
2:B:84:TRP:HA	2:B:87:ARG:HG2	1.93	0.50
2:B:99:CYS:C	2:B:101:ALA:H	2.19	0.50
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.50
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.93	0.50
6:F:299:LEU:HD11	6:F:300:ILE:HG13	1.93	0.50
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.50
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.50
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.50
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.50
10:P:205:ASP:OD1	10:P:205:ASP:O	2.30	0.50
11:Q:64:LEU:HG	16:W:84:LEU:HD22	1.93	0.50
14:T:140:CYS:HB2	14:T:143:GLU:CG	2.40	0.50
17:X:30:HIS:CE1	18:Z:63:GLU:HG3	2.47	0.50
18:Z:80:ASP:O	18:Z:84:LEU:HG	2.11	0.50
19:a:4:GLU:O	19:a:7:PRO:HD2	2.11	0.50
22:r:6:ARG:HG2	22:r:6:ARG:O	2.11	0.50
2:B:117:PHE:HA	8:H:39:ILE:HG21	1.94	0.50
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.44	0.50
4:D:338:ARG:NH1	18:Z:23:ARG:CA	2.75	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
5:E:129:TYR:CE2	5:E:167:LEU:HG	2.47	0.50
7:G:272:ARG:HH11	7:G:274:LEU:HD23	1.77	0.50
10:P:238:GLN:HB2	10:P:270:ARG:HG2	1.94	0.50
14:T:140:CYS:O	14:T:144:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:140:PHE:O	18:Z:141:THR:C	2.55	0.50
1:A:102:LEU:HD11	1:A:106:TRP:HE1	1.77	0.49
2:B:68:ARG:HD3	2:B:70:ARG:CG	2.41	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.94	0.49
3:C:186:ILE:HG13	3:C:187:LEU:N	2.27	0.49
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.49
4:D:289:SER:N	4:D:293:LEU:HG	2.27	0.49
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.49
6:F:126:LYS:CD	6:F:275:LEU:HB2	2.42	0.49
7:G:401:LEU:HD23	7:G:496:MET:HE1	1.92	0.49
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.49
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.93	0.49
1:A:61:THR:CG2	8:H:290:TRP:CZ3	2.91	0.49
1:A:103:ALA:O	1:A:107:THR:HG23	2.13	0.49
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.13	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.49
12:R:32:THR:OG1	12:R:33:HIS:N	2.39	0.49
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.49
19:a:32:GLY:HA3	19:a:60:TYR:CG	2.47	0.49
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.49
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.49
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.49
10:P:360:ARG:O	10:P:361:TRP:HB2	2.13	0.49
14:T:138:LEU:HD13	14:T:144:ILE:CD1	2.43	0.49
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.49
5:E:129:TYR:HD2	5:E:167:LEU:O	1.94	0.49
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.47	0.49
6:F:225:LEU:N	11:Q:160:TYR:HE2	2.07	0.49
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.94	0.49
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.92	0.49
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.49
17:X:82:PHE:HB3	19:a:64:LYS:HZ2	1.77	0.49
1:A:106:TRP:CE3	24:b:201:3PE:H331	2.48	0.49
2:B:164:CYS:SG	25:B:301:SF4:S4	3.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.49
5:E:137:THR:HG22	6:F:370:LEU:HD21	1.95	0.49
5:E:138:PRO:CG	6:F:122:PRO:HB3	2.38	0.49
5:E:199:ASP:O	5:E:202:GLU:HB3	2.11	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
10:P:64:PHE:CZ	10:P:211:ASP:HB3	2.48	0.49
13:S:25:GLN:O	13:S:26:ARG:C	2.55	0.49
14:T:88:LYS:NZ	14:T:96:GLU:H	2.11	0.49
20:b:23:PHE:CB	24:b:201:3PE:H2D2	2.37	0.49
3:C:75:VAL:HG22	3:C:85:ILE:HG23	1.94	0.49
4:D:213:PHE:O	4:D:217:VAL:HG13	2.13	0.49
5:E:78:VAL:CG1	5:E:104:LEU:HD13	2.42	0.49
9:I:48:VAL:O	20:b:10:LYS:NZ	2.42	0.49
9:I:68:ARG:HH21	18:Z:25:LEU:CD2	2.26	0.49
10:P:70:VAL:HG12	10:P:97:MET:SD	2.52	0.49
10:P:122:HIS:HB2	12:R:46:VAL:HG22	1.94	0.49
20:b:68:SER:O	20:b:69:HIS:C	2.56	0.49
1:A:57:LEU:O	1:A:58:VAL:C	2.54	0.49
4:D:82:LEU:O	4:D:99:LEU:HG	2.12	0.49
4:D:266:ARG:NH1	9:I:60:ILE:HA	2.27	0.49
6:F:163:TYR:CE1	23:s:80:PHE:HB3	2.48	0.49
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.49
8:H:155:LEU:O	8:H:315:PRO:HG3	2.12	0.49
8:H:296:LEU:HD21	24:I:301:3PE:H351	1.95	0.49
18:Z:121:ILE:HG23	18:Z:122:GLY:N	2.25	0.49
3:C:149:LEU:CD1	16:W:80:ARG:HH21	2.19	0.49
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.28	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.48	0.49
6:F:379:CYS:SG	25:F:502:SF4:S1	3.11	0.49
8:H:17:MET:CE	8:H:225:MET:HB3	2.41	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.95	0.49
10:P:315:THR:HB	10:P:318:LYS:H	1.78	0.49
16:W:122:LEU:HD11	16:W:126:TYR:CE2	2.48	0.49
18:Z:89:GLU:HG2	18:Z:128:ARG:NH1	2.27	0.49
20:b:26:TRP:CZ3	24:b:201:3PE:H2G2	2.48	0.49
2:B:175:TYR:OH	4:D:117:HIS:HE1	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.49
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.49
3:C:131:LEU:O	3:C:139:ARG:HG3	2.13	0.49
4:D:166:ARG:CZ	18:Z:8:GLN:HG2	2.43	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.43	0.49
14:T:90:TYR:HE2	14:T:92:LYS:HB3	1.78	0.49
17:X:115:LEU:HD13	17:X:117:TRP:CZ3	2.48	0.49
1:A:18:ILE:O	1:A:21:ALA:HB3	2.13	0.48
2:B:68:ARG:HG2	2:B:69:SER:N	2.29	0.48
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.42	0.48
5:E:129:TYR:CD2	5:E:167:LEU:O	2.66	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.48
6:F:333:GLU:OE2	6:F:334:THR:HG23	2.13	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.48
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.48
12:R:67:GLN:HG2	12:R:109:LEU:HD21	1.95	0.48
16:W:42:TRP:O	16:W:43:TYR:C	2.55	0.48
20:b:48:ALA:O	20:b:49:THR:C	2.53	0.48
3:C:48:PRO:HD3	4:D:162:GLN:OE1	2.13	0.48
4:D:198:THR:HA	8:H:32:GLN:HG2	1.94	0.48
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.48
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.96	0.48
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.48
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.48
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.48
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.48
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.48
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.48
12:R:32:THR:HA	12:R:59:PHE:HZ	1.78	0.48
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.48
16:W:32:LYS:HG2	33:W:201:EHZ:C19	2.44	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
2:B:95:PHE:CE1	2:B:131:MET:HE2	2.40	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.48
3:C:107:PHE:CE2	3:C:140:ILE:HD13	2.48	0.48
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.48
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.95	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
14:T:119:ILE:HG13	14:T:135:ALA:HB1	1.95	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.96	0.48
17:X:22:SER:CB	19:a:47:LEU:HB3	2.42	0.48
2:B:99:CYS:HB3	4:D:141:TYR:CD2	2.47	0.48
4:D:279:THR:HG22	4:D:280:ALA:N	2.29	0.48
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.48
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.48
5:E:81:VAL:HG21	5:E:104:LEU:HD21	1.94	0.48
5:E:164:PRO:C	5:E:166:LYS:H	2.21	0.48
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.48
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.48
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.48
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
9:I:114:ILE:HD13	12:R:106:TYR:CD1	2.48	0.48
10:P:235:THR:O	10:P:236:VAL:C	2.56	0.48
12:R:43:TYR:CD1	12:R:44:ARG:HB2	2.49	0.48
14:T:103:HIS:HD1	14:T:140:CYS:HG	1.53	0.48
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.48
22:r:12:ARG:HE	22:r:20:LEU:HD21	1.78	0.48
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.48	0.48
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.48
5:E:142:ARG:O	5:E:143:ASP:HB2	2.13	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
8:H:142:TYR:CA	8:H:289:LEU:CD1	2.75	0.48
9:I:49:ASP:O	9:I:50:MET:C	2.55	0.48
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.48
10:P:318:LYS:O	10:P:322:ILE:HG13	2.13	0.48
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.14	0.48
12:R:31:ILE:HD11	12:R:37:VAL:HG23	1.96	0.48
14:T:117:GLU:HG2	16:W:43:TYR:CZ	2.48	0.48
19:a:7:PRO:HD3	34:q:201:CDL:H181	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:CD2	4:D:103:GLY:HA3	2.47	0.48
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.44	0.48
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.28	0.48
9:I:49:ASP:O	9:I:53:ALA:N	2.41	0.48
12:R:79:CYS:O	12:R:88:HIS:CE1	2.67	0.48
18:Z:72:MET:O	18:Z:73:PRO:C	2.56	0.48
19:a:3:PHE:CB	34:q:201:CDL:H162	2.44	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.76	0.48
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.48
4:D:375:MET:HE1	7:G:126:LEU:CA	2.43	0.48
5:E:143:ASP:O	5:E:144:SER:C	2.55	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
7:G:541:PRO:HB2	7:G:561:PRO:CG	2.44	0.48
10:P:55:VAL:HG12	10:P:123:SER:HA	1.96	0.48
10:P:170:LEU:HG	10:P:171:ASN:N	2.28	0.48
14:T:104:PHE:CZ	14:T:118:ILE:HG21	2.48	0.48
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.48
22:r:109:ASP:O	22:r:110:GLN:OE1	2.32	0.48
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.49	0.48
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.49	0.48
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.41	0.48
6:F:410:ASP:O	6:F:413:TRP:HB3	2.14	0.48
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.48
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.48
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.48
10:P:111:ARG:NH1	10:P:138:ASN:O	2.44	0.48
10:P:304:LEU:O	10:P:307:LEU:HB3	2.14	0.48
4:D:88:HIS:O	4:D:88:HIS:CG	2.66	0.48
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.13	0.48
4:D:248:SER:C	18:Z:19:ILE:HG21	2.39	0.48
5:E:164:PRO:C	5:E:166:LYS:N	2.72	0.48
8:H:300:LEU:HD23	20:b:25:VAL:HG11	1.95	0.48
10:P:318:LYS:HA	10:P:321:ARG:HH12	1.78	0.48
21:q:23:LEU:HD11	21:q:33:ILE:HG12	1.96	0.48
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.47
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.14	0.47
6:F:296:LEU:HD13	6:F:337:MET:CE	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.14	0.47
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.47
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.47
8:H:318:MET:HG2	19:a:40:ARG:HH22	1.78	0.47
10:P:79:GLN:NE2	10:P:102:GLN:O	2.47	0.47
10:P:311:GLU:O	10:P:312:PRO:C	2.57	0.47
12:R:32:THR:O	12:R:33:HIS:C	2.57	0.47
17:X:20:VAL:CG2	17:X:24:VAL:HG21	2.40	0.47
19:a:3:PHE:O	19:a:6:LEU:HG	2.15	0.47
20:b:23:PHE:HD1	24:b:201:3PE:H3B2	1.77	0.47
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.47
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.48	0.47
5:E:45:GLU:H	5:E:45:GLU:CD	2.21	0.47
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.47
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	0.47
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.44	0.47
7:G:401:LEU:HD23	7:G:496:MET:CE	2.43	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.47
10:P:237:LYS:HZ2	10:P:322:ILE:HG23	1.79	0.47
18:Z:58:ARG:CZ	20:b:49:THR:HG21	2.44	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.47
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.78	0.47
1:A:49:LEU:CD2	4:D:80:MET:HG2	2.43	0.47
2:B:135:GLY:HA2	25:B:301:SF4:S3	2.54	0.47
3:C:124:ARG:HD2	11:Q:140:LYS:HZ1	1.79	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.47
5:E:179:CYS:H	6:F:125:CYS:HB2	1.79	0.47
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.47
8:H:187:ILE:CD1	24:I:301:3PE:H242	2.41	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
10:P:108:TRP:CZ2	31:P:401:NDP:H2A	2.49	0.47
10:P:228:LEU:HD11	10:P:288:PHE:HZ	1.78	0.47
10:P:335:LEU:O	10:P:336:GLU:HB2	2.15	0.47
14:T:87:LEU:CD2	14:T:104:PHE:HZ	2.12	0.47
19:a:37:ARG:HG3	19:a:59:ARG:NH1	2.29	0.47
19:a:45:TRP:O	19:a:49:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:12:ARG:HB3	22:r:20:LEU:CD2	2.43	0.47
24:A:401:3PE:H262	24:A:401:3PE:C32	2.45	0.47
2:B:92:PRO:HG3	2:B:119:VAL:HG13	1.96	0.47
2:B:123:ALA:CB	30:H:401:UQ9:O2	2.62	0.47
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.47
4:D:260:GLU:OE2	18:Z:26:PRO:HD2	2.14	0.47
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.47
6:F:46:TYR:O	6:F:48:ARG:HG2	2.13	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.47
6:F:425:CYS:SG	25:F:502:SF4:S4	3.13	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.96	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:66:THR:HA	8:H:124:ASN:OD1	2.13	0.47
14:T:82:ARG:NH1	14:T:126:PHE:HA	2.29	0.47
17:X:17:GLU:HB3	17:X:19:LYS:HG3	1.96	0.47
20:b:19:LEU:HD21	24:b:201:3PE:H332	1.95	0.47
1:A:63:LEU:O	1:A:67:LEU:HG	2.14	0.47
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.47
6:F:127:ASP:O	6:F:131:MET:HG3	2.14	0.47
7:G:82:ILE:HG21	7:G:100:TRP:HB3	1.96	0.47
9:I:188:GLU:OE1	12:R:56:ASN:CB	2.63	0.47
10:P:76:MET:HE1	10:P:254:LYS:CE	2.45	0.47
16:W:29:ASN:O	16:W:29:ASN:OD1	2.33	0.47
17:X:36:CYS:O	17:X:39:THR:HG22	2.15	0.47
20:b:16:GLU:CD	24:b:201:3PE:H12	2.39	0.47
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.73	0.47
6:F:254:ILE:O	6:F:258:GLY:N	2.48	0.47
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.50	0.47
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.47
7:G:462:PHE:CD1	7:G:465:VAL:HB	2.50	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
8:H:306:SER:OG	20:b:33:PRO:HG3	2.15	0.47
14:T:132:ASP:HB3	16:W:40:ARG:HH12	1.78	0.47
15:V:116:ILE:O	15:V:116:ILE:CG2	2.61	0.47
16:W:58:THR:HB	16:W:61:GLN:HB3	1.94	0.47
21:q:6:VAL:CG1	34:q:201:CDL:HA21	2.45	0.47
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.95	0.47
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.47
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.47
4:D:254:ARG:HH11	22:r:25:GLN:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:299:GLN:HB3	22:r:104:TRP:CE3	2.49	0.47
4:D:359:ASP:O	7:G:150:ARG:NH2	2.48	0.47
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.47
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.47
5:E:92:LEU:HG	5:E:92:LEU:O	2.15	0.47
5:E:191:TYR:O	5:E:192:TYR:C	2.58	0.47
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.47
6:F:166:ALA:HB1	23:s:80:PHE:CD1	2.50	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.47
9:I:48:VAL:HG12	20:b:10:LYS:HZ2	1.80	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.47
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.03	0.47
10:P:245:VAL:HA	10:P:265:PHE:CD2	2.49	0.47
1:A:54:LYS:O	1:A:55:PHE:C	2.58	0.47
3:C:73:GLN:O	3:C:74:GLN:C	2.57	0.47
5:E:70:PRO:HG2	6:F:236:PHE:CE2	2.50	0.47
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.50	0.47
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.97	0.47
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.47
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	2.30	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:358:THR:HG22	10:P:359:TYR:H	1.79	0.47
15:V:50:GLN:HE22	22:r:94:ALA:H	1.63	0.47
18:Z:10:MET:O	18:Z:11:PRO:C	2.56	0.47
19:a:66:LEU:H	19:a:66:LEU:CD1	2.27	0.47
23:s:76:ASN:HB3	23:s:79:THR:HB	1.96	0.47
2:B:90:LEU:O	2:B:119:VAL:HA	2.14	0.47
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.47
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
9:I:107:PRO:O	9:I:108:SER:C	2.57	0.47
10:P:209:ARG:O	10:P:210:GLU:HB2	2.15	0.47
10:P:318:LYS:O	10:P:319:VAL:C	2.58	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
13:S:16:LEU:HD21	13:S:95:LEU:HD12	1.97	0.47
16:W:99:VAL:HG13	16:W:99:VAL:O	2.15	0.47
17:X:32:TYR:HD2	18:Z:71:LEU:HD23	1.80	0.47

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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	0.47
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.50	0.47
2:B:99:CYS:O	2:B:100:CYS:C	2.57	0.47
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.12	0.47
4:D:83:ASN:O	4:D:85:GLY:N	2.48	0.47
4:D:381:HIS:HE1	9:I:161:ALA:O	1.98	0.47
6:F:217:GLU:CD	6:F:224:ARG:HH22	2.23	0.47
6:F:281:HIS:HB3	6:F:358:ASP:CG	2.40	0.47
7:G:82:ILE:HG23	7:G:100:TRP:HB3	1.96	0.47
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.74	0.47
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.97	0.47
10:P:276:LEU:O	10:P:280:ILE:HG13	2.15	0.47
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.48	0.47
12:R:47:ARG:HG3	12:R:48:PHE:CD1	2.50	0.47
12:R:88:HIS:HB2	12:R:89:PRO:HD2	1.96	0.47
16:W:113:THR:O	16:W:113:THR:HG22	2.15	0.47
17:X:69:ASN:OD1	17:X:70:PHE:N	2.47	0.47
1:A:73:LEU:O	8:H:160:TYR:OH	2.30	0.46
2:B:140:LYS:O	2:B:143:PRO:HD2	2.14	0.46
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.50	0.46
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.46
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.46
8:H:180:PRO:HD3	18:Z:43:LEU:HD21	1.97	0.46
8:H:200:LEU:CD2	8:H:282:TYR:HD1	2.28	0.46
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.46
10:P:315:THR:O	10:P:316:LYS:C	2.57	0.46
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.46
15:V:56:LEU:HD12	15:V:57:ASP:CA	2.45	0.46
19:a:59:ARG:HG3	19:a:60:TYR:N	2.29	0.46
20:b:23:PHE:CD1	24:b:201:3PE:H3B2	2.50	0.46
21:q:68:MET:SD	21:q:81:MET:HG2	2.55	0.46
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.46
8:H:310:PHE:O	20:b:38:TYR:HB2	2.15	0.46
27:H:402:PC1:C21	27:H:402:PC1:H252	2.46	0.46
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.97	0.46
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.39	0.46
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.46
19:a:22:SER:O	19:a:23:THR:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:SER:HA	3:C:203:LEU:CD2	2.46	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.97	0.46
5:E:143:ASP:O	5:E:146:SER:N	2.49	0.46
5:E:145:ASP:O	5:E:146:SER:C	2.56	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.46
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.46
9:I:123:CYS:SG	25:I:303:SF4:S4	3.13	0.46
19:a:2:TRP:CH2	34:q:201:CDL:OB8	2.68	0.46
21:q:76:ASP:OD1	21:q:76:ASP:C	2.57	0.46
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.96	0.46
2:B:127:GLN:CD	2:B:127:GLN:N	2.72	0.46
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.98	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.16	0.46
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.48	0.46
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.46
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.46
8:H:26:LYS:HB3	19:a:5:ILE:HG22	1.98	0.46
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.98	0.46
13:S:44:LEU:CD1	13:S:91:MET:HG2	2.45	0.46
1:A:58:VAL:CG2	8:H:286:MET:HE1	2.45	0.46
2:B:124:SER:H	30:H:401:UQ9:H3MB	1.79	0.46
3:C:67:ILE:HD11	15:V:47:TYR:CD2	2.51	0.46
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.46
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.46
5:E:73:HIS:ND1	11:Q:166:TRP:CE3	2.84	0.46
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.39	0.46
6:F:299:LEU:CD1	6:F:300:ILE:N	2.67	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.46
10:P:287:THR:HG23	10:P:289:ILE:HD11	1.97	0.46
10:P:357:ARG:NH2	10:P:364:SER:O	2.47	0.46
12:R:54:GLU:HB2	21:q:124:TYR:CD1	2.51	0.46
13:S:34:ARG:O	13:S:38:VAL:HG23	2.16	0.46
17:X:115:LEU:HD13	17:X:117:TRP:CZ2	2.51	0.46
18:Z:28:ARG:O	18:Z:28:ARG:CG	2.64	0.46
20:b:69:HIS:CD2	20:b:71:GLN:H	2.33	0.46
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.46
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
9:I:53:ALA:O	9:I:54:THR:C	2.56	0.46
10:P:207:PHE:CD2	10:P:241:TYR:HD1	2.33	0.46
12:R:54:GLU:HB2	21:q:124:TYR:HD1	1.81	0.46
15:V:22:GLU:O	15:V:26:ILE:HG12	2.16	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.59	0.46
19:a:46:TYR:HD2	19:a:47:LEU:HD12	1.81	0.46
20:b:19:LEU:CD2	24:b:201:3PE:H332	2.46	0.46
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.46
4:D:256:ASP:CG	18:Z:23:ARG:HA	2.39	0.46
5:E:245:GLN:HB3	6:F:256:ARG:O	2.16	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
6:F:300:ILE:HD13	6:F:307:VAL:HG22	1.96	0.46
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.46
7:G:35:PHE:O	7:G:101:ASN:HA	2.16	0.46
7:G:655:ARG:NH1	13:S:59:SER:H	2.14	0.46
8:H:140:ILE:HG13	8:H:141:SER:N	2.29	0.46
10:P:153:ALA:HB3	10:P:194:VAL:CG2	2.46	0.46
14:T:87:LEU:CD2	14:T:122:MET:HE1	2.46	0.46
15:V:56:LEU:HD13	15:V:60:LYS:HE2	1.98	0.46
17:X:139:GLU:CD	17:X:139:GLU:H	2.23	0.46
18:Z:62:ILE:O	18:Z:66:GLU:HG3	2.16	0.46
21:q:98:PRO:O	21:q:99:THR:C	2.59	0.46
6:F:224:ARG:HD3	11:Q:164:PHE:CE1	2.51	0.46
8:H:19:PHE:HB2	19:a:12:MET:HG2	1.97	0.46
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.46
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.46
9:I:62:MET:SD	18:Z:35:MET:HG2	2.56	0.46
10:P:261:LYS:HB2	10:P:263:PHE:CE1	2.51	0.46
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.50	0.46
2:B:136:THR:HG21	2:B:177:VAL:CG2	2.44	0.46
5:E:136:THR:HB	28:E:301:FES:S2	2.56	0.46
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
8:H:302:MET:SD	20:b:26:TRP:CD1	3.09	0.46
16:W:32:LYS:HZ2	33:W:201:EHZ:C19	2.28	0.46
17:X:35:GLN:O	17:X:36:CYS:CB	2.64	0.46
17:X:107:PHE:O	17:X:110:CYS:SG	2.73	0.46
20:b:28:LEU:O	20:b:32:MET:HG2	2.15	0.46
34:q:201:CDL:H141	34:q:201:CDL:H321	1.97	0.46
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:SER:HB2	4:D:123:LEU:HD21	1.98	0.46
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.46
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.46
5:E:221:ARG:HB2	5:E:225:GLU:HG2	1.98	0.46
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.46
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.46
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.46
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.46
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.46
8:H:179:TRP:HE1	18:Z:43:LEU:HG	1.81	0.46
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.46
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.50	0.46
9:I:61:LEU:O	24:I:301:3PE:H332	2.15	0.46
10:P:66:GLY:O	10:P:69:VAL:N	2.48	0.46
19:a:50:ARG:HA	19:a:53:ARG:NH1	2.31	0.46
20:b:45:ILE:N	20:b:80:TRP:HH2	2.14	0.46
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.51	0.45
4:D:152:SER:O	4:D:153:ILE:C	2.57	0.45
4:D:248:SER:HB2	18:Z:19:ILE:HD13	1.97	0.45
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.45
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.45
13:S:20:ARG:HG3	13:S:54:LEU:CB	2.43	0.45
13:S:25:GLN:HG3	13:S:26:ARG:H	1.80	0.45
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.28	0.45
2:B:123:ALA:CA	30:H:401:UQ9:H3MB	2.46	0.45
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.80	0.45
3:C:132:LEU:HD11	4:D:300:TRP:CZ2	2.50	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
4:D:140:ASP:O	4:D:143:SER:O	2.35	0.45
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.45
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.98	0.45
7:G:32:ILE:HD11	7:G:45:PRO:HG3	1.98	0.45
7:G:35:PHE:CE1	7:G:40:SER:CB	2.99	0.45
7:G:97:MET:HB2	7:G:100:TRP:NE1	2.30	0.45
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.45
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.45
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.45
13:S:19:ILE:HD12	13:S:94:VAL:CG1	2.44	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
19:a:50:ARG:HG2	19:a:54:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:14:VAL:HA	21:q:23:LEU:HD22	1.98	0.45
22:r:109:ASP:O	22:r:110:GLN:CG	2.64	0.45
1:A:106:TRP:CH2	8:H:291:LYS:HA	2.51	0.45
4:D:88:HIS:C	4:D:90:ALA:N	2.73	0.45
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	3.05	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.31	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.45
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.45
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.45
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.45
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	0.45
8:H:312:ALA:CB	20:b:38:TYR:HB3	2.44	0.45
27:I:302:PC1:H112	18:Z:29:GLY:HA3	1.98	0.45
10:P:170:LEU:HD12	10:P:171:ASN:H	1.81	0.45
17:X:122:LEU:HD23	20:b:82:LYS:HG2	1.98	0.45
19:a:2:TRP:O	19:a:3:PHE:C	2.56	0.45
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
5:E:60:LYS:O	5:E:61:ARG:C	2.57	0.45
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.51	0.45
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.51	0.45
6:F:51:TRP:CB	6:F:133:HIS:O	2.64	0.45
10:P:218:ALA:HB2	10:P:280:ILE:CG2	2.47	0.45
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.45
16:W:42:TRP:CZ2	16:W:93:LEU:HB2	2.51	0.45
17:X:5:VAL:CG1	17:X:7:LEU:HG	2.46	0.45
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.45
3:C:130:ASN:ND2	3:C:141:ARG:HE	2.13	0.45
4:D:97:LEU:HD23	4:D:111:PRO:HA	1.98	0.45
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.45
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.45
5:E:39:VAL:HG21	7:G:163:LYS:NZ	2.31	0.45
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.45
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.45
6:F:300:ILE:CG2	6:F:306:GLY:C	2.90	0.45
7:G:163:LYS:HE2	12:R:97:LYS:NZ	2.31	0.45
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
9:I:60:ILE:CG2	24:I:301:3PE:H111	2.46	0.45
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.45
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.45
17:X:123:GLY:CA	18:Z:66:GLU:OE2	2.52	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.47	0.45
7:G:35:PHE:CD1	7:G:40:SER:HB2	2.51	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
10:P:259:VAL:H	10:P:261:LYS:HG2	1.82	0.45
14:T:83:VAL:HG21	14:T:145:VAL:HG22	1.99	0.45
18:Z:94:GLU:HA	18:Z:97:ILE:HG12	1.99	0.45
21:q:74:PHE:HD2	21:q:75:TRP:CD1	2.33	0.45
2:B:99:CYS:O	2:B:102:VAL:N	2.45	0.45
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.32	0.45
5:E:52:PHE:O	5:E:99:LYS:HG3	2.17	0.45
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.45
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.45
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.80	0.45
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.45
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.99	0.45
12:R:89:PRO:HG2	12:R:106:TYR:CZ	2.51	0.45
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.45
17:X:32:TYR:CD2	18:Z:71:LEU:HD23	2.52	0.45
34:q:201:CDL:H321	34:q:201:CDL:C14	2.47	0.45
3:C:100:ARG:NH1	15:V:86:LYS:NZ	2.64	0.45
3:C:101:ASP:OD1	15:V:86:LYS:HE3	2.16	0.45
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.45
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.98	0.45
7:G:176:CYS:SG	25:G:802:SF4:S1	3.14	0.45
7:G:341:ILE:HD12	7:G:555:ILE:CG1	2.47	0.45
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.52	0.45
9:I:188:GLU:OE1	12:R:56:ASN:HB2	2.16	0.45
10:P:245:VAL:HA	10:P:265:PHE:HD2	1.82	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
14:T:130:ILE:CG2	14:T:131:PRO:CD	2.95	0.45
17:X:18:VAL:HG21	18:Z:74:LEU:HD11	1.99	0.45
21:q:71:LYS:HB2	21:q:73:THR:HG23	1.98	0.45
2:B:127:GLN:OE1	2:B:127:GLN:N	2.50	0.45
3:C:133:SER:O	3:C:133:SER:OG	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:257:ARG:CG	6:F:261:TRP:CD2	2.93	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.45
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.45
7:G:450:LYS:HG3	7:G:450:LYS:O	2.17	0.45
8:H:224:PHE:CE2	30:H:401:UQ9:C14	3.00	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
9:I:58:ALA:HB2	18:Z:36:PHE:CE2	2.52	0.45
10:P:238:GLN:HB3	10:P:326:ASP:OD2	2.17	0.45
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.45
15:V:56:LEU:HD11	15:V:57:ASP:OD1	2.17	0.45
17:X:127:LYS:HD2	20:b:70:PRO:O	2.17	0.45
17:X:142:TYR:HB3	18:Z:115:ARG:NH1	2.31	0.45
18:Z:121:ILE:HD11	18:Z:136:ALA:HB3	1.98	0.45
20:b:20:VAL:HA	24:b:201:3PE:H282	1.99	0.45
3:C:149:LEU:O	16:W:23:ILE:HD11	2.17	0.45
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.45
4:D:198:THR:HG21	8:H:275:ALA:HB1	1.99	0.45
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.47	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.31	0.45
8:H:13:ILE:HD13	19:a:16:LEU:HD23	1.98	0.45
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.45
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.45
14:T:118:ILE:CG2	14:T:122:MET:HE3	2.47	0.45
14:T:119:ILE:CD1	14:T:138:LEU:HD11	2.43	0.45
14:T:133:ILE:HG23	14:T:134:ASP:N	2.32	0.45
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.45
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.52	0.45
21:q:85:GLU:CG	21:q:98:PRO:HB3	2.36	0.45
2:B:127:GLN:NE2	8:H:212:ASN:O	2.50	0.44
3:C:78:SER:C	3:C:80:LEU:H	2.24	0.44
3:C:80:LEU:HD12	4:D:396:THR:HG22	1.97	0.44
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.44
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.18	0.44
5:E:69:TYR:HE2	5:E:80:PRO:HG2	1.81	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.44

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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	0.44
8:H:89:LEU:HD12	8:H:89:LEU:HA	1.87	0.44
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.44
10:P:64:PHE:CE1	10:P:209:ARG:O	2.69	0.44
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.44
16:W:20:VAL:HG21	16:W:80:ARG:CZ	2.48	0.44
20:b:38:TYR:O	20:b:39:THR:C	2.59	0.44
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.52	0.44
4:D:90:ALA:O	4:D:193:ASP:OD2	2.35	0.44
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.44
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.44
4:D:266:ARG:NH2	9:I:59:ARG:O	2.50	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.57	0.44
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.44
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.44
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.44
8:H:280:PHE:HD2	8:H:284:GLN:HG3	1.81	0.44
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.44
22:r:5:THR:HG22	22:r:5:THR:O	2.18	0.44
3:C:107:PHE:CE1	3:C:133:SER:HB3	2.53	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	2.18	0.44
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.83	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
6:F:297:LYS:HB2	6:F:333:GLU:HB2	2.00	0.44
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.44
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:20:LEU:CA	19:a:12:MET:SD	3.05	0.44
8:H:277:TYR:CE2	24:I:301:3PE:H271	2.53	0.44
10:P:209:ARG:CA	10:P:352:VAL:HG22	2.47	0.44
16:W:58:THR:HB	16:W:61:GLN:H	1.82	0.44
17:X:82:PHE:HB3	19:a:64:LYS:NZ	2.32	0.44
1:A:48:ARG:C	1:A:49:LEU:HD22	2.43	0.44
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.44
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.44
5:E:177:GLY:O	28:E:301:FES:S1	2.75	0.44
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.17	0.44
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.99	0.44
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.51	0.44
8:H:293:PHE:CE1	24:I:301:3PE:H32	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:I:301:3PE:H241	24:I:301:3PE:H272	1.60	0.44
10:P:55:VAL:HA	10:P:79:GLN:O	2.17	0.44
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.44
10:P:310:PHE:O	10:P:311:GLU:C	2.60	0.44
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.44
18:Z:131:GLU:O	18:Z:134:SER:N	2.51	0.44
2:B:120:VAL:HG21	30:H:401:UQ9:H1M	1.91	0.44
2:B:147:LYS:HD2	2:B:147:LYS:HA	1.75	0.44
3:C:98:PHE:HE1	15:V:44:TYR:CE1	2.35	0.44
3:C:197:PHE:CZ	4:D:121:GLU:HB2	2.53	0.44
6:F:231:ALA:O	6:F:239:PRO:HA	2.18	0.44
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.44
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.28	0.44
6:F:382:CYS:HA	7:G:74:ASN:O	2.17	0.44
7:G:32:ILE:CG2	7:G:98:LYS:HD2	2.47	0.44
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.17	0.44
27:H:402:PC1:H342	27:H:402:PC1:H371	1.84	0.44
10:P:140:ASP:O	10:P:143:ASP:N	2.51	0.44
10:P:168:SER:O	10:P:202:ARG:HA	2.17	0.44
10:P:231:LEU:HD11	10:P:290:PRO:HB2	2.00	0.44
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.44
14:T:79:ILE:O	14:T:83:VAL:HG23	2.17	0.44
18:Z:75:PHE:CD1	19:a:46:TYR:HE2	2.35	0.44
2:B:94:THR:HG21	2:B:104:MET:SD	2.57	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.44
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.44
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.44
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:66:THR:O	27:H:402:PC1:H153	2.18	0.44
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.44
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.44
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.44
9:I:50:MET:O	9:I:51:LYS:C	2.60	0.44
10:P:81:ILE:HD13	12:R:46:VAL:HG11	2.00	0.44
10:P:140:ASP:O	10:P:141:PHE:C	2.61	0.44
17:X:50:GLU:OE1	17:X:55:ARG:HB3	2.18	0.44
18:Z:143:TYR:HE2	19:a:36:LYS:HZ2	1.65	0.44
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.44
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.44
5:E:90:GLY:HA3	5:E:126:VAL:HG12	1.99	0.44
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.32	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
7:G:303:THR:HB	7:G:614:GLY:HA3	1.98	0.44
8:H:99:ASN:CG	19:a:40:ARG:HG3	2.42	0.44
8:H:171:HIS:CE1	18:Z:53:TRP:CE3	3.06	0.44
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.44
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.44
21:q:55:PHE:CD1	22:r:26:LEU:CD2	2.96	0.44
1:A:105:GLU:OE2	1:A:110:GLY:HA3	2.18	0.44
4:D:145:MET:O	4:D:146:CYS:C	2.59	0.44
4:D:376:GLU:HG2	7:G:121:LEU:CD1	2.47	0.44
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.44
6:F:333:GLU:H	6:F:333:GLU:CD	2.25	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.44
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.44
10:P:278:LYS:O	10:P:282:GLY:N	2.51	0.44
10:P:305:PHE:CB	10:P:314:THR:HG22	2.47	0.44
10:P:361:TRP:O	10:P:364:SER:HB3	2.18	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.44
14:T:92:LYS:O	14:T:92:LYS:HG2	2.16	0.44
2:B:97:LEU:HB2	2:B:134:ALA:O	2.18	0.44
2:B:117:PHE:HA	8:H:39:ILE:CG2	2.48	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:140:MET:HE1	6:F:366:ALA:HA	2.00	0.44
6:F:226:LYS:HD3	6:F:226:LYS:HA	1.84	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.44
7:G:466:LEU:HD13	7:G:500:ILE:CG1	2.48	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
8:H:63:PRO:HD2	8:H:66:THR:HG21	2.00	0.44
8:H:186:PHE:CE2	24:I:301:3PE:H2B1	2.52	0.44
9:I:60:ILE:HG23	24:I:301:3PE:H111	1.99	0.44
10:P:220:TYR:HA	10:P:223:PHE:CD2	2.51	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
18:Z:72:MET:SD	20:b:53:TYR:HB2	2.57	0.44
3:C:78:SER:C	3:C:80:LEU:N	2.76	0.43
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
4:D:376:GLU:HG2	7:G:121:LEU:HD12	1.98	0.43
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.43
17:X:52:ASP:CB	18:Z:116:TRP:HB2	2.46	0.43
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.83	0.43
6:F:44:ASN:HB2	6:F:59:ARG:HD3	1.99	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
7:G:422:TRP:HZ2	7:G:441:ARG:HB3	1.82	0.43
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.43
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.43
9:I:35:THR:HG22	22:r:107:SER:HA	1.97	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.00	0.43
13:S:16:LEU:CB	13:S:69:TYR:CD1	2.97	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.43
17:X:66:CYS:O	17:X:67:ALA:C	2.62	0.43
20:b:6:SER:OG	20:b:10:LYS:HD2	2.18	0.43
1:A:23:TRP:O	1:A:26:GLN:HG3	2.19	0.43
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.43
3:C:124:ARG:HD2	11:Q:140:LYS:HZ2	1.84	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.43
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.43
8:H:128:SER:HA	8:H:210:GLY:O	2.19	0.43
8:H:196:ALA:C	8:H:198:PHE:N	2.76	0.43
27:H:402:PC1:H342	27:H:402:PC1:H251	1.99	0.43
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.43
10:P:104:THR:HG22	10:P:106:LEU:HD12	2.00	0.43
10:P:170:LEU:O	10:P:171:ASN:CG	2.61	0.43
14:T:133:ILE:O	14:T:136:GLU:N	2.46	0.43
16:W:97:ILE:C	16:W:99:VAL:N	2.73	0.43
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.43
3:C:167:ARG:CZ	3:C:186:ILE:HG22	2.49	0.43
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.43
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.96	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.43
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
7:G:462:PHE:CZ	7:G:466:LEU:HD21	2.54	0.43
8:H:5:ASN:CG	19:a:23:THR:HA	2.43	0.43
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.52	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.97	0.43
8:H:138:GLN:HG3	8:H:139:THR:N	2.34	0.43
8:H:257:THR:O	8:H:260:MET:HB3	2.19	0.43
14:T:113:LEU:O	14:T:116:VAL:HB	2.17	0.43
17:X:20:VAL:O	19:a:50:ARG:NH1	2.51	0.43
18:Z:68:ARG:HG3	18:Z:69:ILE:N	2.34	0.43
1:A:63:LEU:O	1:A:64:LEU:C	2.61	0.43
2:B:194:CYS:SG	4:D:138:ARG:NE	2.91	0.43
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
4:D:339:GLN:NE2	9:I:37:LYS:HZ2	2.15	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.01	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.27	0.43
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
8:H:33:LEU:HD21	22:r:25:GLN:HG2	2.01	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
10:P:81:ILE:HG23	10:P:106:LEU:HD13	2.00	0.43
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.43
14:T:87:LEU:CD2	14:T:104:PHE:CE1	2.94	0.43
14:T:109:GLY:O	14:T:110:LEU:C	2.61	0.43
19:a:12:MET:HE2	19:a:12:MET:HB3	1.90	0.43
3:C:149:LEU:HD21	11:Q:59:LEU:HD22	2.00	0.43
4:D:88:HIS:CE1	4:D:92:HIS:O	2.72	0.43
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.43
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.43
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.43
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.48	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
9:I:78:PHE:HB3	22:r:8:ILE:HG22	1.99	0.43
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.43
10:P:142:GLU:O	10:P:146:VAL:CG1	2.62	0.43
16:W:25:SER:OG	16:W:34:ARG:NH2	2.52	0.43
18:Z:108:GLU:O	18:Z:109:SER:C	2.61	0.43
21:q:7:LEU:CD2	34:q:201:CDL:H311	2.49	0.43
1:A:73:LEU:O	1:A:76:PRO:HD2	2.18	0.43
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.43
8:H:157:ASN:ND2	8:H:164:THR:OG1	2.49	0.43
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.43
8:H:200:LEU:CD1	8:H:201:THR:N	2.70	0.43
9:I:162:CYS:SG	25:I:304:SF4:S2	3.17	0.43
10:P:76:MET:HE1	10:P:254:LYS:HE2	2.01	0.43
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.43
10:P:259:VAL:N	10:P:261:LYS:HG2	2.33	0.43
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.00	0.43
10:P:358:THR:O	10:P:362:LEU:HG	2.19	0.43
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.43
17:X:10:LEU:HD12	17:X:13:LEU:HD12	2.01	0.43
17:X:35:GLN:HB2	17:X:70:PHE:CD1	2.53	0.43
24:b:201:3PE:H281	24:b:201:3PE:H252	1.85	0.43
3:C:240:ALA:O	3:C:241:PHE:C	2.62	0.43
4:D:279:THR:HA	15:V:12:VAL:CG1	2.49	0.43
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.43
6:F:88:ARG:HA	6:F:88:ARG:HD3	1.85	0.43
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.43
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.43
7:G:82:ILE:HG22	7:G:100:TRP:HE3	1.83	0.43
8:H:17:MET:HE1	8:H:225:MET:HE3	2.01	0.43
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.43
10:P:172:ALA:H	10:P:202:ARG:HH21	1.67	0.43
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.43
14:T:113:LEU:HD22	16:W:71:MET:HE2	2.01	0.43
16:W:47:PRO:HG3	16:W:63:ARG:NH2	2.26	0.43
21:q:21:ARG:HD2	21:q:21:ARG:HA	1.80	0.43
1:A:52:SER:O	1:A:55:PHE:N	2.51	0.43
1:A:81:THR:O	20:b:46:ASN:ND2	2.52	0.43
1:A:106:TRP:CH2	8:H:295:PRO:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.51	0.43
5:E:70:PRO:HG2	6:F:236:PHE:CD2	2.54	0.43
5:E:124:LYS:HB3	5:E:125:PRO:HD2	2.01	0.43
8:H:19:PHE:CD2	19:a:11:ILE:HB	2.53	0.43
8:H:90:PRO:O	8:H:91:MET:C	2.60	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.59	0.43
8:H:303:TRP:HB2	20:b:25:VAL:CG1	2.49	0.43
9:I:42:LYS:HA	9:I:42:LYS:HD3	1.84	0.43
10:P:73:LEU:HD23	10:P:73:LEU:HA	1.89	0.43
10:P:153:ALA:HB2	10:P:191:VAL:HG23	2.01	0.43
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.82	0.43
14:T:93:ILE:HD11	14:T:118:ILE:HD11	2.00	0.43
16:W:57:ILE:HG23	16:W:107:MET:HE1	2.00	0.43
16:W:83:ASP:O	16:W:86:VAL:CG2	2.66	0.43
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.43
19:a:52:ARG:HG3	19:a:57:VAL:O	2.18	0.43
21:q:138:VAL:O	21:q:139:PRO:C	2.62	0.43
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.43
5:E:189:ASP:CG	6:F:163:TYR:HB3	2.44	0.43
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.43
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
8:H:21:THR:HG21	30:H:401:UQ9:H16	2.01	0.43
8:H:134:ARG:HH21	8:H:200:LEU:CD1	2.32	0.43
13:S:58:CYS:SG	13:S:59:SER:N	2.92	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.42
5:E:78:VAL:HG12	5:E:104:LEU:CD1	2.44	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
6:F:126:LYS:HG3	6:F:275:LEU:HD22	2.01	0.42
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.42
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.42
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
10:P:81:ILE:HD11	12:R:46:VAL:HG11	2.00	0.42
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.42
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.42
15:V:56:LEU:CD1	15:V:57:ASP:OD1	2.67	0.42
16:W:23:ILE:HG22	16:W:24:PHE:HD1	1.81	0.42
18:Z:44:ILE:HD13	18:Z:44:ILE:HA	1.85	0.42
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.42
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.42
6:F:127:ASP:HB3	6:F:245:VAL:HG21	2.00	0.42
6:F:296:LEU:HD22	6:F:337:MET:HE1	2.01	0.42
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.42
7:G:281:ILE:HD12	7:G:282:ASN:N	2.34	0.42
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.42
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.54	0.42
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.42
13:S:16:LEU:HD21	13:S:95:LEU:HG	2.00	0.42
16:W:36:ARG:O	16:W:39:TYR:N	2.51	0.42
16:W:71:MET:O	16:W:74:ALA:N	2.43	0.42
1:A:60:ILE:O	1:A:61:THR:C	2.61	0.42
1:A:99:SER:HB3	24:b:201:3PE:C38	2.49	0.42
2:B:81:LEU:CD2	27:B:303:PC1:H352	2.48	0.42
4:D:264:ASN:O	9:I:65:GLU:OE1	2.38	0.42
5:E:109:MET:HE2	7:G:196:GLY:CA	2.49	0.42
5:E:136:THR:HG21	6:F:122:PRO:HG3	2.01	0.42
6:F:50:ASP:O	6:F:55:GLY:HA3	2.19	0.42
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.42
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.42
8:H:8:THR:O	8:H:9:LEU:CB	2.67	0.42
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.42
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.54	0.42
9:I:92:PRO:HB3	21:q:92:CYS:HB2	2.01	0.42
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.42
10:P:306:GLY:HA2	10:P:312:PRO:HB3	2.01	0.42
18:Z:94:GLU:HA	18:Z:97:ILE:HD11	2.01	0.42
19:a:51:ASP:CA	19:a:54:ILE:HD12	2.49	0.42
21:q:13:GLN:HE22	34:q:201:CDL:CA3	2.28	0.42
4:D:279:THR:HG23	15:V:13:GLY:CA	2.26	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.55	0.42
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.42
7:G:651:PRO:HB3	13:S:58:CYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:14:LEU:HD23	8:H:14:LEU:HA	1.86	0.42
8:H:20:LEU:N	19:a:12:MET:SD	2.92	0.42
10:P:179:LYS:O	10:P:180:SER:C	2.63	0.42
10:P:376:ASN:O	10:P:377:TYR:C	2.61	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
11:Q:64:LEU:HD12	16:W:85:LEU:HD21	2.00	0.42
16:W:42:TRP:CE2	16:W:93:LEU:HB2	2.54	0.42
21:q:6:VAL:HG13	34:q:201:CDL:CA2	2.47	0.42
1:A:73:LEU:N	1:A:74:PRO:HD2	2.34	0.42
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.01	0.42
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.42
9:I:94:SER:HB2	9:I:95:PRO:CD	2.34	0.42
10:P:197:GLU:HB3	10:P:259:VAL:HG22	1.99	0.42
10:P:231:LEU:CD1	10:P:290:PRO:HB2	2.49	0.42
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.42
12:R:64:ILE:HD12	12:R:64:ILE:HA	1.95	0.42
18:Z:129:THR:O	18:Z:130:LYS:C	2.61	0.42
19:a:37:ARG:NH2	19:a:51:ASP:OD2	2.52	0.42
1:A:99:SER:HB3	24:b:201:3PE:C39	2.48	0.42
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.42
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.42
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.42
4:D:448:VAL:HG21	8:H:204:GLU:OE2	2.13	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.42
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.43	0.42
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
10:P:169:HIS:CD2	10:P:181:LEU:HD11	2.49	0.42
10:P:235:THR:HG21	10:P:323:HIS:CD2	2.55	0.42
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.85	0.42
13:S:16:LEU:HD13	13:S:19:ILE:HD11	2.02	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.54	0.42
17:X:26:LYS:HD3	17:X:95:GLN:OE1	2.19	0.42
17:X:39:THR:HG23	17:X:40:ASN:N	2.33	0.42
24:b:201:3PE:H361	24:b:201:3PE:H391	1.89	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.37	0.42
5:E:78:VAL:O	5:E:82:LEU:HB2	2.20	0.42
5:E:181:ASN:HB3	5:E:193:GLU:HB2	2.01	0.42
5:E:233:LEU:CD2	6:F:43:THR:HA	2.48	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.42
7:G:117:MET:SD	7:G:143:SER:HB2	2.59	0.42
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
8:H:39:ILE:HG13	21:q:31:ASN:ND2	2.35	0.42
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.42
9:I:152:CYS:SG	25:I:303:SF4:S3	3.17	0.42
9:I:152:CYS:SG	25:I:303:SF4:S1	3.17	0.42
10:P:207:PHE:O	10:P:241:TYR:HA	2.20	0.42
10:P:220:TYR:CG	10:P:226:VAL:HG13	2.55	0.42
10:P:265:PHE:N	10:P:265:PHE:CD1	2.87	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
15:V:37:HIS:O	15:V:38:PHE:C	2.63	0.42
16:W:38:LEU:O	16:W:39:TYR:C	2.62	0.42
17:X:38:LYS:O	17:X:42:GLU:HG3	2.20	0.42
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.52	0.42
18:Z:79:LYS:O	18:Z:80:ASP:C	2.63	0.42
19:a:37:ARG:CB	19:a:48:MET:HE2	2.50	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42
22:r:18:GLN:OE1	22:r:18:GLN:N	2.53	0.42
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.42
4:D:147:ASN:O	4:D:148:GLU:C	2.62	0.42
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.26	0.42
6:F:291:GLU:OE2	6:F:292:MET:N	2.53	0.42
6:F:383:THR:N	6:F:384:PRO:CD	2.79	0.42
6:F:412:LEU:HD12	6:F:412:LEU:HA	1.85	0.42
8:H:23:VAL:HG11	19:a:9:LEU:CD2	2.43	0.42
8:H:68:MET:HG3	8:H:68:MET:O	2.19	0.42
8:H:199:ASP:O	8:H:279:ARG:CD	2.57	0.42
9:I:93:LEU:O	21:q:93:MET:CG	2.65	0.42
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.42
10:P:316:LYS:O	10:P:320:GLU:HG2	2.19	0.42
11:Q:85:ASN:C	11:Q:87:MET:N	2.76	0.42
12:R:42:ASP:C	12:R:43:TYR:O	2.61	0.42
16:W:76:VAL:HG13	16:W:82:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.42
21:q:50:GLU:HA	21:q:59:HIS:O	2.20	0.42
1:A:25:PRO:HG3	8:H:60:PRO:CD	2.45	0.42
1:A:102:LEU:HD23	24:b:201:3PE:H371	2.02	0.42
2:B:69:SER:O	2:B:70:ARG:C	2.61	0.42
2:B:92:PRO:CD	2:B:119:VAL:HG13	2.50	0.42
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.53	0.42
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.42
4:D:145:MET:HE3	4:D:214:TYR:CD2	2.55	0.42
4:D:338:ARG:HH12	18:Z:23:ARG:CA	2.30	0.42
5:E:196:THR:O	5:E:199:ASP:HB2	2.19	0.42
7:G:155:GLU:N	7:G:155:GLU:CD	2.78	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.42
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.52	0.42
8:H:30:TYR:CZ	19:a:1:MET:O	2.71	0.42
20:b:5:ILE:HD12	20:b:6:SER:N	2.34	0.42
20:b:7:ALA:C	20:b:9:LEU:H	2.27	0.42
1:A:56:PHE:CZ	1:A:60:ILE:HD11	2.55	0.42
2:B:116:ARG:NH2	9:I:86:TYR:H	2.17	0.42
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.42
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.42
6:F:296:LEU:HD22	6:F:337:MET:HE3	2.02	0.42
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.42
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.42
8:H:202:GLU:HA	8:H:210:GLY:N	2.34	0.42
10:P:242:VAL:HG13	10:P:243:ALA:N	2.35	0.42
10:P:293:LEU:HD12	10:P:294:PRO:HD2	2.01	0.42
12:R:60:ALA:O	12:R:61:ILE:C	2.63	0.42
17:X:70:PHE:CE1	17:X:117:TRP:CZ3	3.08	0.42
18:Z:97:ILE:HG13	18:Z:98:MET:N	2.30	0.42
20:b:61:GLY:O	20:b:63:MET:HG3	2.20	0.42
1:A:24:LEU:HD13	1:A:24:LEU:O	2.20	0.41
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.84	0.41
4:D:271:ARG:HG2	8:H:281:ARG:CG	2.44	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.41
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:80:LYS:O	14:T:84:LEU:HG	2.20	0.41
20:b:60:ASP:OD1	20:b:60:ASP:C	2.61	0.41
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.55	0.41
21:q:56:PHE:CD1	21:q:59:HIS:NE2	2.77	0.41
1:A:60:ILE:HD13	1:A:60:ILE:HA	1.83	0.41
4:D:101:LEU:HD11	4:D:106:VAL:CG2	2.39	0.41
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.41
4:D:368:ARG:NH2	9:I:165:ASP:HB2	2.35	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
6:F:261:TRP:CE2	6:F:265:PHE:CZ	3.08	0.41
7:G:689:LEU:HD12	7:G:689:LEU:HA	1.79	0.41
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
11:Q:52:LEU:HD23	16:W:19:SER:O	2.20	0.41
11:Q:158:LYS:HE3	11:Q:158:LYS:HB3	1.91	0.41
13:S:21:VAL:HG23	13:S:91:MET:HE1	2.02	0.41
16:W:45:GLU:O	16:W:46:VAL:C	2.62	0.41
16:W:55:LEU:HB3	16:W:57:ILE:HG12	2.01	0.41
17:X:117:TRP:CD1	17:X:117:TRP:N	2.87	0.41
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
21:q:74:PHE:HE2	21:q:75:TRP:HE1	1.68	0.41
22:r:12:ARG:HH21	22:r:20:LEU:CD1	2.33	0.41
1:A:111:LEU:HD13	8:H:290:TRP:HB3	2.02	0.41
2:B:114:MET:O	2:B:115:ASP:C	2.62	0.41
27:B:303:PC1:H111	27:B:303:PC1:H133	1.72	0.41
3:C:168:GLU:CA	3:C:186:ILE:CD1	2.97	0.41
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.50	0.41
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.41
4:D:259:GLU:C	4:D:261:MET:N	2.75	0.41
4:D:384:LEU:HD23	4:D:384:LEU:HA	1.89	0.41
5:E:65:ILE:HG21	5:E:80:PRO:HB2	2.01	0.41
5:E:179:CYS:C	5:E:181:ASN:N	2.78	0.41
5:E:225:GLU:O	5:E:226:PRO:C	2.60	0.41
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.41
6:F:383:THR:HG21	7:G:120:LEU:HD23	2.00	0.41
7:G:541:PRO:HB2	7:G:561:PRO:CD	2.50	0.41
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.41
14:T:87:LEU:CD2	14:T:122:MET:CE	2.97	0.41
16:W:93:LEU:HD23	16:W:93:LEU:C	2.45	0.41
18:Z:6:VAL:O	18:Z:7:LYS:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:91:LEU:HD13	18:Z:91:LEU:C	2.45	0.41
18:Z:120:LEU:HD12	18:Z:121:ILE:H	1.85	0.41
19:a:34:LYS:O	19:a:35:GLU:C	2.63	0.41
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.41
1:A:52:SER:O	1:A:55:PHE:HB2	2.21	0.41
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.41
3:C:180:HIS:CD2	3:C:182:ASP:H	2.37	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
5:E:67:LYS:O	5:E:68:ASN:C	2.63	0.41
6:F:70:LEU:O	6:F:71:LYS:C	2.63	0.41
6:F:94:PRO:CG	6:F:97:LEU:HD12	2.45	0.41
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.41
7:G:94:MET:HE3	7:G:94:MET:HB3	1.97	0.41
7:G:127:ASP:HA	12:R:106:TYR:HH	1.83	0.41
7:G:450:LYS:CD	7:G:453:GLN:HG3	2.32	0.41
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.21	0.41
10:P:324:ILE:HD13	10:P:324:ILE:HA	1.81	0.41
12:R:38:TYR:HE2	12:R:44:ARG:NE	2.19	0.41
12:R:55:VAL:HG22	12:R:56:ASN:N	2.35	0.41
13:S:19:ILE:O	13:S:53:ILE:HD12	2.20	0.41
14:T:82:ARG:O	14:T:86:VAL:HG23	2.20	0.41
14:T:90:TYR:CD2	14:T:92:LYS:HB3	2.54	0.41
18:Z:10:MET:HB3	18:Z:11:PRO:HD2	2.03	0.41
21:q:5:GLU:HG2	21:q:9:ARG:HE	1.85	0.41
22:r:113:LEU:HD12	22:r:113:LEU:HA	1.76	0.41
1:A:20:VAL:O	1:A:21:ALA:C	2.62	0.41
1:A:55:PHE:HD1	1:A:55:PHE:HA	1.74	0.41
2:B:100:CYS:SG	25:B:301:SF4:S3	3.19	0.41
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.84	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
4:D:198:THR:OG1	4:D:261:MET:SD	2.78	0.41
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.35	0.41
6:F:217:GLU:OE2	6:F:224:ARG:NH2	2.53	0.41
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.51	0.41
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	0.41
6:F:413:TRP:CH2	6:F:436:GLN:HG2	2.56	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:272:ARG:HH11	7:G:274:LEU:CD2	2.33	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:132:ASP:O	16:W:40:ARG:NH2	2.53	0.41
21:q:56:PHE:HD2	22:r:27:ARG:HH22	1.68	0.41
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.41
3:C:77:VAL:HG22	3:C:83:LEU:HD13	2.03	0.41
3:C:241:PHE:O	3:C:242:PRO:C	2.62	0.41
4:D:198:THR:N	4:D:199:PRO:CD	2.83	0.41
5:E:134:CYS:SG	5:E:175:CYS:HA	2.60	0.41
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.41
7:G:36:VAL:O	7:G:37:ASP:C	2.63	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:598:ASN:ND2	7:G:600:GLU:OE2	2.51	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.41
9:I:130:ILE:HD11	9:I:145:TYR:HE1	1.86	0.41
10:P:96:LEU:C	10:P:96:LEU:CD1	2.94	0.41
12:R:48:PHE:CE2	12:R:53:LYS:HB2	2.56	0.41
19:a:49:GLU:O	19:a:50:ARG:C	2.61	0.41
2:B:92:PRO:HG3	2:B:119:VAL:CG1	2.51	0.41
3:C:124:ARG:HH12	3:C:125:PHE:HZ	1.56	0.41
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.82	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:404:GLY:HA2	7:G:684:LEU:HD11	1.99	0.41
8:H:16:ALA:O	19:a:12:MET:HG2	2.20	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	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
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.41
10:P:56:ALA:HA	10:P:125:VAL:O	2.20	0.41
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.41
18:Z:99:LYS:HE3	18:Z:99:LYS:HB2	1.77	0.41
19:a:41:VAL:O	19:a:42:GLN:C	2.64	0.41
20:b:25:VAL:O	20:b:26:TRP:C	2.64	0.41
2:B:94:THR:O	2:B:94:THR:OG1	2.36	0.41
2:B:137:LEU:HD11	2:B:142:ALA:HA	2.03	0.41
2:B:210:ARG:NE	21:q:78:ASP:OD1	2.53	0.41
3:C:160:ILE:HB	4:D:286:TYR:CE1	2.56	0.41
4:D:82:LEU:HD13	8:H:126:LYS:HD2	2.02	0.41
6:F:61:ASP:O	6:F:256:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:113:LEU:HD13	6:F:149:MET:SD	2.60	0.41
6:F:280:GLY:O	6:F:356:VAL:HB	2.20	0.41
6:F:300:ILE:HD13	6:F:307:VAL:CG2	2.51	0.41
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.41
9:I:149:MET:CE	9:I:185:TYR:HD2	2.34	0.41
27:I:302:PC1:H222	18:Z:35:MET:HE1	2.02	0.41
10:P:228:LEU:HD11	10:P:288:PHE:CZ	2.54	0.41
15:V:98:LYS:HG2	15:V:100:TRP:CZ2	2.55	0.41
17:X:143:HIS:CG	17:X:143:HIS:O	2.73	0.41
18:Z:19:ILE:HG22	18:Z:20:ASP:N	2.36	0.41
21:q:6:VAL:O	34:q:201:CDL:HA62	2.20	0.41
2:B:145:LEU:O	2:B:146:ARG:C	2.64	0.41
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.41
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.56	0.41
4:D:119:GLY:O	4:D:123:LEU:HD23	2.21	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.03	0.41
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.54	0.41
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.41
4:D:299:GLN:OE1	22:r:104:TRP:HB2	2.20	0.41
4:D:338:ARG:NH2	18:Z:23:ARG:CB	2.83	0.41
4:D:339:GLN:HE21	9:I:37:LYS:HZ2	1.68	0.41
5:E:48:PRO:HD3	5:E:94:ILE:CG2	2.51	0.41
5:E:67:LYS:HE2	5:E:67:LYS:HB2	1.88	0.41
5:E:129:TYR:HE2	5:E:167:LEU:HG	1.86	0.41
5:E:133:VAL:HG22	5:E:185:VAL:CG1	2.45	0.41
5:E:145:ASP:OD1	5:E:145:ASP:N	2.54	0.41
5:E:193:GLU:HG3	5:E:217:PRO:HG3	2.02	0.41
5:E:241:GLY:HA3	6:F:63:TYR:CZ	2.56	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:116:ASN:OD1	6:F:116:ASN:C	2.63	0.41
6:F:208:GLU:OE1	6:F:210:THR:N	2.52	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.41
7:G:184:ARG:O	7:G:185:PHE:C	2.64	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
8:H:23:VAL:CG2	19:a:9:LEU:HG	2.51	0.41
8:H:249:ILE:CD1	17:X:99:HIS:HB3	2.49	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
9:I:149:MET:HE2	9:I:185:TYR:HD2	1.86	0.41
9:I:162:CYS:HB3	9:I:165:ASP:HA	2.02	0.41
27:I:302:PC1:H382	27:I:302:PC1:H352	1.88	0.41
10:P:96:LEU:HD12	10:P:97:MET:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:177:SER:O	10:P:182:ARG:NH2	2.53	0.41
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	2.03	0.41
14:T:99:SER:HB2	14:T:102:SER:HB2	2.03	0.41
14:T:120:MET:O	14:T:121:ALA:C	2.63	0.41
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.35	0.41
19:a:50:ARG:HA	19:a:53:ARG:HH11	1.85	0.41
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
2:B:126:ARG:HD2	8:H:213:VAL:O	2.20	0.41
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.41
3:C:128:VAL:HG22	3:C:143:LYS:HB3	2.03	0.41
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.41
6:F:45:LEU:O	6:F:46:TYR:HB2	2.21	0.41
6:F:300:ILE:CG2	6:F:306:GLY:CA	2.95	0.41
6:F:363:ILE:O	6:F:364:VAL:C	2.64	0.41
7:G:49:VAL:HB	7:G:91:ALA:HA	2.03	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.41
8:H:42:PRO:HD2	8:H:45:ILE:CD1	2.51	0.41
10:P:75:ARG:HH21	16:W:113:THR:HG23	1.86	0.41
10:P:243:ALA:O	10:P:244:ASP:C	2.63	0.41
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.41
14:T:123:GLU:HG2	14:T:130:ILE:HD12	2.02	0.41
15:V:56:LEU:C	15:V:56:LEU:CD1	2.85	0.41
17:X:33:GLY:CA	18:Z:70:ALA:HB1	2.50	0.41
18:Z:11:PRO:O	18:Z:12:PRO:C	2.64	0.41
18:Z:72:MET:N	18:Z:73:PRO:CD	2.83	0.41
20:b:69:HIS:HD2	20:b:70:PRO:CD	2.26	0.41
21:q:89:TRP:HB2	21:q:98:PRO:HD3	2.03	0.41
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.20	0.40
2:B:84:TRP:CZ3	27:B:303:PC1:H351	2.56	0.40
2:B:96:GLY:HA3	26:B:302:UQ1:HM32	1.89	0.40
3:C:102:HIS:CE1	15:V:48:THR:CG2	2.89	0.40
3:C:229:PHE:O	11:Q:123:ASN:ND2	2.54	0.40
4:D:99:LEU:HD12	4:D:99:LEU:C	2.44	0.40
4:D:310:VAL:C	4:D:312:ASP:H	2.29	0.40
5:E:167:LEU:HD23	5:E:168:PHE:HE1	1.86	0.40
5:E:187:ILE:HB	5:E:190:ASN:ND2	2.36	0.40
6:F:47:GLY:O	6:F:48:ARG:HB2	2.21	0.40
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.54	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
10:P:315:THR:H	10:P:318:LYS:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:38:TYR:HE2	12:R:44:ARG:HE	1.69	0.40
14:T:140:CYS:HB2	14:T:143:GLU:HB2	2.02	0.40
16:W:24:PHE:HB2	16:W:83:ASP:OD2	2.20	0.40
16:W:44:ARG:O	16:W:47:PRO:HG2	2.20	0.40
17:X:38:LYS:HD2	17:X:131:VAL:HG12	2.02	0.40
18:Z:8:GLN:O	18:Z:10:MET:HG3	2.21	0.40
1:A:2:ASN:ND2	18:Z:143:TYR:CE1	2.89	0.40
1:A:16:THR:O	1:A:20:VAL:HG23	2.22	0.40
1:A:18:ILE:HG12	8:H:222:LEU:CD2	2.51	0.40
1:A:62:PHE:HD1	8:H:144:VAL:CG2	2.35	0.40
2:B:91:TRP:HA	2:B:120:VAL:HG12	2.01	0.40
2:B:124:SER:O	2:B:125:PRO:C	2.63	0.40
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.40
4:D:378:LEU:HD23	7:G:126:LEU:HB2	2.03	0.40
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.40
5:E:142:ARG:HB3	5:E:182:ALA:HB3	2.03	0.40
5:E:190:ASN:O	5:E:191:TYR:C	2.63	0.40
5:E:238:LYS:HB3	5:E:242:PHE:CG	2.57	0.40
7:G:314:LEU:HD23	7:G:583:ILE:HG13	2.02	0.40
8:H:23:VAL:O	8:H:23:VAL:CG1	2.69	0.40
8:H:87:VAL:HB	8:H:88:PRO:HD3	2.03	0.40
8:H:179:TRP:NE1	18:Z:43:LEU:HG	2.37	0.40
8:H:296:LEU:CD2	24:I:301:3PE:H351	2.50	0.40
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.40
10:P:180:SER:HB2	10:P:321:ARG:HH21	1.87	0.40
13:S:25:GLN:CG	13:S:26:ARG:N	2.82	0.40
17:X:112:LEU:HD13	17:X:118:VAL:HG22	2.03	0.40
19:a:17:VAL:O	19:a:18:ILE:C	2.62	0.40
19:a:58:ASN:ND2	19:a:60:TYR:OH	2.53	0.40
2:B:106:HIS:O	2:B:109:ALA:HB3	2.22	0.40
3:C:243:ALA:C	7:G:105:ASN:ND2	2.80	0.40
4:D:158:LEU:O	4:D:392:PRO:HG2	2.21	0.40
4:D:240:LEU:O	4:D:241:LEU:C	2.62	0.40
4:D:304:LYS:HD2	4:D:318:VAL:HG23	2.04	0.40
5:E:39:VAL:HG11	7:G:163:LYS:HZ2	1.84	0.40
5:E:78:VAL:CA	5:E:104:LEU:HD13	2.46	0.40
7:G:169:VAL:HG12	7:G:231:LEU:HB2	2.03	0.40
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.40
8:H:42:PRO:HD2	8:H:45:ILE:HD11	2.03	0.40
8:H:119:SER:OG	8:H:211:PHE:HB2	2.22	0.40
8:H:306:SER:CB	8:H:310:PHE:HE2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.55	0.40
11:Q:57:GLU:O	11:Q:58:LYS:C	2.64	0.40
13:S:47:ALA:O	13:S:48:HIS:HD2	2.05	0.40
1:A:48:ARG:NE	1:A:48:ARG:HA	2.36	0.40
1:A:69:ILE:O	1:A:72:LEU:N	2.55	0.40
2:B:117:PHE:CD2	2:B:206:LEU:HD21	2.55	0.40
3:C:160:ILE:HG13	4:D:285:ASN:ND2	2.36	0.40
4:D:139:LEU:HD13	4:D:424:ILE:HG12	2.02	0.40
4:D:145:MET:HG2	4:D:148:GLU:OE2	2.20	0.40
4:D:146:CYS:SG	4:D:403:PRO:HD3	2.62	0.40
4:D:269:ARG:O	4:D:273:VAL:HG23	2.21	0.40
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.40
5:E:223:CYS:CB	6:F:133:HIS:CE1	3.04	0.40
6:F:306:GLY:O	6:F:307:VAL:C	2.64	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.09	0.40
7:G:160:VAL:CG1	7:G:161:GLU:N	2.84	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
8:H:251:LEU:HD11	8:H:254:LEU:HB2	2.02	0.40
9:I:91:GLY:HA2	9:I:92:PRO:HD3	1.91	0.40
27:I:302:PC1:C22	18:Z:35:MET:CE	2.98	0.40
18:Z:34:SER:O	18:Z:38:VAL:HG23	2.22	0.40
18:Z:96:ILE:H	18:Z:96:ILE:HG13	1.72	0.40
4:D:144:MET:N	4:D:144:MET:SD	2.95	0.40
4:D:188:THR:HG21	4:D:203:MET:HB2	2.02	0.40
4:D:265:ASN:C	4:D:267:ILE:H	2.29	0.40
4:D:280:ALA:CB	15:V:11:LEU:CG	2.95	0.40
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.37	0.40
6:F:413:TRP:O	6:F:414:GLU:C	2.63	0.40
7:G:32:ILE:CG2	7:G:98:LYS:HA	2.52	0.40
7:G:217:GLU:C	7:G:219:SER:N	2.79	0.40
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.40
7:G:651:PRO:HB3	13:S:58:CYS:CA	2.52	0.40
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.86	0.40
8:H:200:LEU:HD21	8:H:282:TYR:HD1	1.87	0.40
9:I:50:MET:O	9:I:54:THR:N	2.37	0.40
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.40
9:I:201:ILE:O	9:I:205:ILE:HG12	2.21	0.40
10:P:227:PRO:O	10:P:228:LEU:HD23	2.21	0.40
10:P:285:HIS:CE1	10:P:364:SER:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:333:PRO:HB2	10:P:337:ASP:CB	2.50	0.40
12:R:32:THR:HG23	12:R:35:GLY:H	1.85	0.40
14:T:118:ILE:HD13	14:T:118:ILE:HA	1.83	0.40
17:X:4:ILE:HG22	17:X:6:GLU:N	2.28	0.40
19:a:60:TYR:O	19:a:61:TYR:C	2.60	0.40
20:b:26:TRP:CD1	24:b:201:3PE:H3C1	2.57	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	88/115 (76%)	79 (90%)	9 (10%)	0	100	100
2	B	155/224 (69%)	144 (93%)	10 (6%)	1 (1%)	21	52
3	C	196/263 (74%)	184 (94%)	12 (6%)	0	100	100
4	D	383/463 (83%)	355 (93%)	27 (7%)	1 (0%)	36	65
5	E	208/248 (84%)	188 (90%)	20 (10%)	0	100	100
6	F	424/464 (91%)	404 (95%)	20 (5%)	0	100	100
7	G	685/727 (94%)	627 (92%)	58 (8%)	0	100	100
8	H	308/318 (97%)	286 (93%)	21 (7%)	1 (0%)	36	65
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	P	338/377 (90%)	315 (93%)	23 (7%)	0	100	100
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	76 (94%)	5 (6%)	0	100	100
13	S	81/99 (82%)	78 (96%)	3 (4%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
17	X	140/172 (81%)	129 (92%)	11 (8%)	0	100	100
18	Z	137/144 (95%)	129 (94%)	8 (6%)	0	100	100
19	a	64/70 (91%)	60 (94%)	4 (6%)	0	100	100
20	b	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
21	q	116/145 (80%)	114 (98%)	2 (2%)	0	100	100
22	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
23	s	11/104 (11%)	11 (100%)	0	0	100	100
All	All	4121/5036 (82%)	3858 (94%)	260 (6%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
4	D	93	GLY
2	B	195	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/104 (81%)	84 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	73	76
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	332/395 (84%)	331 (100%)	1 (0%)	86	83
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	80
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	86
8	H	276/280 (99%)	276 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	P	297/325 (91%)	296 (100%)	1 (0%)	86	83
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68	74
12	R	70/96 (73%)	69 (99%)	1 (1%)	59	70
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	70
14	T	69/135 (51%)	68 (99%)	1 (1%)	59	70
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	76
19	a	56/60 (93%)	55 (98%)	1 (2%)	51	67
20	b	71/73 (97%)	71 (100%)	0	100	100
21	q	108/131 (82%)	107 (99%)	1 (1%)	70	75
22	r	44/96 (46%)	44 (100%)	0	100	100
23	s	13/95 (14%)	13 (100%)	0	100	100
All	All	3619/4292 (84%)	3607 (100%)	12 (0%)	84	83

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

Mol	Chain	Res	Type
2	B	104	MET
4	D	232	VAL
5	E	244	VAL
7	G	271	MET
10	P	316	LYS
11	Q	96	LYS
12	R	64	ILE
13	S	68	ARG
14	T	103	HIS
18	Z	7	LYS
19	a	66	LEU
21	q	138	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN

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Mol	Chain	Res	Type
2	B	83	ASN
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	54	HIS
3	C	88	HIS
3	C	123	ASN
3	C	130	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	87	GLN
4	D	88	HIS
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	313	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	132	GLN
5	E	152	GLN
5	E	190	ASN
5	E	245	GLN
6	F	44	ASN
6	F	116	ASN
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	101	ASN
7	G	105	ASN
7	G	140	GLN

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Mol	Chain	Res	Type
7	G	164	ASN
7	G	205	GLN
7	G	495	ASN
7	G	498	GLN
7	G	514	ASN
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	32	GLN
8	H	47	GLN
8	H	93	HIS
8	H	169	GLN
8	H	171	HIS
8	H	212	ASN
8	H	258	ASN
8	H	284	GLN
8	H	292	ASN
9	I	126	GLN
10	P	43	HIS
10	P	71	ASN
10	P	79	GLN
10	P	169	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
11	Q	51	GLN
11	Q	88	GLN
13	S	73	GLN
15	V	41	HIS
15	V	50	GLN
16	W	29	ASN
16	W	54	GLN
17	X	30	HIS
17	X	77	HIS
19	a	31	ASN
19	a	42	GLN
20	b	69	HIS

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Mol	Chain	Res	Type
20	b	83	ASN
21	q	13	GLN
21	q	52	ASN
21	q	54	GLN
21	q	87	HIS
21	q	91	HIS
22	r	21	GLN
22	r	110	GLN
23	s	84	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	3PE	A	401	-	45,45,50	0.93	2 (4%)	48,50,55	1.02	2 (4%)
29	FMN	F	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.21	6 (12%)
30	UQ9	H	401	-	35,35,58	0.81	2 (5%)	43,45,73	0.62	1 (2%)
25	SF4	G	802	7	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	SF4	G	801	7	0,12,12	-	-	-		
27	PC1	I	302	-	46,46,53	1.00	2 (4%)	52,54,61	1.09	3 (5%)
31	NDP	P	401	-	51,52,52	1.18	5 (9%)	71,80,80	1.57	10 (14%)
33	EHZ	W	201	-	29,31,37	1.80	7 (24%)	37,41,47	1.94	12 (32%)
25	SF4	I	304	9	0,12,12	-	-	-		
27	PC1	H	402	-	41,41,53	1.05	2 (4%)	47,49,61	1.08	4 (8%)
25	SF4	I	303	9	0,12,12	-	-	-		
27	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.17	3 (7%)
28	FES	E	301	5	0,4,4	-	-	-		
26	UQ1	B	302	-	18,18,18	2.11	2 (11%)	24,25,25	1.75	4 (16%)
24	3PE	I	301	-	50,50,50	0.90	2 (4%)	53,55,55	1.04	4 (7%)
25	SF4	F	502	6	0,12,12	-	-	-		
24	3PE	b	201	-	45,45,50	0.95	2 (4%)	48,50,55	1.11	3 (6%)
28	FES	G	803	7	0,4,4	-	-	-		
34	CDL	q	201	-	56,56,99	1.20	4 (7%)	62,68,111	1.31	8 (12%)
25	SF4	B	301	2	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
24	3PE	A	401	-	-	13/49/49/54	-
29	FMN	F	501	-	-	4/18/18/18	0/3/3/3
30	UQ9	H	401	-	-	13/30/54/81	0/1/1/1
25	SF4	G	802	7	-	-	0/6/5/5
25	SF4	G	801	7	-	-	0/6/5/5
27	PC1	I	302	-	-	12/50/50/57	-
31	NDP	P	401	-	-	6/34/77/77	0/5/5/5
33	EHZ	W	201	-	-	21/39/39/45	-
25	SF4	I	304	9	-	-	0/6/5/5
27	PC1	H	402	-	-	16/45/45/57	-
25	SF4	I	303	9	-	-	0/6/5/5
27	PC1	B	303	-	-	11/38/38/57	-
28	FES	E	301	5	-	-	0/1/1/1
26	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
24	3PE	I	301	-	-	17/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SF4	F	502	6	-	-	0/6/5/5
24	3PE	b	201	-	-	9/49/49/54	-
28	FES	G	803	7	-	-	0/1/1/1
34	CDL	q	201	-	-	12/67/67/110	-
25	SF4	B	301	2	-	-	0/6/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	302	UQ1	C6-C5	7.71	1.49	1.35
33	W	201	EHZ	C15-N2	5.03	1.45	1.33
29	F	501	FMN	C9A-C5A	4.96	1.49	1.41
33	W	201	EHZ	C12-N1	4.93	1.45	1.33
31	P	401	NDP	C5A-C4A	4.39	1.46	1.39
27	I	302	PC1	O31-C31	4.21	1.45	1.33
27	B	303	PC1	O31-C31	4.16	1.45	1.33
34	q	201	CDL	OB8-CB7	4.16	1.45	1.33
27	H	402	PC1	O31-C31	4.15	1.45	1.33
24	b	201	3PE	O31-C31	4.12	1.45	1.33
34	q	201	CDL	OA6-CA5	4.11	1.45	1.34
34	q	201	CDL	OA8-CA7	4.10	1.45	1.33
24	I	301	3PE	O31-C31	4.10	1.45	1.33
27	I	302	PC1	O21-C21	4.09	1.45	1.34
34	q	201	CDL	OB6-CB5	4.08	1.45	1.34
24	A	401	3PE	O31-C31	4.08	1.45	1.33
27	B	303	PC1	O21-C21	4.04	1.45	1.34
24	b	201	3PE	O21-C21	4.02	1.45	1.34
27	H	402	PC1	O21-C21	4.01	1.45	1.34
24	I	301	3PE	O21-C21	3.98	1.45	1.34
24	A	401	3PE	O21-C21	3.92	1.45	1.34
26	B	302	UQ1	C3-C2	3.58	1.49	1.36
29	F	501	FMN	C8-C7	3.26	1.48	1.40
29	F	501	FMN	C4-N3	-2.71	1.33	1.38
33	W	201	EHZ	P1-O7	2.65	1.64	1.54
30	H	401	UQ9	C3-C2	-2.65	1.41	1.48
30	H	401	UQ9	C4-C5	-2.64	1.41	1.48
31	P	401	NDP	C5A-C6A	2.58	1.48	1.41
33	W	201	EHZ	O4-C15	-2.55	1.18	1.23
31	P	401	NDP	C5A-N7A	-2.47	1.34	1.39
29	F	501	FMN	C5A-N5	-2.47	1.34	1.39
33	W	201	EHZ	O3-C12	-2.41	1.18	1.23
33	W	201	EHZ	C9-S1	2.39	1.81	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	W	201	EHZ	P1-OP3	-2.29	1.46	1.54
31	P	401	NDP	C8A-N7A	2.29	1.36	1.31
31	P	401	NDP	C4A-N9A	-2.09	1.33	1.37

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	W	201	EHZ	C8-C9-S1	6.20	121.38	113.56
31	P	401	NDP	C5A-C4A-N3A	-5.70	118.87	126.72
26	B	302	UQ1	CM2-O2-C2	5.33	135.19	116.47
31	P	401	NDP	N3A-C4A-N9A	4.55	134.90	127.17
34	q	201	CDL	OA6-CA5-C11	4.35	120.89	111.48
27	I	302	PC1	O21-C21-C22	4.23	120.63	111.48
34	q	201	CDL	OB6-CB5-C51	4.11	120.38	111.48
24	A	401	3PE	O21-C21-C22	3.77	119.63	111.48
27	B	303	PC1	O21-C21-C22	3.77	119.63	111.48
27	H	402	PC1	O21-C21-C22	3.72	119.53	111.48
24	I	301	3PE	O21-C21-C22	3.68	119.44	111.48
31	P	401	NDP	C2A-N3A-C4A	3.63	120.69	111.83
24	b	201	3PE	C2-O21-C21	-3.57	109.25	117.80
24	b	201	3PE	O21-C21-C22	3.48	119.02	111.48
31	P	401	NDP	C4A-C5A-N7A	-3.47	106.61	110.58
33	W	201	EHZ	O2-C9-C8	-3.20	118.71	123.74
31	P	401	NDP	N3A-C2A-N1A	-3.17	123.78	128.58
33	W	201	EHZ	C14-C13-C12	-3.06	107.30	112.39
33	W	201	EHZ	OP3-P1-O9	-2.96	99.31	110.83
33	W	201	EHZ	C7-C8-C9	-2.95	107.28	113.86
31	P	401	NDP	C4A-N9A-C8A	2.94	108.82	105.74
27	B	303	PC1	O31-C31-C32	2.91	120.70	111.83
27	I	302	PC1	C2-O21-C21	-2.91	110.84	117.80
33	W	201	EHZ	C13-C12-N1	2.90	121.62	116.34
34	q	201	CDL	OA8-CA7-C31	2.86	120.56	111.83
26	B	302	UQ1	C7-C8-C9	-2.81	119.29	127.25
34	q	201	CDL	CA4-OA6-CA5	-2.81	111.07	117.80
24	I	301	3PE	O31-C31-C32	2.77	120.28	111.83
27	B	303	PC1	C2-O21-C21	-2.76	111.18	117.80
27	H	402	PC1	O31-C31-C32	2.71	120.11	111.83
27	I	302	PC1	O31-C31-C32	2.67	119.98	111.83
24	A	401	3PE	O31-C31-C32	2.67	119.96	111.83
24	b	201	3PE	O31-C31-C32	2.58	119.70	111.83
31	P	401	NDP	C5A-N7A-C8A	2.55	107.46	103.45
34	q	201	CDL	OB8-CB7-C71	2.52	119.51	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	501	FMN	O4-C4-C4A	-2.51	119.91	126.53
26	B	302	UQ1	C11-C9-C10	2.49	120.33	114.59
31	P	401	NDP	C3D-C2D-C1D	2.47	106.14	101.46
26	B	302	UQ1	CM5-C5-C6	-2.45	120.43	124.45
33	W	201	EHZ	C5-C6-C7	-2.43	107.98	114.68
29	F	501	FMN	C4A-C10-N1	-2.42	118.65	124.59
33	W	201	EHZ	C10-S1-C9	2.38	108.89	101.84
34	q	201	CDL	CB4-OB6-CB5	-2.28	112.33	117.80
30	H	401	UQ9	C7-C6-C1	-2.26	121.02	124.89
29	F	501	FMN	C4-C4A-N5	2.26	121.32	118.21
27	H	402	PC1	C2-O21-C21	-2.23	112.47	117.80
33	W	201	EHZ	C11-N1-C12	-2.19	118.74	122.82
33	W	201	EHZ	O6-P1-O9	2.19	112.36	106.44
33	W	201	EHZ	O2-C9-S1	-2.18	119.91	122.68
31	P	401	NDP	N9A-C8A-N7A	-2.16	110.88	113.94
27	H	402	PC1	C11-C12-N	-2.15	108.92	115.82
29	F	501	FMN	C4A-C10-N10	2.12	119.52	116.48
31	P	401	NDP	C6A-C5A-N7A	2.08	136.09	132.09
24	I	301	3PE	O31-C31-O32	-2.05	118.49	123.63
29	F	501	FMN	O2-C2-N1	-2.05	118.39	121.80
24	I	301	3PE	C2-O21-C21	-2.05	112.89	117.80
34	q	201	CDL	OA8-CA7-OA9	-2.03	118.56	123.63
29	F	501	FMN	C4-N3-C2	-2.01	122.07	125.64
34	q	201	CDL	OA6-CA5-OA7	-2.00	119.02	123.70
33	W	201	EHZ	O3-C12-N1	-2.00	119.11	123.03

There are no chirality outliers.

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	401	3PE	C11-O13-P-O11
24	A	401	3PE	C12-C11-O13-P
24	A	401	3PE	O32-C31-O31-C3
24	A	401	3PE	C32-C31-O31-C3
24	I	301	3PE	C11-O13-P-O11
24	I	301	3PE	C11-O13-P-O12
24	b	201	3PE	O22-C21-O21-C2
24	b	201	3PE	C22-C21-O21-C2
27	B	303	PC1	C1-O11-P-O12
27	B	303	PC1	C1-O11-P-O14
27	B	303	PC1	C1-O11-P-O13
27	B	303	PC1	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
27	H	402	PC1	C11-O13-P-O12
27	H	402	PC1	C11-O13-P-O14
27	H	402	PC1	C11-O13-P-O11
27	H	402	PC1	C12-C11-O13-P
27	H	402	PC1	O32-C31-O31-C3
27	I	302	PC1	C11-O13-P-O12
27	I	302	PC1	C11-O13-P-O14
27	I	302	PC1	C11-O13-P-O11
27	I	302	PC1	C1-O11-P-O12
27	I	302	PC1	C1-O11-P-O13
29	F	501	FMN	N10-C1'-C2'-O2'
29	F	501	FMN	C5'-O5'-P-O1P
29	F	501	FMN	C5'-O5'-P-O3P
30	H	401	UQ9	C22-C23-C24-C26
30	H	401	UQ9	C22-C23-C24-C25
30	H	401	UQ9	C7-C8-C9-C11
30	H	401	UQ9	C7-C8-C9-C10
31	P	401	NDP	C2N-C3N-C7N-N7N
33	W	201	EHZ	O1-C7-C8-C9
33	W	201	EHZ	C6-C7-C8-C9
33	W	201	EHZ	S1-C10-C11-N1
33	W	201	EHZ	C16-C17-C20-O6
33	W	201	EHZ	C20-O6-P1-O7
33	W	201	EHZ	C20-O6-P1-O9
33	W	201	EHZ	C20-O6-P1-OP3
34	q	201	CDL	CA3-OA5-PA1-OA2
34	q	201	CDL	CA3-OA5-PA1-OA3
34	q	201	CDL	CA3-OA5-PA1-OA4
27	I	302	PC1	O32-C31-O31-C3
27	I	302	PC1	C32-C31-O31-C3
27	B	303	PC1	O22-C21-O21-C2
27	H	402	PC1	C32-C31-O31-C3
30	H	401	UQ9	C20-C19-C21-C22
30	H	401	UQ9	C18-C19-C21-C22
24	A	401	3PE	C22-C21-O21-C2
24	I	301	3PE	C32-C31-O31-C3
24	b	201	3PE	C32-C31-O31-C3
30	H	401	UQ9	C25-C24-C26-C27
30	H	401	UQ9	C15-C14-C16-C17
30	H	401	UQ9	C23-C24-C26-C27
30	H	401	UQ9	C13-C14-C16-C17
30	H	401	UQ9	C19-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
24	I	301	3PE	O32-C31-O31-C3
24	b	201	3PE	O32-C31-O31-C3
34	q	201	CDL	C12-C13-C14-C15
24	A	401	3PE	O22-C21-O21-C2
34	q	201	CDL	C31-CA7-OA8-CA6
27	I	302	PC1	C11-C12-N-C15
27	H	402	PC1	C24-C25-C26-C27
34	q	201	CDL	OA9-CA7-OA8-CA6
27	I	302	PC1	C11-C12-N-C13
34	q	201	CDL	C51-CB5-OB6-CB4
27	I	302	PC1	C11-C12-N-C14
34	q	201	CDL	OB7-CB5-OB6-CB4
24	I	301	3PE	C22-C21-O21-C2
24	A	401	3PE	C31-C32-C33-C34
24	I	301	3PE	C24-C25-C26-C27
27	B	303	PC1	C2-C1-O11-P
33	W	201	EHZ	N2-C15-C16-C17
24	b	201	3PE	C2A-C2B-C2C-C2D
27	B	303	PC1	C32-C31-O31-C3
24	I	301	3PE	O22-C21-O21-C2
27	B	303	PC1	C32-C33-C34-C35
33	W	201	EHZ	C3-C4-C5-C6
24	A	401	3PE	C3-C2-O21-C21
27	B	303	PC1	O32-C31-O31-C3
27	H	402	PC1	C22-C23-C24-C25
27	B	303	PC1	O13-C11-C12-N
27	H	402	PC1	O13-C11-C12-N
33	W	201	EHZ	O4-C15-C16-O5
24	A	401	3PE	O11-C1-C2-C3
27	H	402	PC1	O22-C21-O21-C2
33	W	201	EHZ	C18-C17-C20-O6
33	W	201	EHZ	C19-C17-C20-O6
24	A	401	3PE	C2E-C2F-C2G-C2H
33	W	201	EHZ	C11-C10-S1-C9
24	A	401	3PE	O11-C1-C2-O21
27	H	402	PC1	C22-C21-O21-C2
24	I	301	3PE	O21-C2-C3-O31
27	H	402	PC1	C27-C28-C29-C2A
24	A	401	3PE	C11-O13-P-O14
24	I	301	3PE	C1-O11-P-O12
24	I	301	3PE	C1-O11-P-O13
24	I	301	3PE	C1-O11-P-O14

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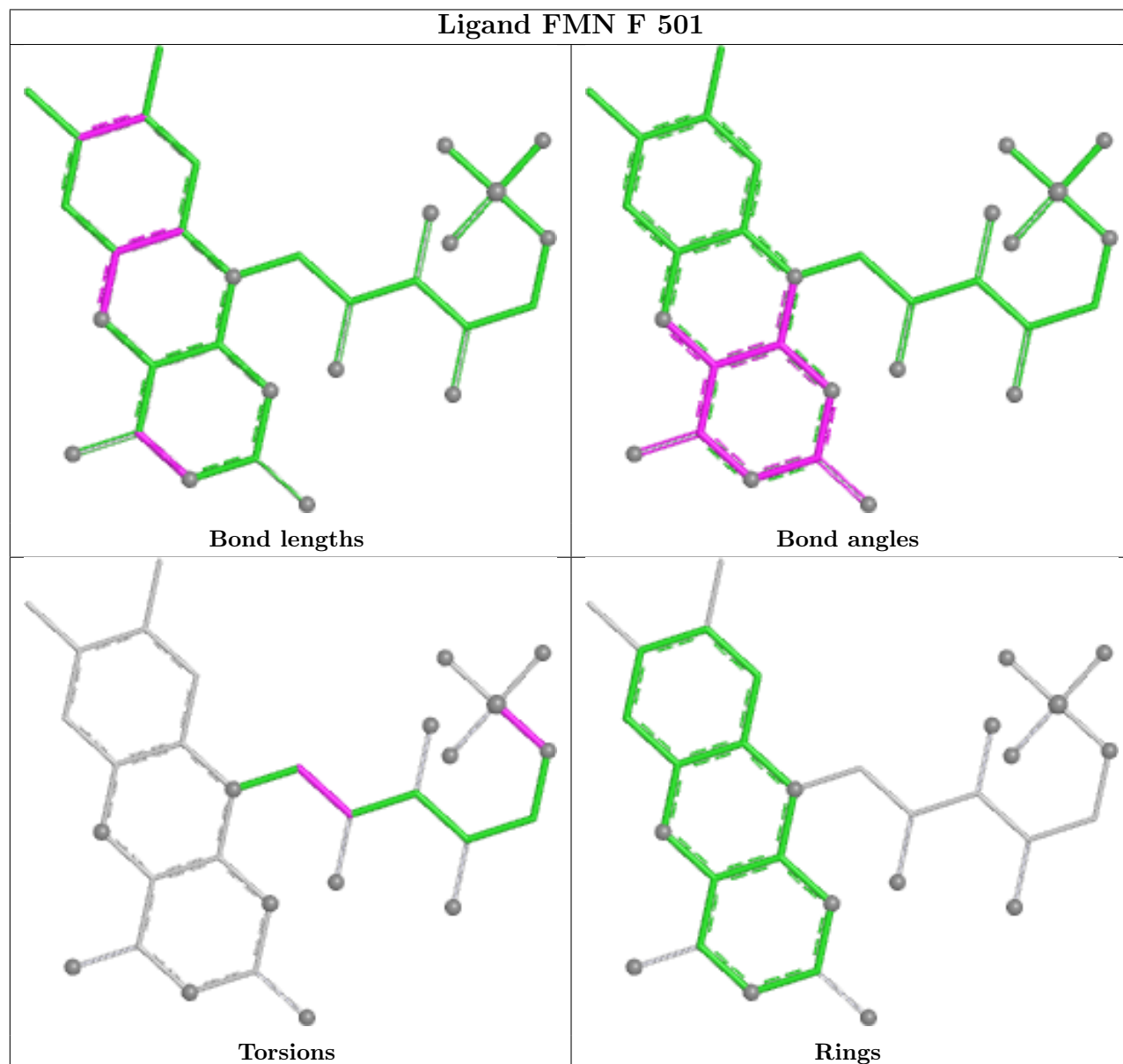
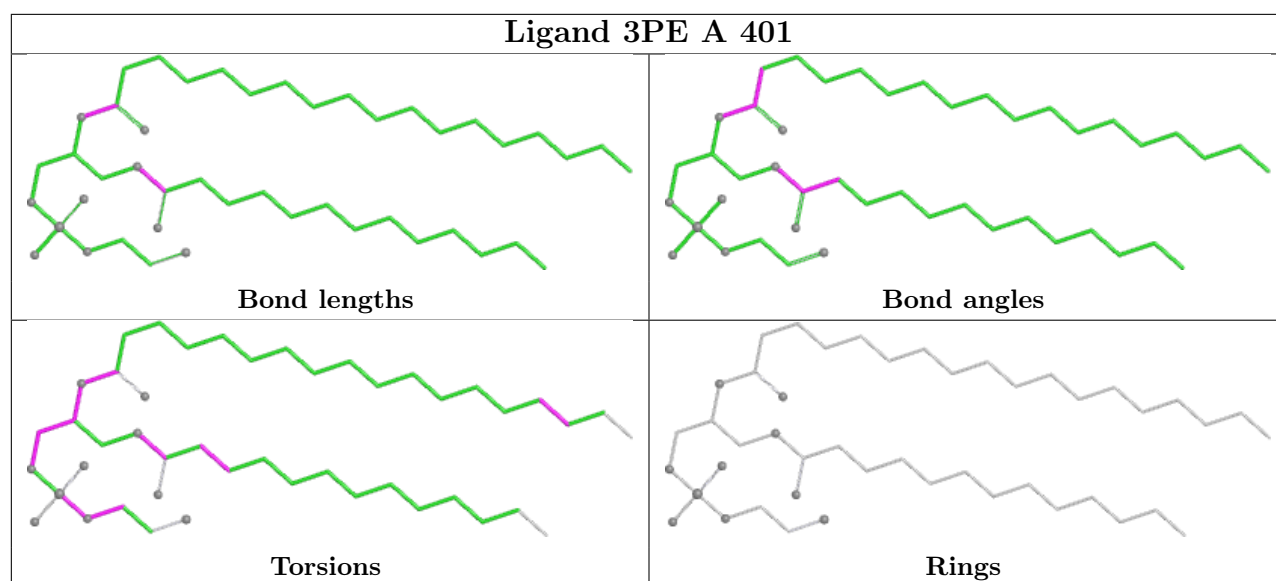
Mol	Chain	Res	Type	Atoms
24	I	301	3PE	C11-O13-P-O14
27	H	402	PC1	C1-O11-P-O14
24	A	401	3PE	C2-C1-O11-P
34	q	201	CDL	CA4-CA3-OA5-PA1
33	W	201	EHZ	C5-C6-C7-O1
24	b	201	3PE	C2B-C2C-C2D-C2E
27	B	303	PC1	C34-C35-C36-C37
33	W	201	EHZ	C2-C3-C4-C5
33	W	201	EHZ	N2-C15-C16-O5
24	I	301	3PE	C37-C38-C39-C3A
33	W	201	EHZ	O2-C9-S1-C10
30	H	401	UQ9	C12-C11-C9-C10
31	P	401	NDP	O4D-C1D-N1N-C6N
31	P	401	NDP	PN-O3-PA-O2A
34	q	201	CDL	C1-CB2-OB2-PB2
27	I	302	PC1	C2E-C2F-C2G-C2H
24	b	201	3PE	C24-C25-C26-C27
24	I	301	3PE	C35-C36-C37-C38
24	I	301	3PE	C33-C34-C35-C36
31	P	401	NDP	C2D-C1D-N1N-C6N
29	F	501	FMN	C5'-O5'-P-O2P
30	H	401	UQ9	C12-C11-C9-C8
33	W	201	EHZ	C15-C16-C17-C18
27	H	402	PC1	C11-C12-N-C13
33	W	201	EHZ	O5-C16-C17-C18
33	W	201	EHZ	O4-C15-C16-C17
24	I	301	3PE	C1-C2-C3-O31
33	W	201	EHZ	C15-C16-C17-C20
34	q	201	CDL	C32-C31-CA7-OA8
27	H	402	PC1	C35-C36-C37-C38
27	H	402	PC1	C11-C12-N-C14
31	P	401	NDP	C2N-C3N-C7N-O7N
27	I	302	PC1	C2C-C2D-C2E-C2F
24	b	201	3PE	C39-C3A-C3B-C3C
24	b	201	3PE	C2C-C2D-C2E-C2F
24	I	301	3PE	C2-C1-O11-P
34	q	201	CDL	C11-CA5-OA6-CA4
31	P	401	NDP	PN-O3-PA-O1A

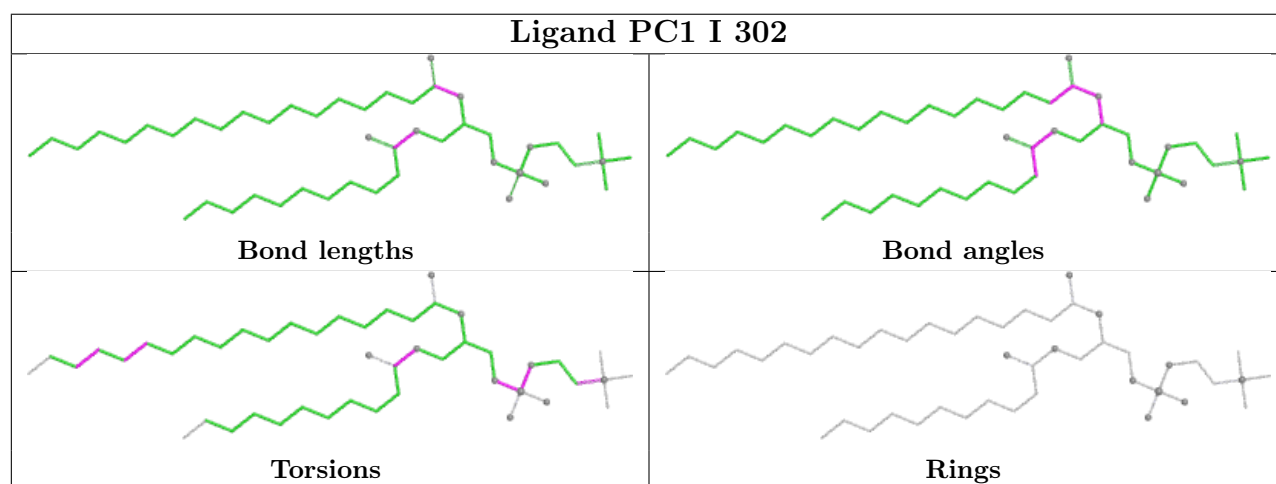
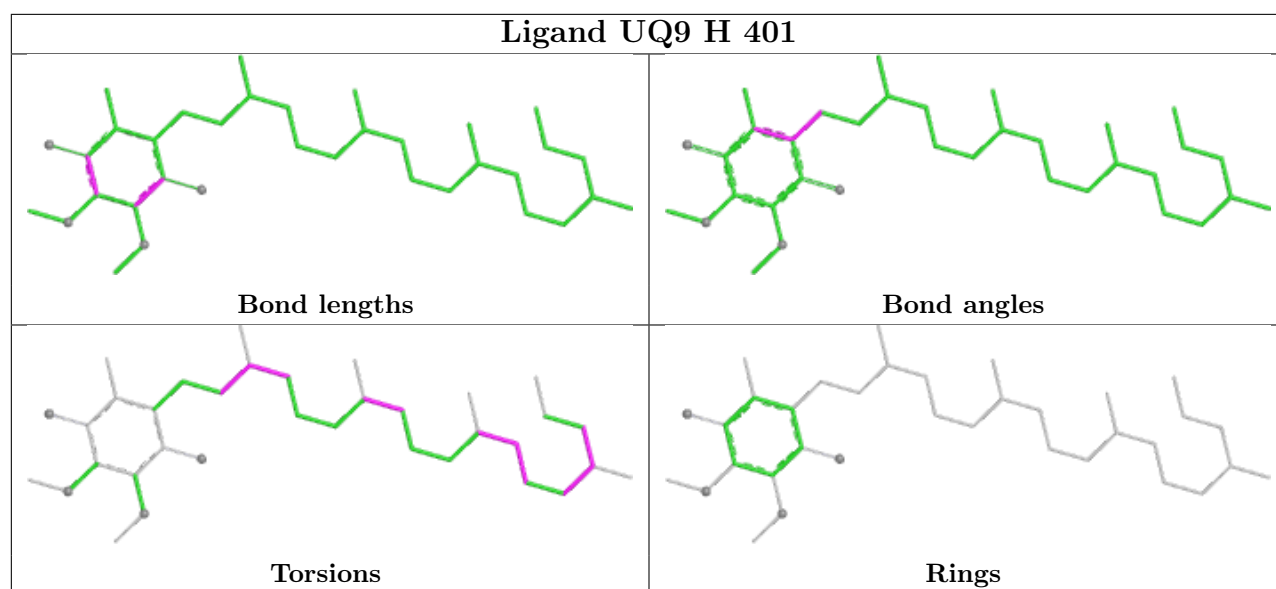
There are no ring outliers.

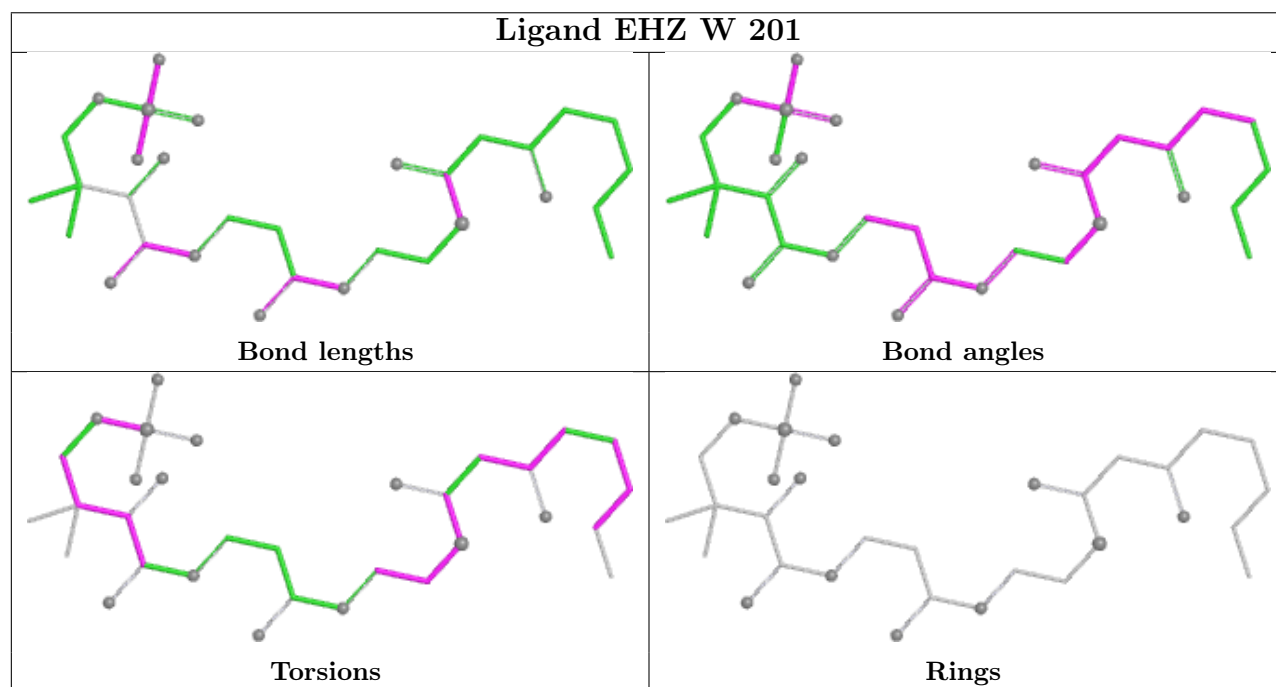
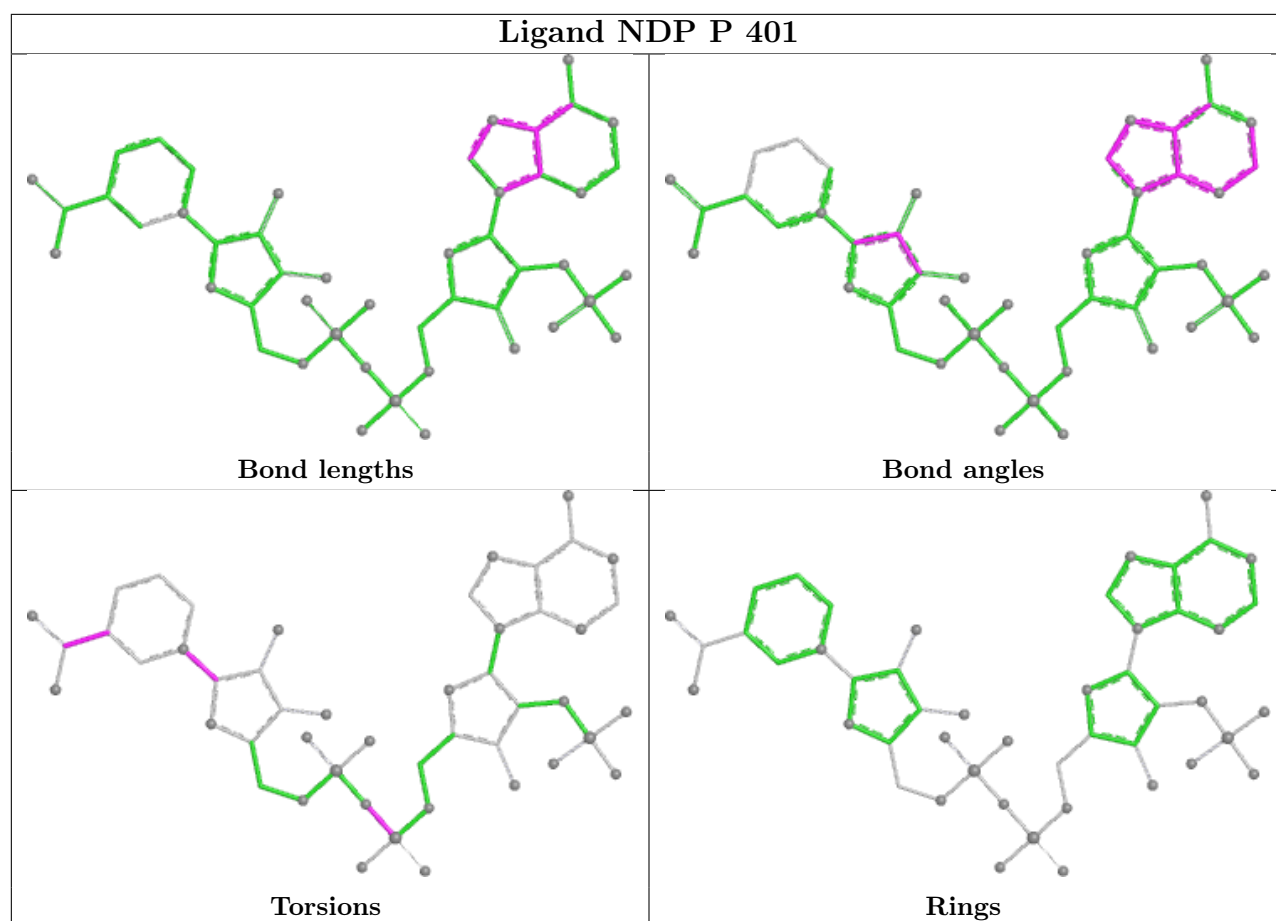
19 monomers are involved in 168 short contacts:

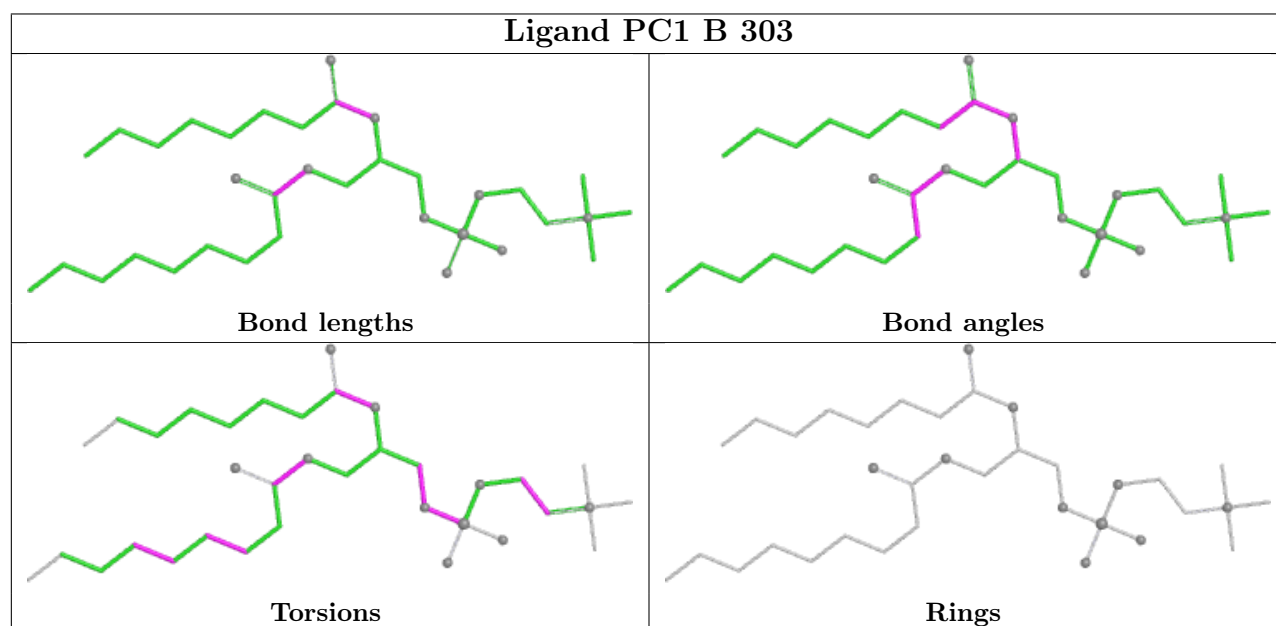
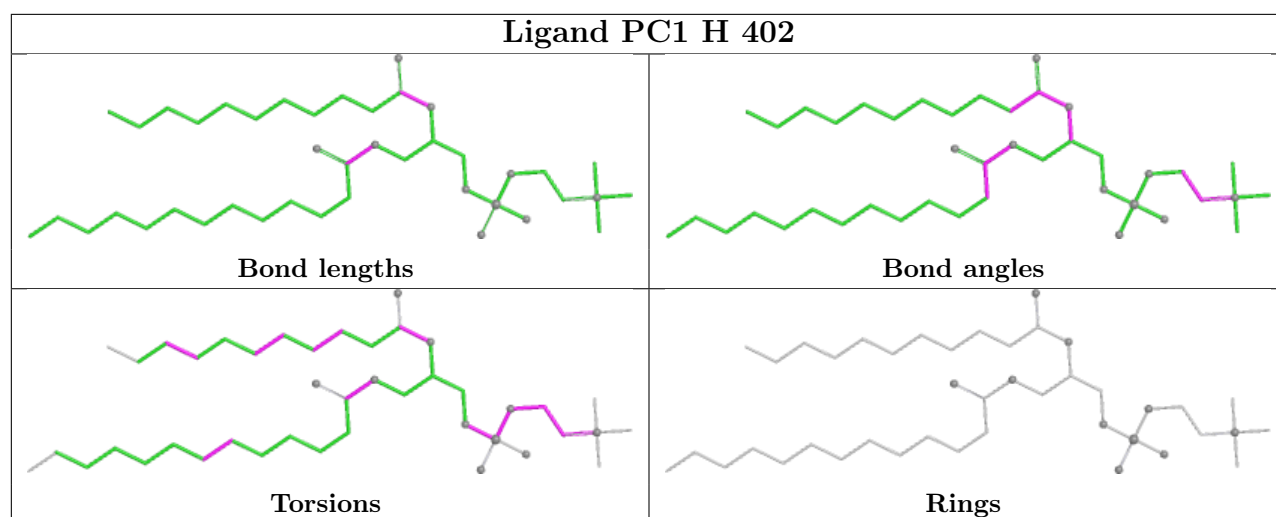
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	401	3PE	5	0
29	F	501	FMN	1	0
30	H	401	UQ9	14	0
25	G	802	SF4	7	0
27	I	302	PC1	13	0
31	P	401	NDP	7	0
33	W	201	EHZ	7	0
25	I	304	SF4	5	0
27	H	402	PC1	8	0
25	I	303	SF4	11	0
27	B	303	PC1	7	0
28	E	301	FES	5	0
26	B	302	UQ1	5	0
24	I	301	3PE	13	0
25	F	502	SF4	10	0
24	b	201	3PE	18	0
28	G	803	FES	5	0
34	q	201	CDL	21	0
25	B	301	SF4	6	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.

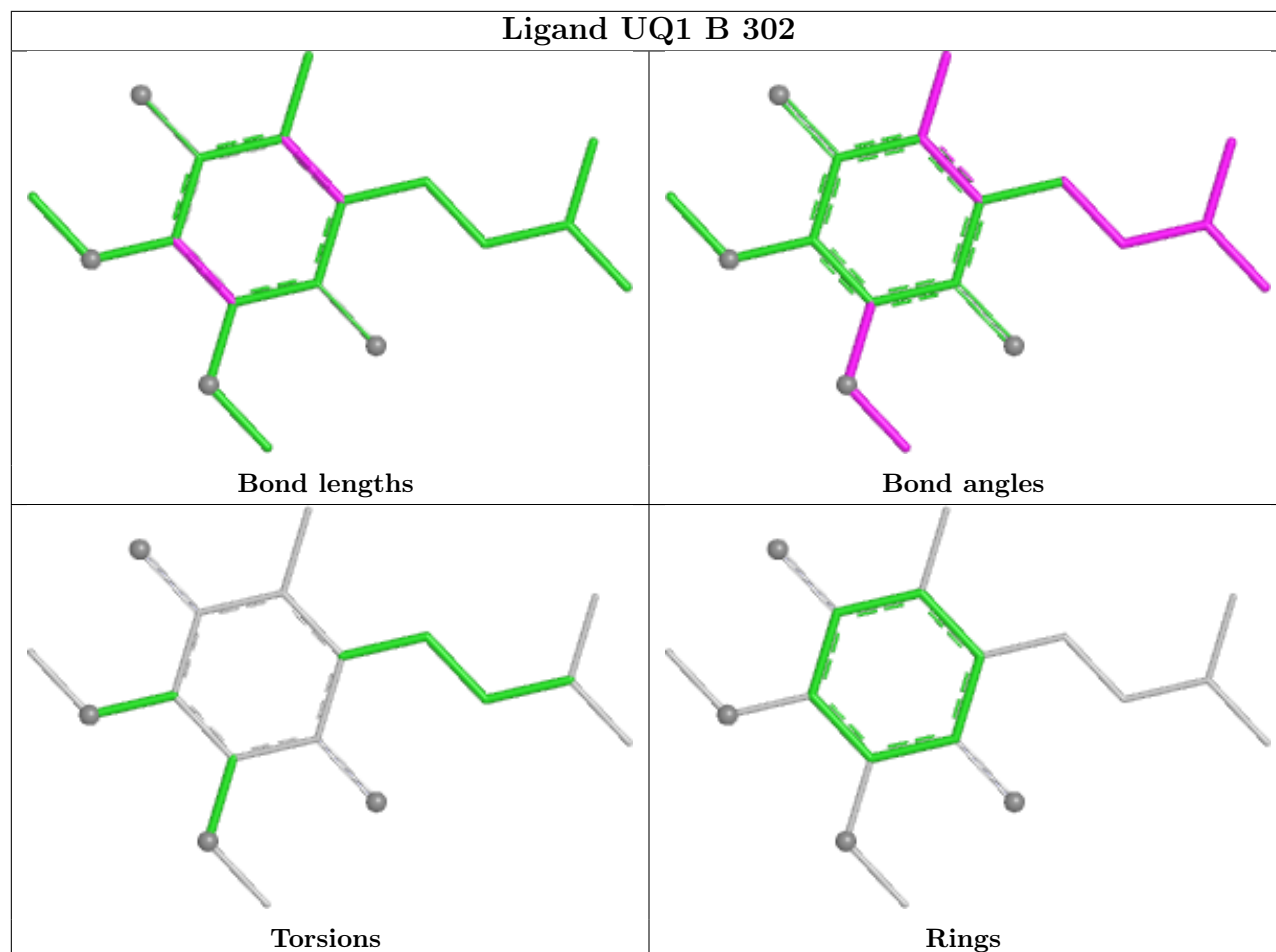




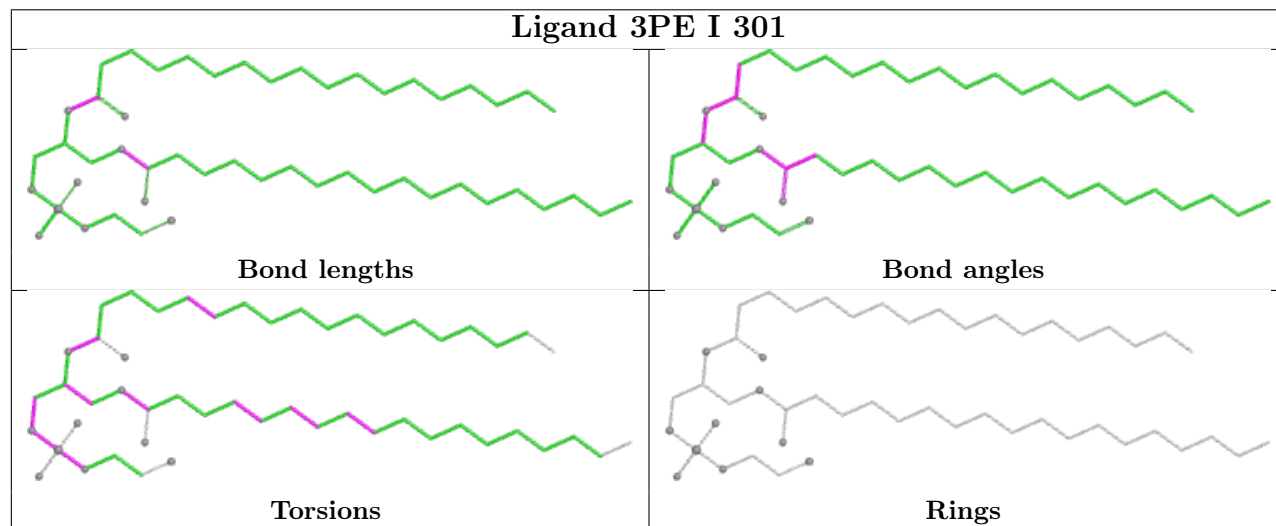


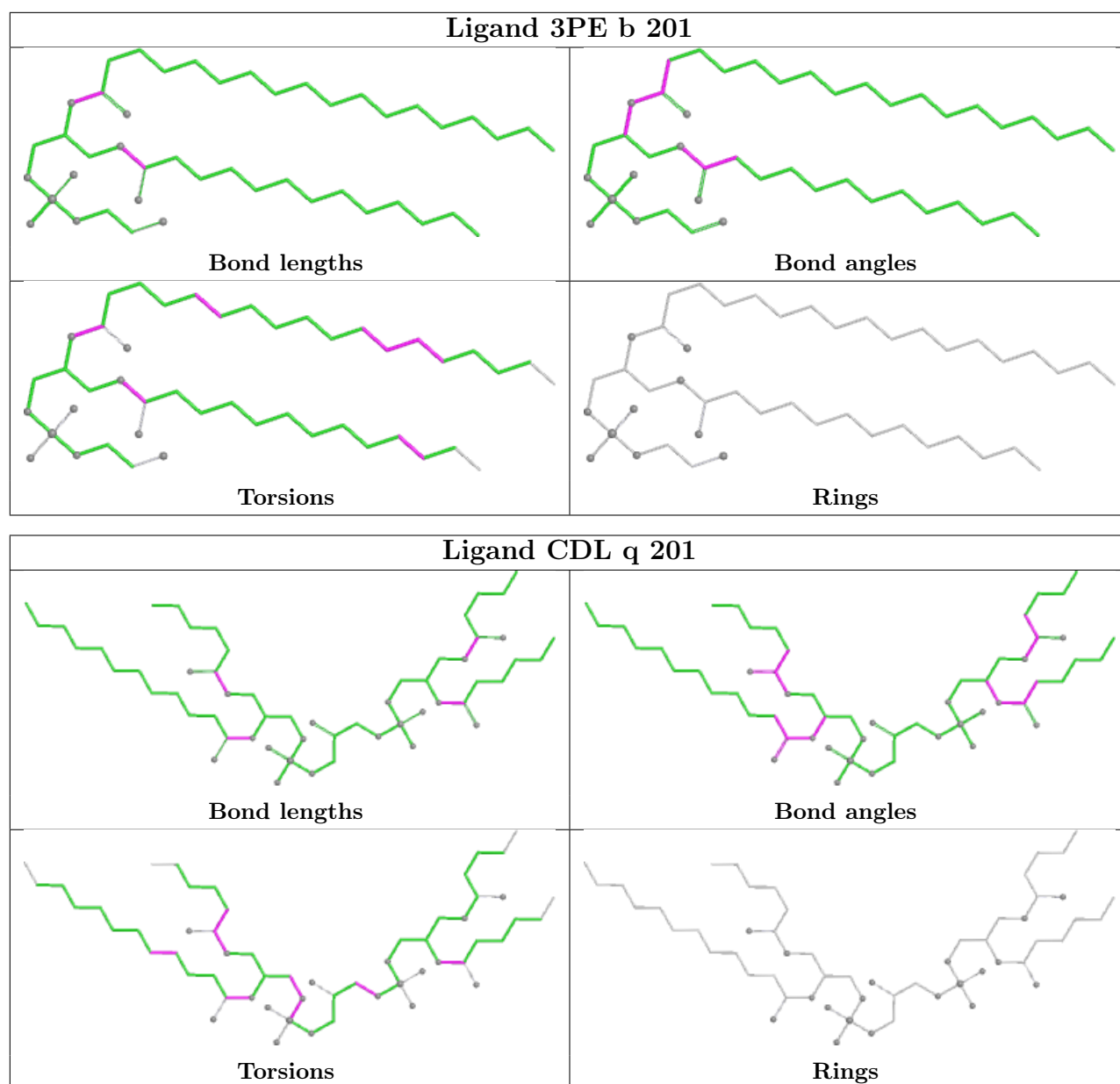


Ligand UQ1 B 302



Ligand 3PE I 301





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.

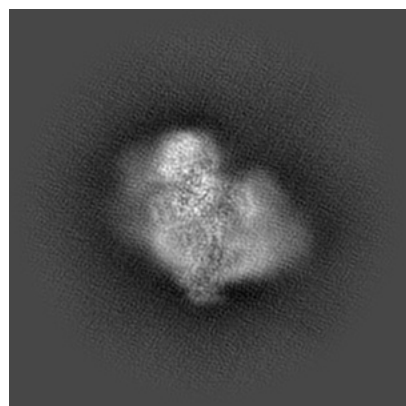
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38511. These allow visual inspection of the internal detail of the map and identification of artifacts.

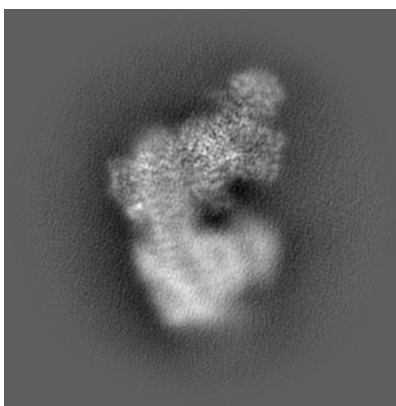
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

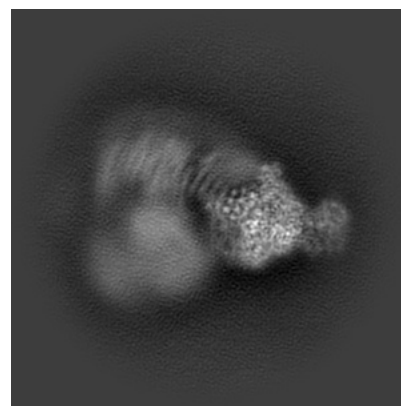
6.1.1 Primary map



X

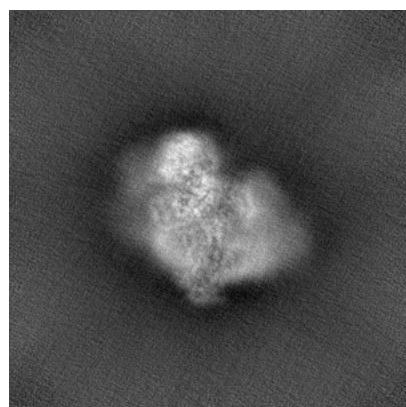


Y

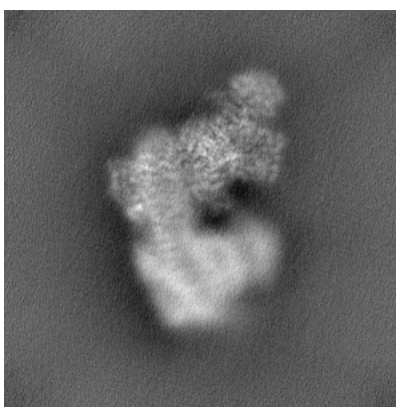


Z

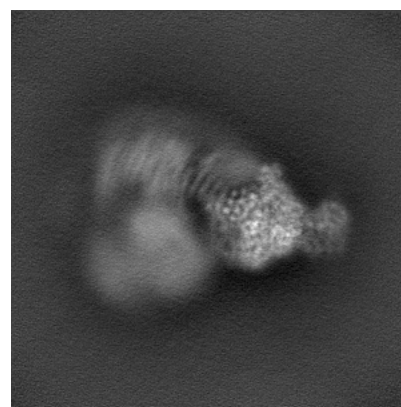
6.1.2 Raw map



X



Y

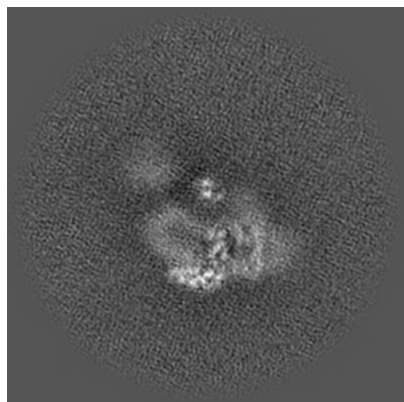


Z

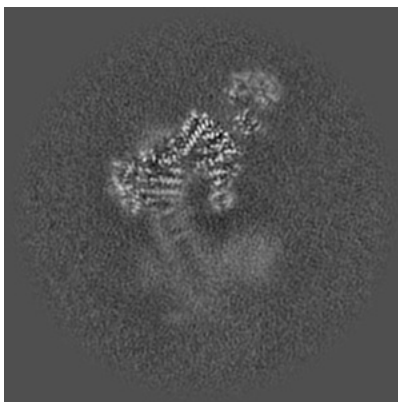
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

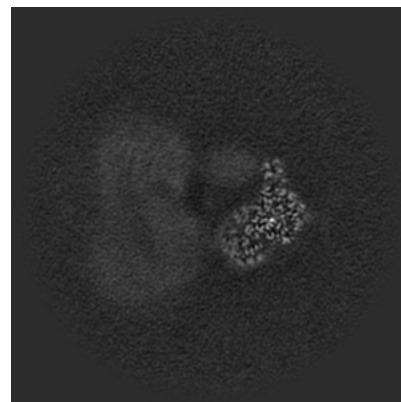
6.2.1 Primary map



X Index: 192

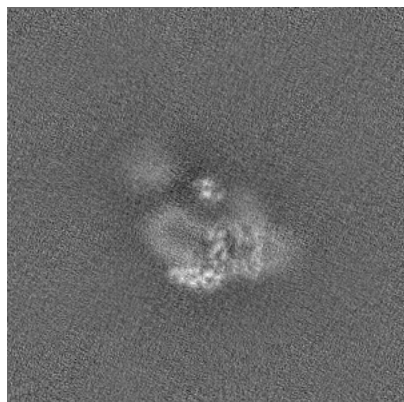


Y Index: 192



Z Index: 192

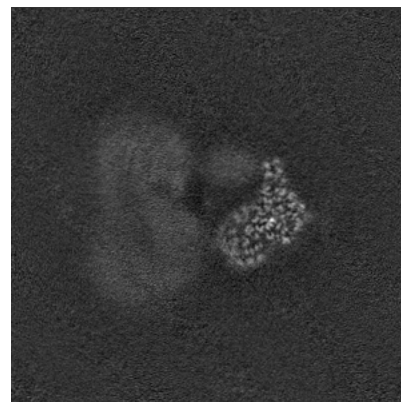
6.2.2 Raw map



X Index: 192



Y Index: 192

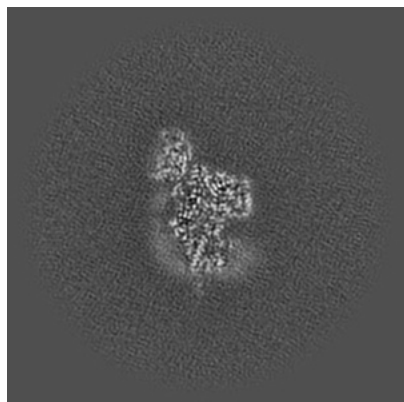


Z Index: 192

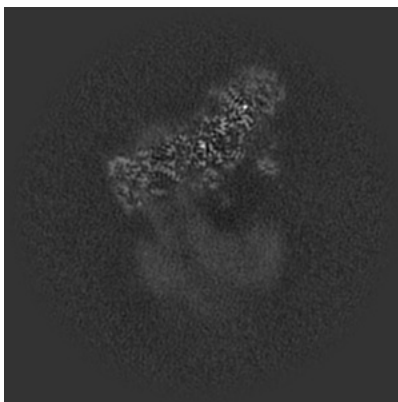
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

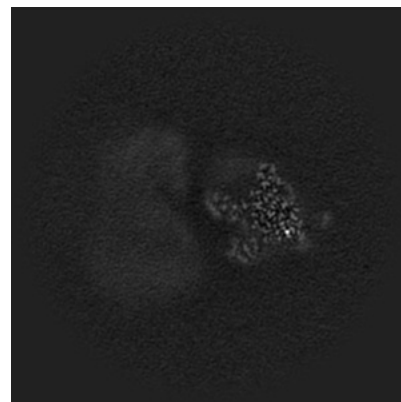
6.3.1 Primary map



X Index: 244

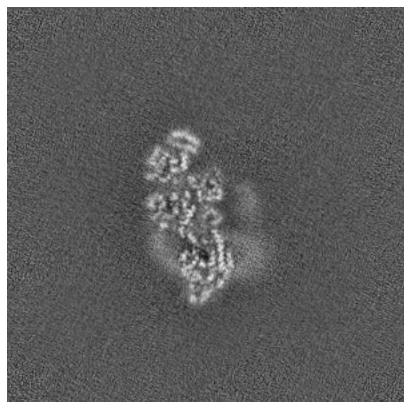


Y Index: 178

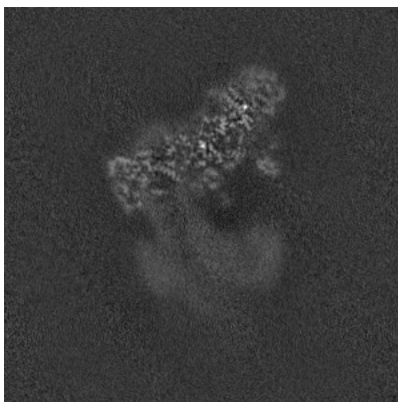


Z Index: 204

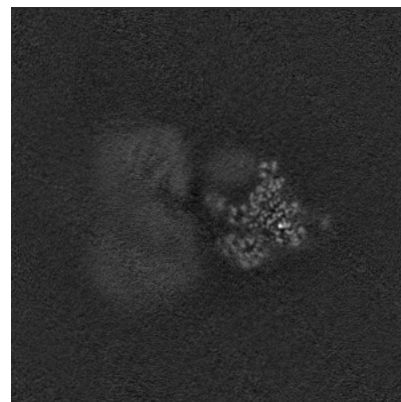
6.3.2 Raw map



X Index: 232



Y Index: 178

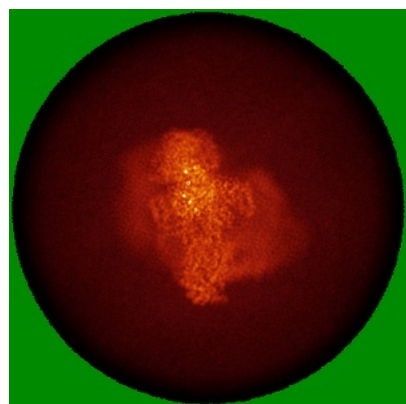


Z Index: 199

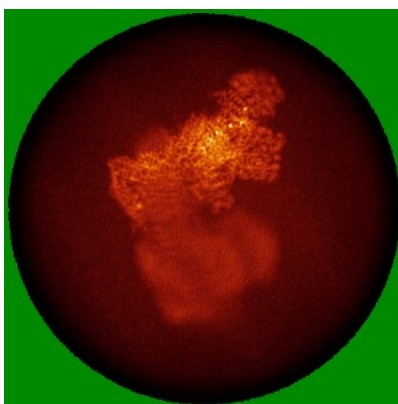
The images above show the largest variance slices of the map in three orthogonal directions.

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

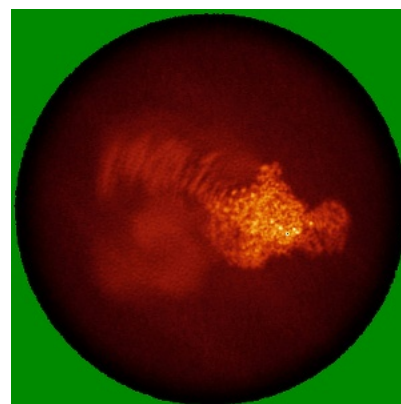
6.4.1 Primary map



X

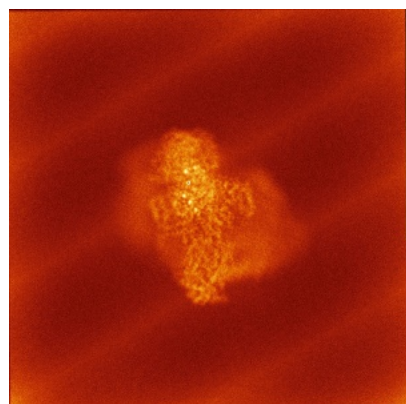


Y

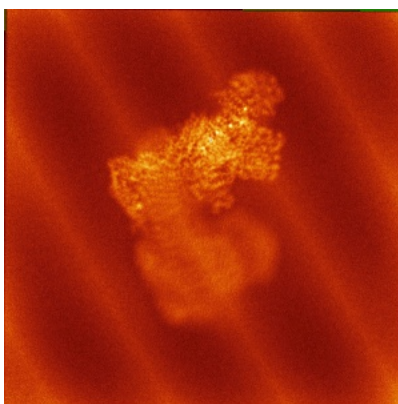


Z

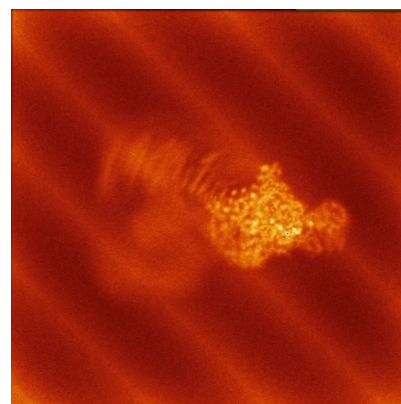
6.4.2 Raw map



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 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

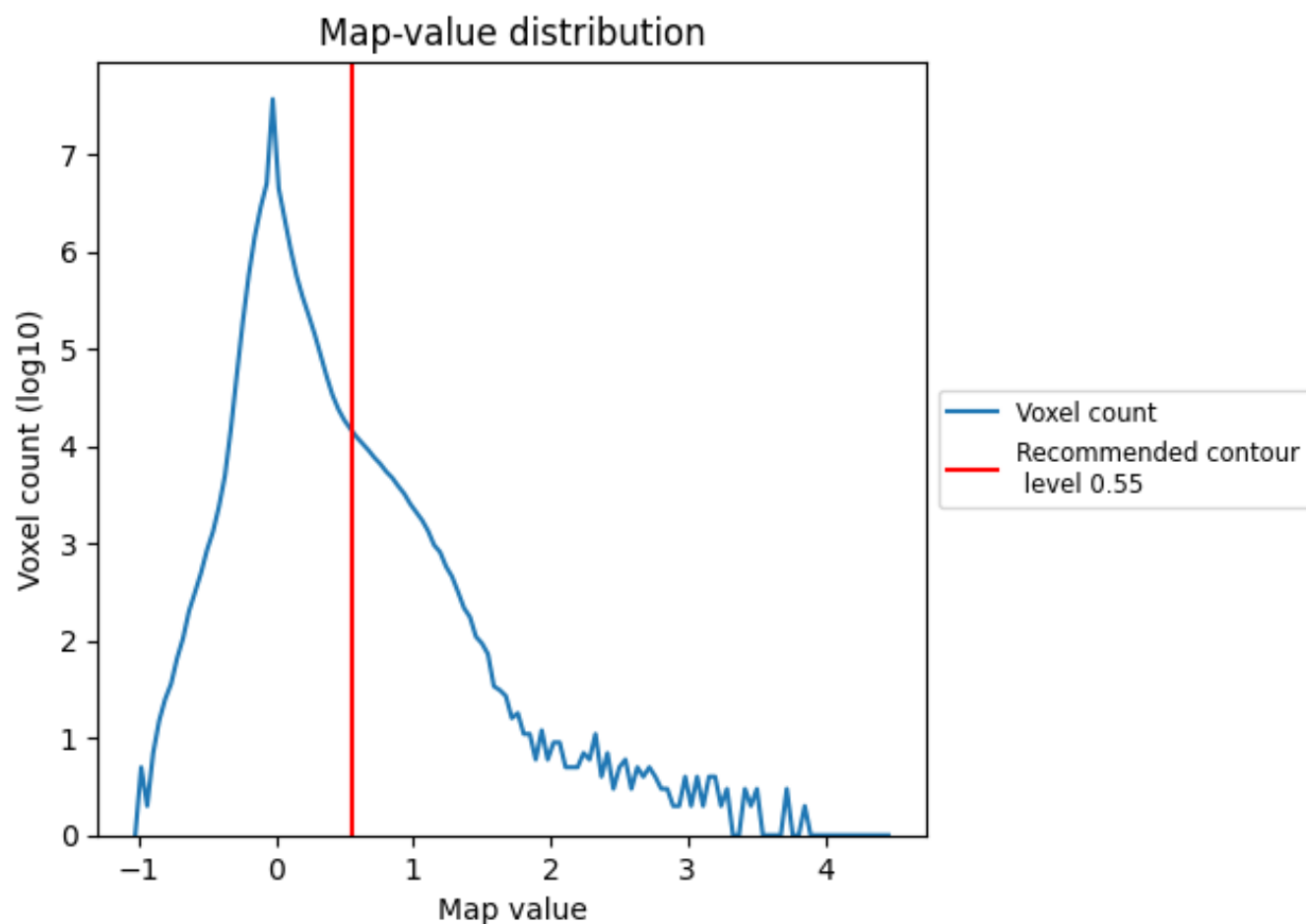
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

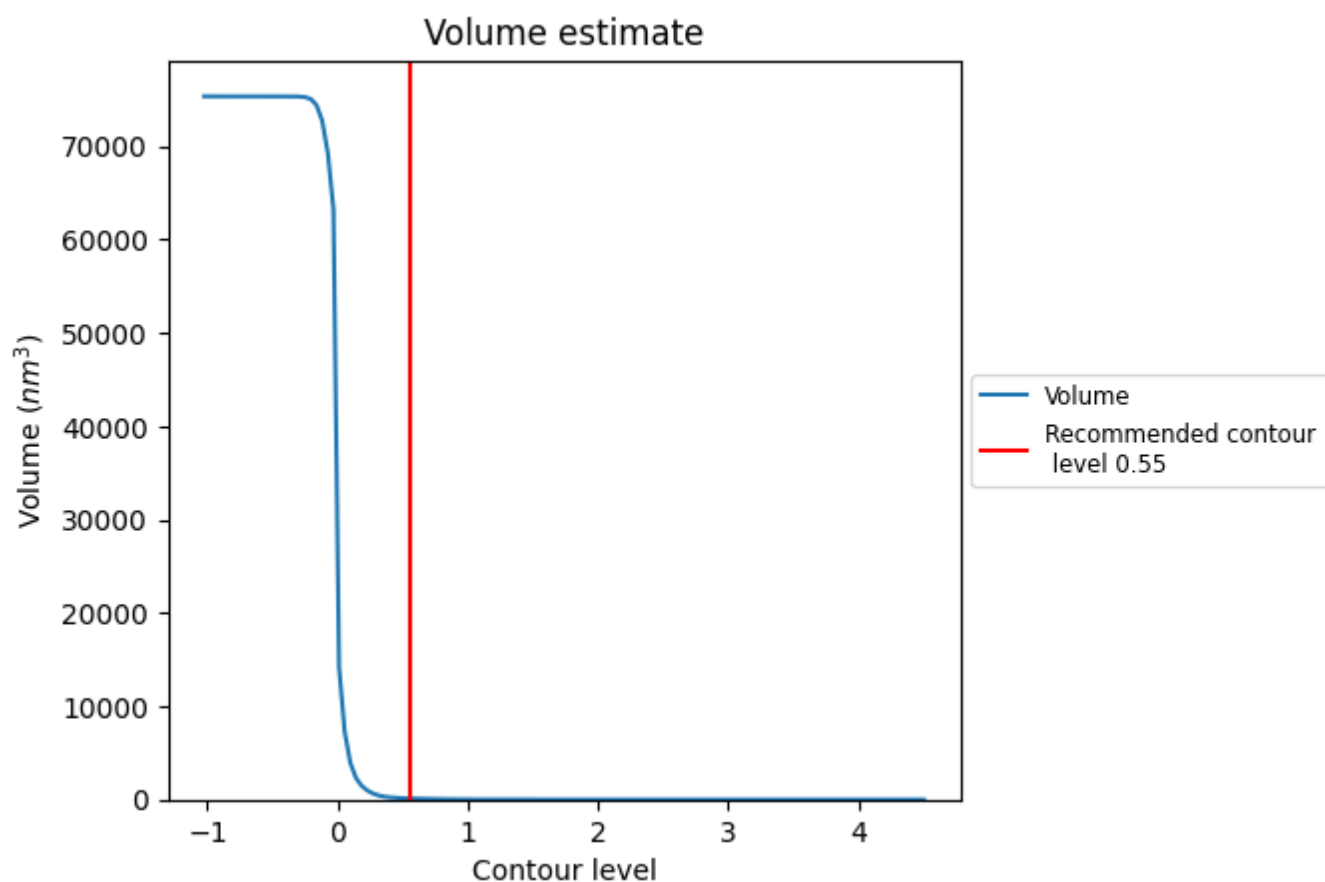
This section contains the results of statistical analysis of the map.

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.

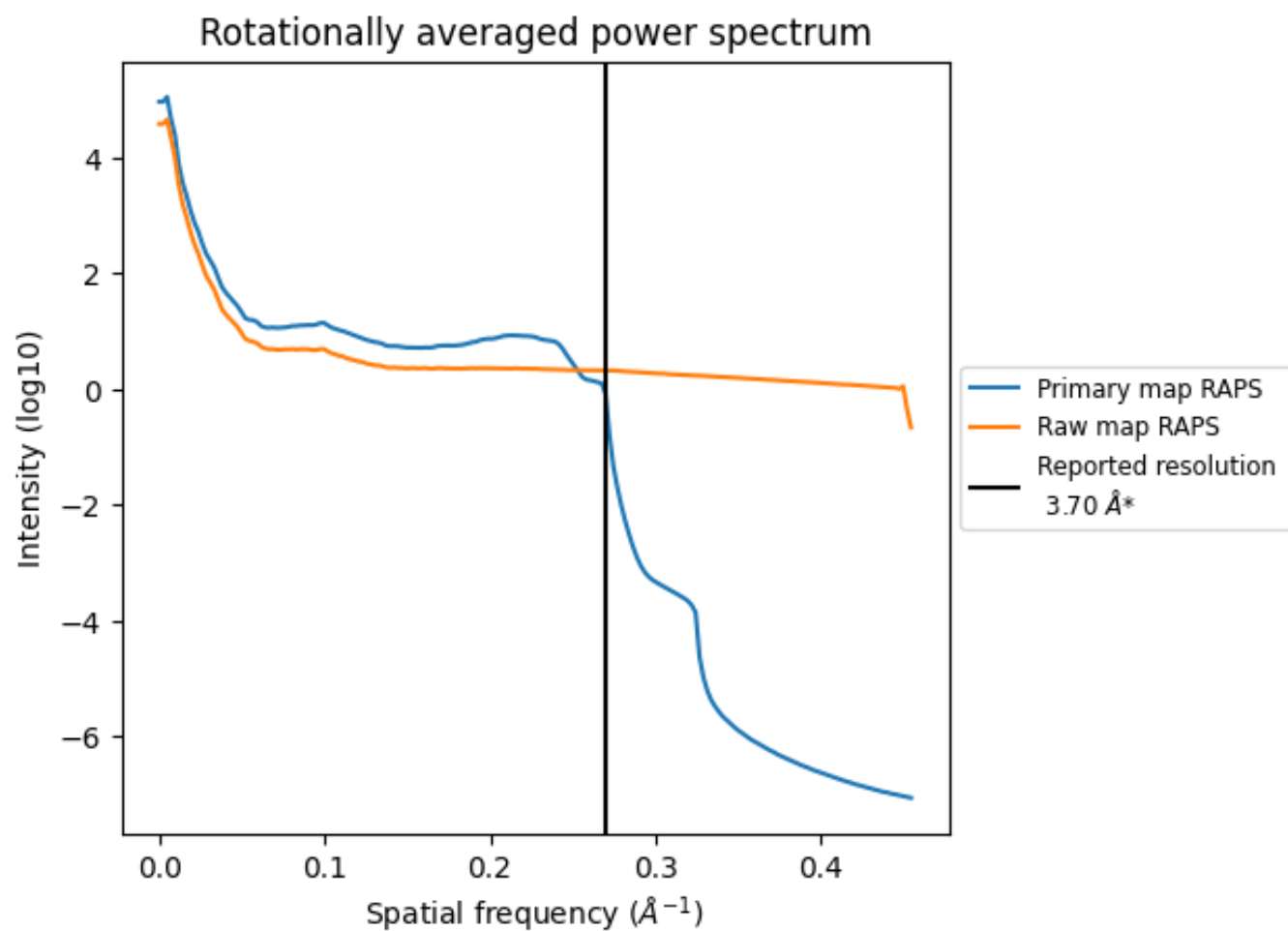
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm³; this corresponds to an approximate mass of 106 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 ⓘ

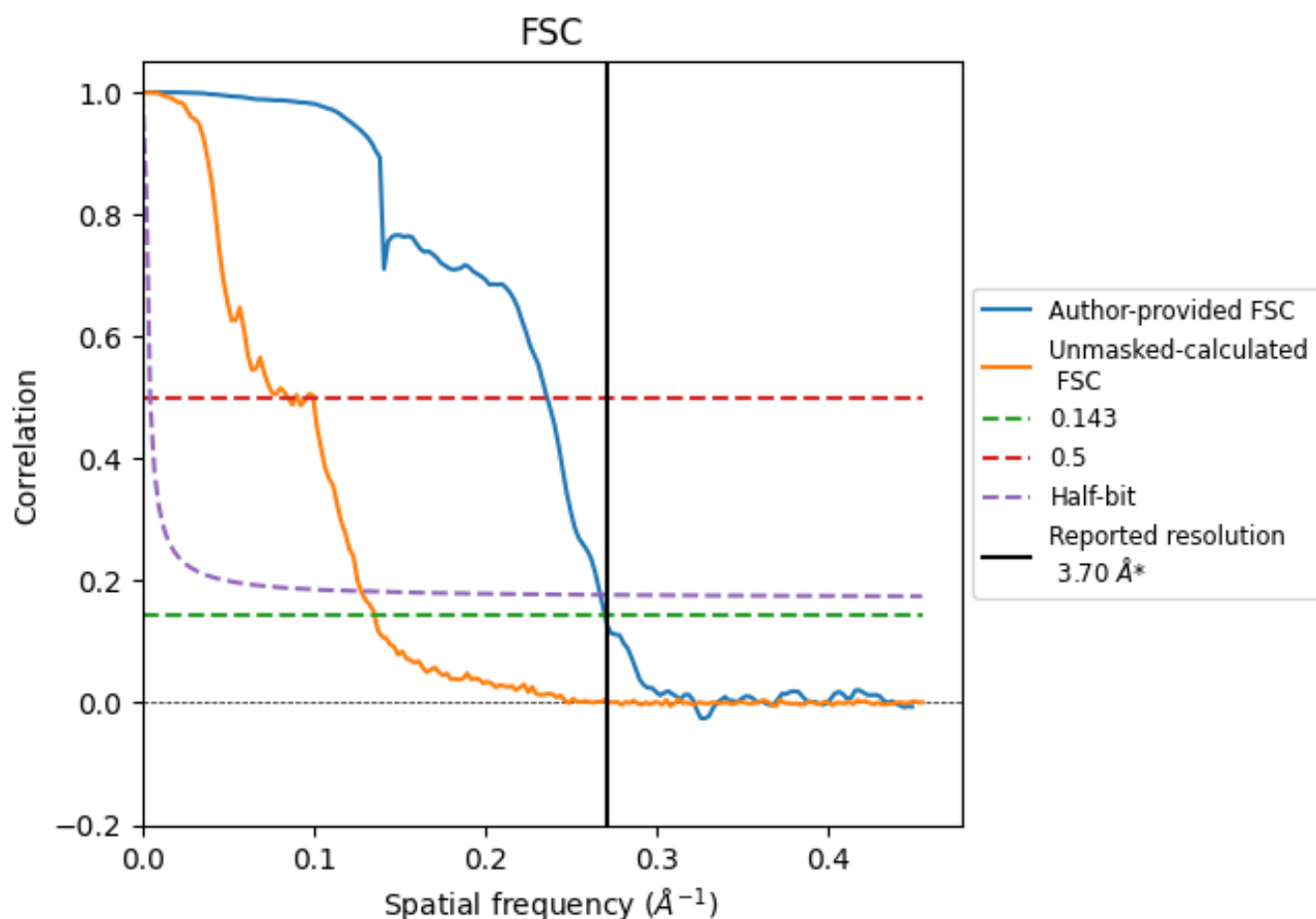


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

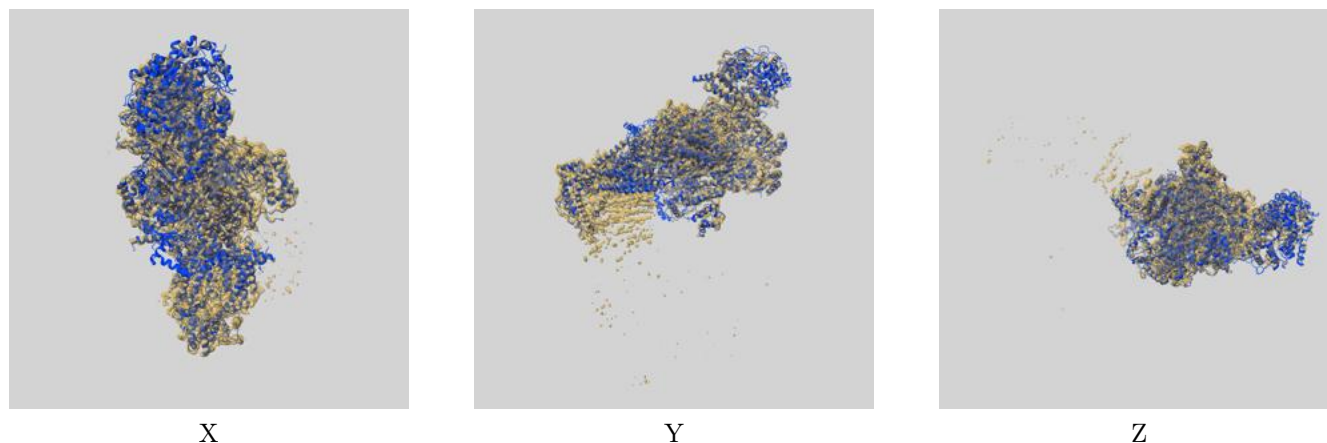
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.24	3.75
Unmasked-calculated*	7.39	11.79	7.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.39 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

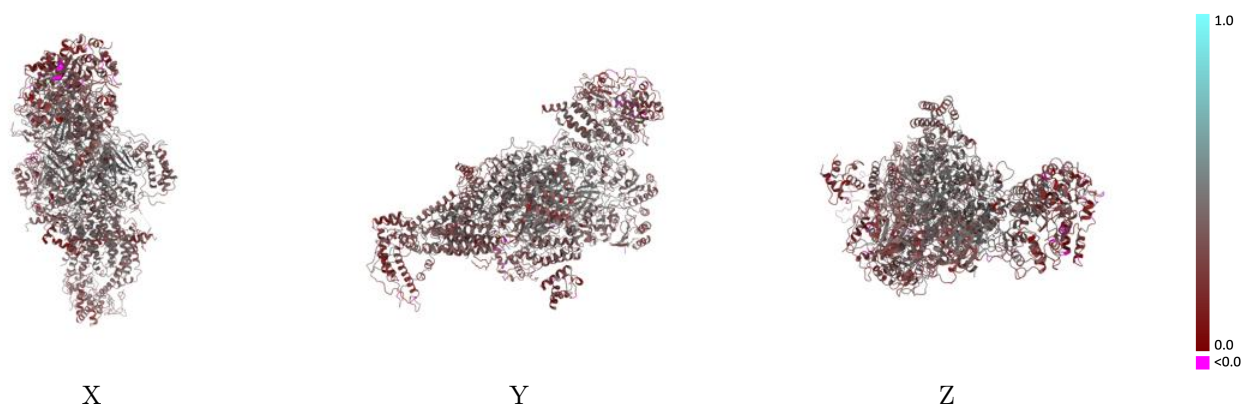
This section contains information regarding the fit between EMDB map EMD-38511 and PDB model 8XNQ. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



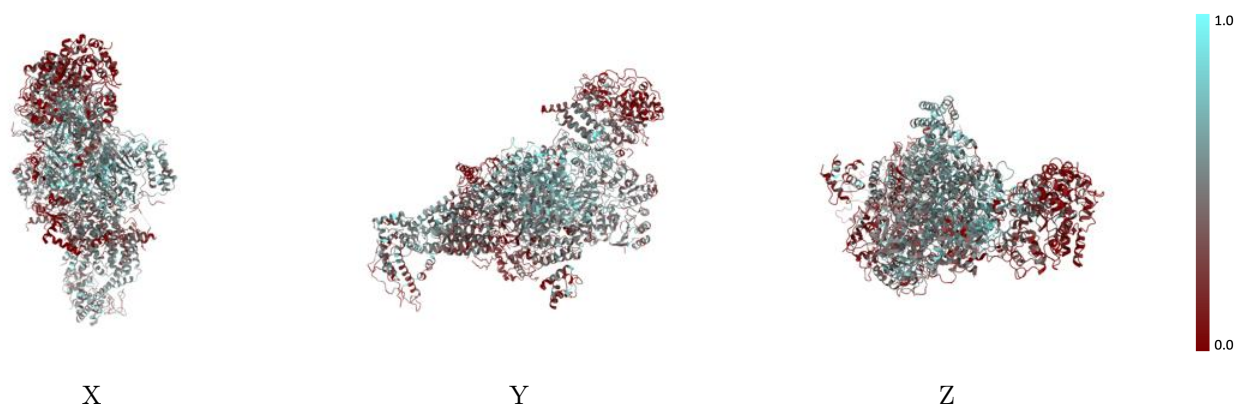
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



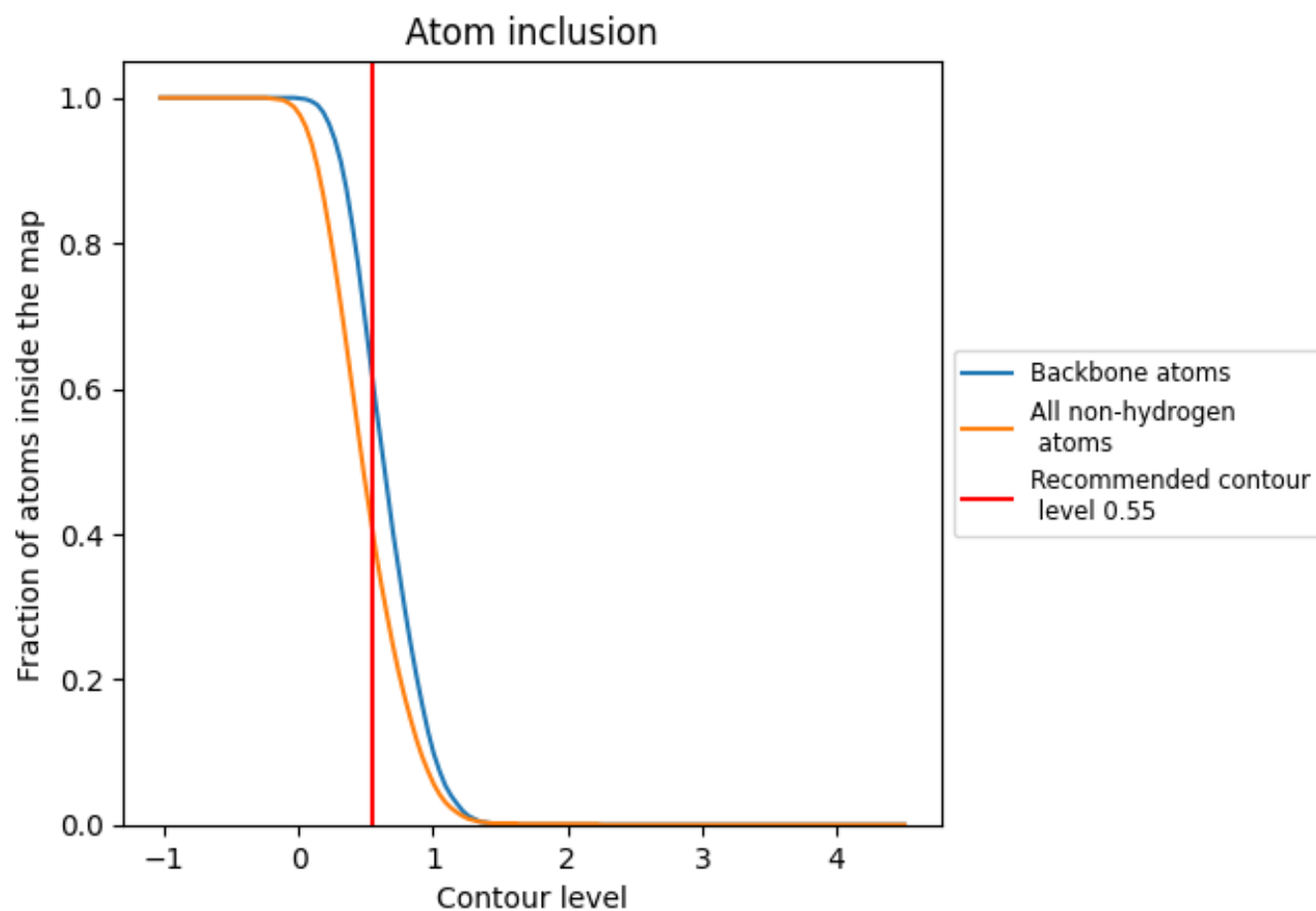
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



At the recommended contour level, 61% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.4040	 0.3450
A	 0.3300	 0.3340
B	 0.5340	 0.4150
C	 0.5760	 0.4210
D	 0.5680	 0.4250
E	 0.1700	 0.2710
F	 0.2510	 0.2970
G	 0.5050	 0.3790
H	 0.4440	 0.3780
I	 0.5700	 0.4170
P	 0.2900	 0.2930
Q	 0.3650	 0.3800
R	 0.1870	 0.2610
S	 0.4290	 0.3140
T	 0.2490	 0.2230
V	 0.5470	 0.3520
W	 0.3800	 0.3520
X	 0.4080	 0.2550
Z	 0.4250	 0.2830
a	 0.5420	 0.3630
b	 0.3870	 0.3080
q	 0.0470	 0.2820
r	 0.1770	 0.3070
s	 0.0090	 0.1520

