



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:00 PM UTC

PDB ID : 7ASK / pdb_00007ask
EMDB ID : EMD-11895
Title : 43S preinitiation complex from Trypanosoma cruzi with the kDDX60 helicase bound with ATP
Authors : Bochler, A.; Brito Querido, J.; Prilepskaja, T.; Soufari, H.; Del Cistia, M.L.; Kuhn, L.; Rimoldi Ribeiro, A.; Valasek, L.S.; Hashem, Y.
Deposited on : 2020-10-27
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

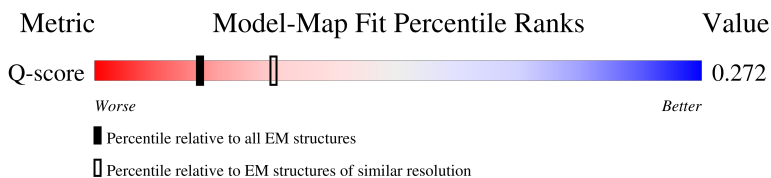
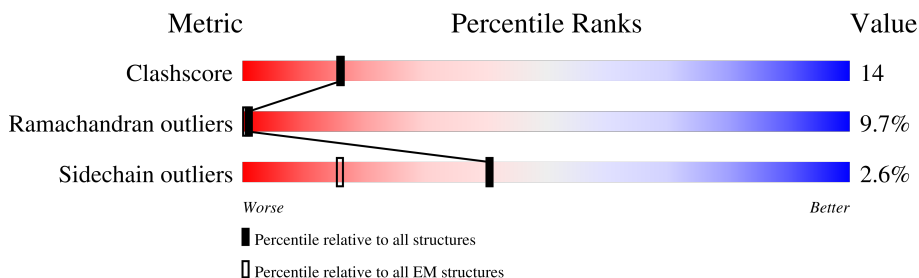
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	F	2174	

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
3	ADP	F	2202	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12285 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.

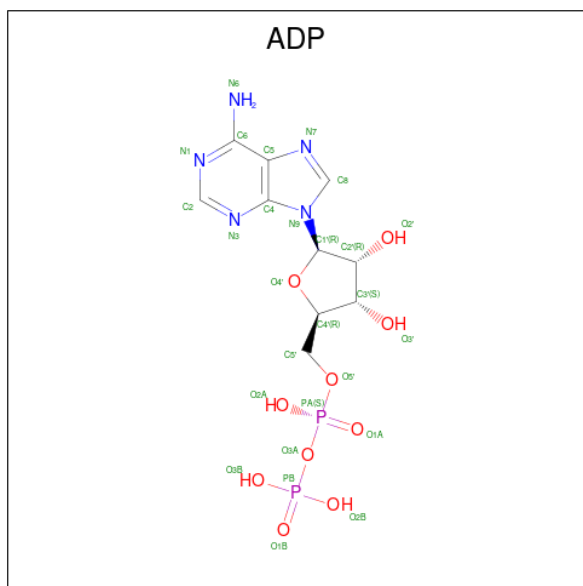
- Molecule 1 is a protein called kDDX60.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	1523	Total	C	N	O	S	0	0
			12257	7734	2165	2292	66		

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
2	F	1	Total	Mg	0
			1	1	

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

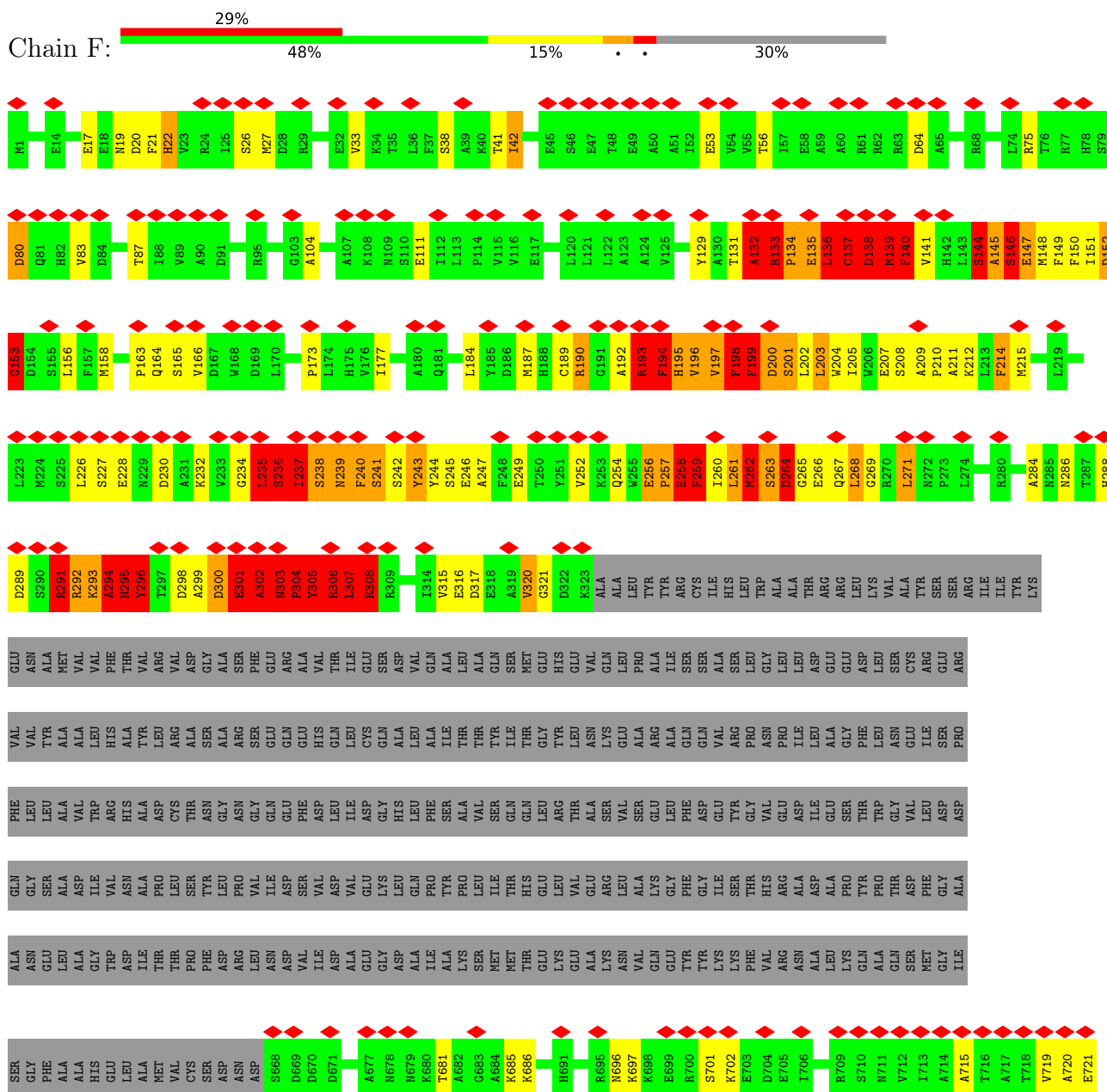


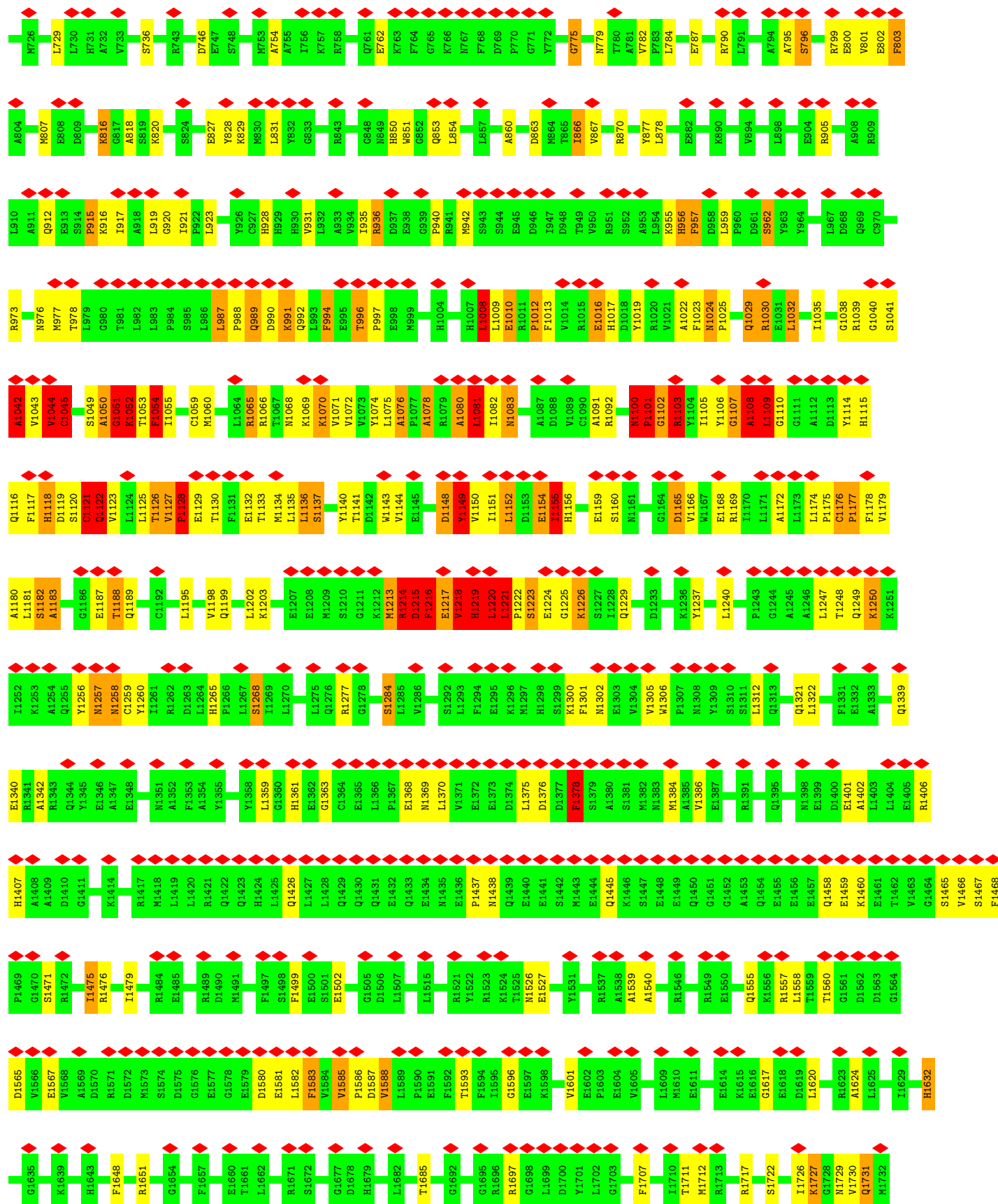
Mol	Chain	Residues	Atoms					AltConf
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: kDDX60





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.221	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0344	Depositor
Map size ($\text{\AA}$)	490.5, 490.5, 490.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.635, 1.635, 1.635	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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	F	1.62	74/12495 (0.6%)	2.05	355/16839 (2.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	4	187

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1149	TYR	C-N	30.49	1.72	1.33
1	F	304	PRO	CA-C	-28.52	1.19	1.52
1	F	305	TYR	CA-C	-23.98	1.20	1.52
1	F	259	PHE	CA-C	23.46	1.81	1.52
1	F	291	ARG	C-N	-23.04	1.03	1.33
1	F	1152	LEU	C-N	22.38	1.64	1.33
1	F	1215	ASP	C-N	-20.83	1.04	1.33
1	F	1183	ALA	N-CA	-20.73	1.19	1.46
1	F	296	TYR	N-CA	-20.67	1.19	1.46
1	F	306	ARG	N-CA	20.60	1.72	1.46
1	F	1052	LYS	C-N	20.05	1.58	1.33
1	F	303	ASN	C-N	18.79	1.55	1.33
1	F	1039	ARG	C-N	18.21	1.67	1.33
1	F	194	PHE	C-N	-18.07	1.08	1.33
1	F	1137	SER	N-CA	-17.52	1.21	1.46
1	F	305	TYR	C-O	15.64	1.43	1.24
1	F	195	HIS	C-N	-15.60	1.12	1.33
1	F	1044	VAL	C-N	15.29	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	259	PHE	C-N	14.96	1.56	1.33
1	F	1149	TYR	N-CA	-14.64	1.27	1.46
1	F	198	PHE	C-N	-14.20	1.14	1.33
1	F	197	VAL	N-CA	13.78	1.61	1.46
1	F	1221	LEU	C-N	13.69	1.65	1.33
1	F	153	GLY	N-CA	-13.49	1.25	1.45
1	F	1122	GLN	C-N	13.45	1.54	1.33
1	F	307	LEU	CA-C	-13.22	1.35	1.52
1	F	1219	HIS	C-N	13.18	1.51	1.33
1	F	1076	ALA	C-N	12.82	1.63	1.33
1	F	1108	ALA	N-CA	-12.78	1.29	1.46
1	F	304	PRO	C-N	-12.77	1.15	1.33
1	F	296	TYR	C-N	12.55	1.49	1.34
1	F	133	ARG	C-N	11.34	1.60	1.33
1	F	301	GLU	C-N	-10.76	1.18	1.33
1	F	292	ARG	N-CA	-10.52	1.32	1.45
1	F	303	ASN	C-O	10.42	1.34	1.24
1	F	199	PHE	N-CA	10.24	1.58	1.46
1	F	239	ASN	CA-C	-10.23	1.38	1.52
1	F	234	GLY	C-N	-10.14	1.19	1.33
1	F	265	GLY	N-CA	-9.97	1.30	1.45
1	F	305	TYR	C-N	9.53	1.47	1.33
1	F	292	ARG	C-N	9.51	1.48	1.33
1	F	136	LEU	C-N	9.28	1.47	1.33
1	F	305	TYR	N-CA	-9.16	1.34	1.46
1	F	294	ALA	C-N	-9.07	1.21	1.33
1	F	146	SER	C-N	9.05	1.46	1.33
1	F	1108	ALA	C-N	8.89	1.46	1.33
1	F	147	GLU	C-N	8.81	1.48	1.33
1	F	134	PRO	CA-C	8.79	1.64	1.52
1	F	1155	ILE	N-CA	-8.75	1.29	1.46
1	F	1103	ARG	C-N	-8.45	1.22	1.33
1	F	294	ALA	N-CA	-8.26	1.35	1.45
1	F	1042	ALA	C-N	-7.87	1.23	1.33
1	F	1051	GLY	C-N	7.85	1.45	1.33
1	F	1040	GLY	N-CA	-7.61	1.34	1.45
1	F	1042	ALA	N-CA	-7.54	1.36	1.46
1	F	239	ASN	C-N	7.43	1.43	1.33
1	F	199	PHE	C-N	7.43	1.44	1.33
1	F	293	LYS	C-N	7.21	1.42	1.33
1	F	1182	SER	C-N	-7.16	1.23	1.33
1	F	236	SER	C-N	-6.99	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	198	PHE	CA-C	-6.89	1.43	1.53
1	F	195	HIS	C-O	-6.86	1.15	1.24
1	F	301	GLU	C-O	-6.80	1.09	1.23
1	F	292	ARG	C-O	-6.63	1.15	1.23
1	F	259	PHE	N-CA	-6.51	1.37	1.45
1	F	258	GLU	C-N	6.42	1.41	1.33
1	F	293	LYS	C-O	6.31	1.31	1.23
1	F	240	PHE	C-N	6.04	1.41	1.33
1	F	1176	CYS	C-N	5.92	1.47	1.33
1	F	293	LYS	N-CA	-5.89	1.38	1.45
1	F	140	PHE	C-N	-5.74	1.26	1.33
1	F	295	ASN	C-N	5.56	1.41	1.33
1	F	262	MET	C-O	5.33	1.29	1.23
1	F	256	GLU	C-N	5.12	1.45	1.33

All (355) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1051	GLY	O-C-N	-28.78	84.72	122.42
1	F	1136	LEU	O-C-N	24.22	148.00	122.08
1	F	1155	ILE	N-CA-CB	22.96	150.53	111.50
1	F	152	ASP	O-C-N	-21.91	97.94	123.13
1	F	306	ARG	N-CA-CB	21.42	146.69	110.49
1	F	305	TYR	N-CA-CB	21.14	146.22	110.49
1	F	262	MET	O-C-N	-20.35	102.94	123.29
1	F	296	TYR	N-CA-C	20.35	154.14	110.80
1	F	193	ARG	CA-C-N	20.32	160.35	121.54
1	F	193	ARG	C-N-CA	20.32	160.35	121.54
1	F	139	MET	O-C-N	-17.58	94.87	123.00
1	F	1154	GLU	O-C-N	-17.45	99.38	122.59
1	F	146	SER	O-C-N	-17.31	98.94	122.30
1	F	198	PHE	O-C-N	-17.00	103.11	122.84
1	F	303	ASN	CA-C-O	16.93	135.43	120.71
1	F	304	PRO	CA-C-O	-16.85	101.82	121.03
1	F	198	PHE	N-CA-C	-16.66	85.80	110.46
1	F	1148	ASP	O-C-N	16.60	145.03	123.12
1	F	1127	VAL	O-C-N	16.45	139.85	121.10
1	F	259	PHE	N-CA-CB	-16.43	85.61	111.56
1	F	239	ASN	CA-C-O	-16.14	99.96	119.49
1	F	1122	GLN	CA-C-O	-16.02	97.60	120.51
1	F	1125	LEU	CB-CA-C	-15.83	90.68	110.94
1	F	1039	ARG	CA-C-N	15.37	147.24	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1039	ARG	C-N-CA	15.37	147.24	121.57
1	F	234	GLY	O-C-N	15.28	142.56	122.70
1	F	1220	LEU	O-C-N	-15.24	103.00	122.82
1	F	1039	ARG	O-C-N	-14.79	102.92	122.59
1	F	147	GLU	O-C-N	-14.72	103.01	122.59
1	F	1148	ASP	CA-C-N	14.54	149.31	121.54
1	F	1148	ASP	C-N-CA	14.54	149.31	121.54
1	F	133	ARG	CA-C-N	14.52	137.98	119.84
1	F	133	ARG	C-N-CA	14.52	137.98	119.84
1	F	259	PHE	CA-C-O	-14.39	106.05	121.45
1	F	1137	SER	N-CA-CB	14.19	135.63	110.37
1	F	258	GLU	CA-C-N	14.13	145.04	121.87
1	F	258	GLU	C-N-CA	14.13	145.04	121.87
1	F	296	TYR	O-C-N	14.09	141.33	122.59
1	F	238	SER	CA-C-N	14.02	143.03	120.60
1	F	238	SER	C-N-CA	14.02	143.03	120.60
1	F	236	SER	O-C-N	-13.93	109.36	123.29
1	F	152	ASP	CA-C-N	13.34	147.56	121.41
1	F	152	ASP	C-N-CA	13.34	147.56	121.41
1	F	304	PRO	N-CA-C	13.12	130.60	110.80
1	F	134	PRO	CA-C-O	-12.66	97.56	120.60
1	F	139	MET	CA-C-N	-12.60	99.68	120.72
1	F	139	MET	C-N-CA	-12.60	99.68	120.72
1	F	256	GLU	CA-C-N	12.59	135.58	119.84
1	F	256	GLU	C-N-CA	12.59	135.58	119.84
1	F	1050	ALA	CA-C-N	-12.39	102.50	122.20
1	F	1050	ALA	C-N-CA	-12.39	102.50	122.20
1	F	307	LEU	O-C-N	12.38	139.06	122.59
1	F	238	SER	CB-CA-C	-12.29	84.59	109.79
1	F	236	SER	CA-C-N	12.17	139.85	122.94
1	F	236	SER	C-N-CA	12.17	139.85	122.94
1	F	1218	VAL	O-C-N	-12.10	110.27	122.97
1	F	133	ARG	O-C-N	-11.99	108.10	121.53
1	F	199	PHE	CA-C-N	11.94	144.34	121.54
1	F	199	PHE	C-N-CA	11.94	144.34	121.54
1	F	1152	LEU	O-C-N	-11.88	109.51	123.41
1	F	306	ARG	CA-C-N	11.80	144.08	121.54
1	F	306	ARG	C-N-CA	11.80	144.08	121.54
1	F	263	SER	O-C-N	-11.67	109.75	123.28
1	F	303	ASN	CB-CA-C	11.41	126.00	110.37
1	F	132	ALA	CA-C-N	11.33	144.60	121.48
1	F	132	ALA	C-N-CA	11.33	144.60	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	304	PRO	O-C-N	11.21	135.65	123.10
1	F	302	ALA	O-C-N	11.12	137.38	122.59
1	F	258	GLU	O-C-N	-10.99	103.87	122.11
1	F	136	LEU	N-CA-CB	-10.96	91.96	110.49
1	F	137	CYS	O-C-N	-10.91	108.21	122.72
1	F	1109	LEU	CA-C-N	10.70	138.07	121.37
1	F	1109	LEU	C-N-CA	10.70	138.07	121.37
1	F	293	LYS	O-C-N	-10.66	110.13	123.24
1	F	1177	PRO	CB-CA-C	10.59	129.03	111.56
1	F	138	ASP	CA-C-N	-10.47	102.86	121.70
1	F	138	ASP	C-N-CA	-10.47	102.86	121.70
1	F	153	GLY	CA-C-N	-10.45	101.58	121.54
1	F	153	GLY	C-N-CA	-10.45	101.58	121.54
1	F	147	GLU	CA-C-N	10.24	137.65	123.11
1	F	147	GLU	C-N-CA	10.24	137.65	123.11
1	F	137	CYS	N-CA-C	-10.22	93.70	109.65
1	F	259	PHE	N-CA-C	10.03	123.90	108.96
1	F	303	ASN	CA-C-N	10.00	130.40	119.90
1	F	303	ASN	C-N-CA	10.00	130.40	119.90
1	F	1121	CYS	O-C-N	-9.97	109.33	122.59
1	F	136	LEU	CA-C-O	-9.79	106.52	120.51
1	F	300	ASP	CA-C-N	-9.72	104.20	121.70
1	F	300	ASP	C-N-CA	-9.72	104.20	121.70
1	F	259	PHE	CB-CA-C	-9.71	89.04	111.09
1	F	292	ARG	CA-C-N	9.67	137.71	122.62
1	F	292	ARG	C-N-CA	9.67	137.71	122.62
1	F	266	GLU	CA-C-N	9.38	138.58	121.70
1	F	266	GLU	C-N-CA	9.38	138.58	121.70
1	F	193	ARG	O-C-N	-9.37	110.13	122.59
1	F	1052	LYS	O-C-N	9.25	133.36	122.17
1	F	135	GLU	CA-C-O	-9.21	110.89	121.58
1	F	1108	ALA	CA-C-N	9.08	138.88	121.54
1	F	1108	ALA	C-N-CA	9.08	138.88	121.54
1	F	196	VAL	CA-C-N	-8.94	110.72	123.06
1	F	196	VAL	C-N-CA	-8.94	110.72	123.06
1	F	1445	GLN	N-CA-C	-8.94	104.43	114.62
1	F	1560	THR	N-CA-C	-8.88	104.49	114.62
1	F	295	ASN	N-CA-C	8.85	129.65	110.80
1	F	1045	CYS	O-C-N	-8.59	113.32	123.03
1	F	293	LYS	CA-C-N	8.55	136.99	121.85
1	F	293	LYS	C-N-CA	8.55	136.99	121.85
1	F	199	PHE	N-CA-CB	-8.53	97.88	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	301	GLU	CA-C-O	-8.48	106.38	120.80
1	F	238	SER	N-CA-C	8.40	122.54	109.52
1	F	237	ILE	CA-C-N	8.40	135.77	122.59
1	F	237	ILE	C-N-CA	8.40	135.77	122.59
1	F	307	LEU	CA-C-N	8.40	137.82	122.54
1	F	307	LEU	C-N-CA	8.40	137.82	122.54
1	F	239	ASN	CB-CA-C	8.13	127.48	110.32
1	F	920	GLY	CA-C-N	8.00	128.10	120.43
1	F	920	GLY	C-N-CA	8.00	128.10	120.43
1	F	263	SER	CA-C-N	-7.96	111.55	122.30
1	F	263	SER	C-N-CA	-7.96	111.55	122.30
1	F	294	ALA	O-C-N	7.93	132.29	123.33
1	F	234	GLY	CA-C-N	7.91	136.64	121.54
1	F	234	GLY	C-N-CA	7.91	136.64	121.54
1	F	195	HIS	CA-C-N	7.71	133.70	122.99
1	F	195	HIS	C-N-CA	7.71	133.70	122.99
1	F	291	ARG	O-C-N	-7.70	111.93	122.94
1	F	1220	LEU	CA-C-N	7.66	140.50	121.80
1	F	1220	LEU	C-N-CA	7.66	140.50	121.80
1	F	194	PHE	O-C-N	7.65	132.77	122.59
1	F	234	GLY	N-CA-C	7.64	131.28	113.18
1	F	292	ARG	O-C-N	-7.55	114.04	123.17
1	F	1076	ALA	O-C-N	7.51	131.10	121.34
1	F	1081	LEU	CA-C-N	7.46	131.05	120.53
1	F	1081	LEU	C-N-CA	7.46	131.05	120.53
1	F	1219	HIS	O-C-N	-7.39	112.76	122.59
1	F	41	THR	CA-C-N	7.33	126.20	120.33
1	F	41	THR	C-N-CA	7.33	126.20	120.33
1	F	197	VAL	N-CA-CB	-7.22	98.82	111.39
1	F	1257	ASN	CA-C-N	7.15	134.57	121.70
1	F	1257	ASN	C-N-CA	7.15	134.57	121.70
1	F	198	PHE	CA-C-O	-7.09	112.88	121.89
1	F	1103	ARG	O-C-N	-7.07	113.19	122.59
1	F	1475	ILE	CA-C-N	6.98	129.94	120.38
1	F	1475	ILE	C-N-CA	6.98	129.94	120.38
1	F	301	GLU	CA-C-N	6.92	134.77	121.54
1	F	301	GLU	C-N-CA	6.92	134.77	121.54
1	F	1177	PRO	N-CA-C	-6.92	98.22	112.47
1	F	144	SER	N-CA-CB	6.81	119.75	110.42
1	F	870	ARG	N-CA-C	-6.75	102.44	111.96
1	F	208	SER	N-CA-C	-6.65	105.45	113.97
1	F	199	PHE	N-CA-C	-6.65	96.18	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	994	PHE	N-CA-C	-6.65	105.46	113.97
1	F	1857	TYR	N-CA-C	-6.63	104.83	113.12
1	F	1302	ASN	N-CA-C	-6.63	106.39	114.75
1	F	1406	ARG	N-CA-C	-6.60	103.28	112.12
1	F	1214	ARG	CA-C-N	6.59	134.32	121.66
1	F	1214	ARG	C-N-CA	6.59	134.32	121.66
1	F	1108	ALA	N-CA-C	6.59	124.83	110.80
1	F	1756	ALA	CA-C-N	6.55	127.39	119.99
1	F	1756	ALA	C-N-CA	6.55	127.39	119.99
1	F	1378	PHE	N-CA-CB	6.54	121.54	110.49
1	F	302	ALA	N-CA-C	6.53	124.70	110.80
1	F	987	LEU	CA-C-N	6.49	127.96	119.84
1	F	987	LEU	C-N-CA	6.49	127.96	119.84
1	F	1176	CYS	CA-C-N	6.49	127.95	119.84
1	F	1176	CYS	C-N-CA	6.49	127.95	119.84
1	F	64	ASP	CA-C-N	6.47	128.96	120.28
1	F	64	ASP	C-N-CA	6.47	128.96	120.28
1	F	299	ALA	CA-C-N	6.45	131.92	122.63
1	F	299	ALA	C-N-CA	6.45	131.92	122.63
1	F	204	TRP	CA-C-N	6.45	133.31	121.70
1	F	204	TRP	C-N-CA	6.45	133.31	121.70
1	F	199	PHE	O-C-N	-6.42	114.64	123.12
1	F	256	GLU	O-C-N	-6.42	113.94	121.32
1	F	262	MET	CA-C-N	6.38	133.55	121.87
1	F	262	MET	C-N-CA	6.38	133.55	121.87
1	F	1620	LEU	CA-C-N	6.36	129.10	120.38
1	F	1620	LEU	C-N-CA	6.36	129.10	120.38
1	F	1125	LEU	CA-C-N	6.31	133.69	122.08
1	F	1125	LEU	C-N-CA	6.31	133.69	122.08
1	F	878	LEU	N-CA-C	-6.28	105.52	113.43
1	F	1183	ALA	N-CA-CB	6.27	121.08	110.49
1	F	104	ALA	N-CA-C	-6.26	106.24	114.31
1	F	1476	ARG	CA-C-N	6.22	128.90	120.38
1	F	1476	ARG	C-N-CA	6.22	128.90	120.38
1	F	1378	PHE	CA-CB-CG	6.20	120.00	113.80
1	F	56	THR	N-CA-C	-6.14	104.57	114.09
1	F	214	PHE	CA-C-N	6.13	130.50	120.63
1	F	214	PHE	C-N-CA	6.13	130.50	120.63
1	F	1182	SER	O-C-N	-6.10	116.27	123.41
1	F	240	PHE	CA-C-N	6.09	132.66	121.70
1	F	240	PHE	C-N-CA	6.09	132.66	121.70
1	F	83	VAL	N-CA-C	-6.08	105.45	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1080	ALA	CA-C-N	6.06	132.61	121.70
1	F	1080	ALA	C-N-CA	6.06	132.61	121.70
1	F	301	GLU	O-C-N	-6.03	113.35	123.00
1	F	1837	PHE	N-CA-CB	6.01	120.65	110.49
1	F	262	MET	CA-C-O	-6.00	114.86	121.28
1	F	1100	ASN	CA-C-N	5.92	127.24	119.84
1	F	1100	ASN	C-N-CA	5.92	127.24	119.84
1	F	942	MET	N-CA-C	-5.92	104.93	113.21
1	F	1215	ASP	CA-C-N	5.91	132.82	121.54
1	F	1215	ASP	C-N-CA	5.91	132.82	121.54
1	F	1256	TYR	N-CA-C	-5.89	100.43	108.38
1	F	1260	TYR	CA-C-N	5.87	128.51	120.46
1	F	1260	TYR	C-N-CA	5.87	128.51	120.46
1	F	1555	GLN	CA-C-N	5.86	132.26	121.70
1	F	1555	GLN	C-N-CA	5.86	132.26	121.70
1	F	296	TYR	N-CA-CB	-5.82	100.65	110.49
1	F	1226	LYS	N-CA-CB	5.80	120.29	110.49
1	F	1791	THR	CA-C-N	5.79	128.36	120.77
1	F	1791	THR	C-N-CA	5.79	128.36	120.77
1	F	1794	TRP	CA-C-N	5.78	130.39	121.19
1	F	1794	TRP	C-N-CA	5.78	130.39	121.19
1	F	1032	LEU	CA-C-N	5.78	128.30	120.38
1	F	1032	LEU	C-N-CA	5.78	128.30	120.38
1	F	800	GLU	N-CA-C	-5.75	104.93	112.41
1	F	1107	GLY	N-CA-C	5.75	121.67	112.58
1	F	962	SER	N-CA-CB	5.73	120.18	110.49
1	F	1141	THR	CA-C-N	5.72	128.27	120.54
1	F	1141	THR	C-N-CA	5.72	128.27	120.54
1	F	991	LYS	CA-C-N	5.72	132.46	121.54
1	F	991	LYS	C-N-CA	5.72	132.46	121.54
1	F	1082	ILE	N-CA-C	5.67	117.09	110.62
1	F	853	GLN	N-CA-C	5.67	119.71	112.34
1	F	1008	LEU	N-CA-CB	5.65	120.05	110.49
1	F	134	PRO	CB-CA-C	-5.63	102.26	111.56
1	F	259	PHE	O-C-N	5.63	129.58	123.10
1	F	1375	LEU	N-CA-C	-5.63	98.81	110.80
1	F	803	PHE	N-CA-CB	5.62	119.99	110.49
1	F	1384	MET	CA-C-N	5.62	128.13	120.54
1	F	1384	MET	C-N-CA	5.62	128.13	120.54
1	F	235	LEU	CA-C-N	-5.61	111.66	122.09
1	F	235	LEU	C-N-CA	-5.61	111.66	122.09
1	F	264	ASP	O-C-N	-5.59	116.70	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1588	VAL	CA-C-N	5.59	126.71	120.06
1	F	1588	VAL	C-N-CA	5.59	126.71	120.06
1	F	215	MET	CA-C-N	5.58	128.08	120.54
1	F	215	MET	C-N-CA	5.58	128.08	120.54
1	F	779	ASN	CA-C-N	5.58	128.22	120.29
1	F	779	ASN	C-N-CA	5.58	128.22	120.29
1	F	136	LEU	O-C-N	-5.58	115.17	122.59
1	F	1137	SER	N-CA-C	-5.58	97.47	109.81
1	F	306	ARG	N-CA-C	-5.55	98.99	110.80
1	F	1070	LYS	CA-C-N	5.54	130.02	121.71
1	F	1070	LYS	C-N-CA	5.54	130.02	121.71
1	F	237	ILE	CA-C-O	-5.54	114.47	120.67
1	F	289	ASP	CA-C-N	5.54	131.66	121.70
1	F	289	ASP	C-N-CA	5.54	131.66	121.70
1	F	307	LEU	CB-CA-C	-5.53	99.41	110.42
1	F	1593	THR	N-CA-C	-5.53	106.44	114.12
1	F	1217	GLU	CA-C-N	5.52	130.44	122.77
1	F	1217	GLU	C-N-CA	5.52	130.44	122.77
1	F	1624	ALA	CA-C-N	5.50	127.59	120.44
1	F	1624	ALA	C-N-CA	5.50	127.59	120.44
1	F	1426	GLN	CA-C-N	5.50	127.65	120.28
1	F	1426	GLN	C-N-CA	5.50	127.65	120.28
1	F	1188	THR	CA-C-N	5.49	132.03	121.54
1	F	1188	THR	C-N-CA	5.49	132.03	121.54
1	F	1051	GLY	N-CA-C	-5.49	108.07	115.21
1	F	209	ALA	CA-C-N	5.48	126.69	119.84
1	F	209	ALA	C-N-CA	5.48	126.69	119.84
1	F	271	LEU	CA-C-N	5.46	126.92	120.09
1	F	271	LEU	C-N-CA	5.46	126.92	120.09
1	F	1527	GLU	CA-C-N	5.45	127.85	120.38
1	F	1527	GLU	C-N-CA	5.45	127.85	120.38
1	F	1322	LEU	CA-C-N	5.45	127.89	120.54
1	F	1322	LEU	C-N-CA	5.45	127.89	120.54
1	F	1376	ASP	N-CA-C	-5.45	99.20	110.80
1	F	1648	PHE	CA-CB-CG	-5.44	108.36	113.80
1	F	136	LEU	N-CA-C	-5.41	99.28	110.80
1	F	1054	PHE	O-C-N	-5.41	115.39	122.59
1	F	1499	PHE	CA-CB-CG	-5.41	108.39	113.80
1	F	1182	SER	CA-C-N	5.40	131.85	121.54
1	F	1182	SER	C-N-CA	5.40	131.85	121.54
1	F	308	ARG	O-C-N	-5.39	115.31	121.99
1	F	1040	GLY	N-CA-C	5.38	121.97	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1155	ILE	N-CA-C	-5.35	96.02	111.00
1	F	1165	ASP	CA-C-N	5.34	128.06	120.53
1	F	1165	ASP	C-N-CA	5.34	128.06	120.53
1	F	237	ILE	O-C-N	-5.33	117.40	123.10
1	F	816	LYS	CA-C-N	5.31	125.98	120.03
1	F	816	LYS	C-N-CA	5.31	125.98	120.03
1	F	1342	ALA	CA-C-N	5.31	127.70	120.54
1	F	1342	ALA	C-N-CA	5.31	127.70	120.54
1	F	305	TYR	CB-CA-C	-5.30	99.87	110.42
1	F	762	GLU	CA-C-N	5.29	127.68	120.54
1	F	762	GLU	C-N-CA	5.29	127.68	120.54
1	F	921	ILE	CA-C-O	-5.29	114.69	118.71
1	F	1229	GLN	N-CA-C	-5.27	106.90	113.38
1	F	1216	PHE	N-CA-CB	5.27	119.39	110.49
1	F	1054	PHE	CA-CB-CG	5.26	119.06	113.80
1	F	303	ASN	N-CA-C	-5.26	102.09	108.14
1	F	1128	PRO	CA-C-N	5.26	129.49	120.71
1	F	1128	PRO	C-N-CA	5.26	129.49	120.71
1	F	1751	HIS	N-CA-CB	5.26	119.38	110.49
1	F	1540	ALA	CA-C-N	5.24	127.56	120.38
1	F	1540	ALA	C-N-CA	5.24	127.56	120.38
1	F	1321	GLN	CA-C-N	5.23	129.51	121.19
1	F	1321	GLN	C-N-CA	5.23	129.51	121.19
1	F	246	GLU	N-CA-C	-5.23	101.35	109.72
1	F	254	GLN	CA-C-N	5.22	127.53	120.38
1	F	254	GLN	C-N-CA	5.22	127.53	120.38
1	F	240	PHE	O-C-N	-5.22	116.99	123.36
1	F	1479	ILE	CA-C-N	5.21	127.52	120.38
1	F	1479	ILE	C-N-CA	5.21	127.52	120.38
1	F	1361	HIS	N-CA-C	-5.21	107.30	113.97
1	F	931	VAL	CA-C-N	5.19	127.75	120.28
1	F	931	VAL	C-N-CA	5.19	127.75	120.28
1	F	1258	ASN	CA-C-N	5.19	128.58	120.75
1	F	1258	ASN	C-N-CA	5.19	128.58	120.75
1	F	284	ALA	CA-C-N	5.18	127.53	120.54
1	F	284	ALA	C-N-CA	5.18	127.53	120.54
1	F	1129	GLU	N-CA-C	-5.18	105.08	111.40
1	F	928	HIS	CA-C-N	5.17	127.47	120.38
1	F	928	HIS	C-N-CA	5.17	127.47	120.38
1	F	746	ASP	CA-C-N	5.17	127.47	120.38
1	F	746	ASP	C-N-CA	5.17	127.47	120.38
1	F	1771	VAL	N-CA-C	5.17	115.38	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	696	ASN	CA-C-N	5.16	131.39	121.54
1	F	696	ASN	C-N-CA	5.16	131.39	121.54
1	F	1010	GLU	N-CA-CB	5.15	119.19	110.49
1	F	923	LEU	CA-C-N	5.14	127.94	120.79
1	F	923	LEU	C-N-CA	5.14	127.94	120.79
1	F	754	ALA	CA-C-N	5.12	127.09	120.44
1	F	754	ALA	C-N-CA	5.12	127.09	120.44
1	F	1122	GLN	CA-C-N	-5.11	114.09	122.67
1	F	1122	GLN	C-N-CA	-5.11	114.09	122.67
1	F	1632	HIS	N-CA-C	-5.11	99.92	110.80
1	F	818	ALA	CA-C-N	5.09	127.41	120.54
1	F	818	ALA	C-N-CA	5.09	127.41	120.54
1	F	111	GLU	CA-C-N	5.09	127.43	120.46
1	F	111	GLU	C-N-CA	5.09	127.43	120.46
1	F	1727	LYS	N-CA-C	-5.08	99.97	110.80
1	F	1155	ILE	CA-C-N	5.08	127.04	120.44
1	F	1155	ILE	C-N-CA	5.08	127.04	120.44
1	F	784	LEU	CA-C-N	5.07	127.39	120.54
1	F	784	LEU	C-N-CA	5.07	127.39	120.54
1	F	729	LEU	N-CA-C	-5.07	106.23	112.72
1	F	252	VAL	CA-C-N	5.06	127.31	120.38
1	F	252	VAL	C-N-CA	5.06	127.31	120.38
1	F	1301	PHE	N-CA-C	-5.06	106.35	112.88
1	F	1121	CYS	N-CA-C	-5.05	100.04	110.80
1	F	973	ARG	CA-C-N	5.05	127.00	120.44
1	F	973	ARG	C-N-CA	5.05	127.00	120.44
1	F	1136	LEU	N-CA-C	5.05	117.18	111.02
1	F	1539	ALA	CA-C-N	5.04	127.80	120.79
1	F	1539	ALA	C-N-CA	5.04	127.80	120.79
1	F	1438	ASN	N-CA-C	-5.03	106.83	113.17
1	F	1502	GLU	CA-C-N	5.02	127.77	120.79
1	F	1502	GLU	C-N-CA	5.02	127.77	120.79
1	F	782	VAL	CA-C-N	5.01	125.03	119.32
1	F	782	VAL	C-N-CA	5.01	125.03	119.32
1	F	1583	PHE	N-CA-CB	5.01	118.96	110.49
1	F	135	GLU	CA-C-N	5.01	131.11	121.54
1	F	135	GLU	C-N-CA	5.01	131.11	121.54

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	296	TYR	CA

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Mol	Chain	Res	Type	Atom
1	F	305	TYR	CA
1	F	1155	ILE	CA
1	F	1697	ARG	CA

All (187) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	1008	LEU	Peptide
1	F	1009	LEU	Peptide
1	F	1012	PRO	Peptide
1	F	1016	GLU	Peptide
1	F	1019	TYR	Peptide
1	F	1022	ALA	Peptide
1	F	1023	PHE	Peptide
1	F	1024	ASN	Peptide
1	F	1038	GLY	Peptide
1	F	1044	VAL	Mainchain
1	F	1045	CYS	Mainchain
1	F	1049	SER	Peptide
1	F	1051	GLY	Peptide,Mainchain
1	F	1052	LYS	Mainchain
1	F	1065	ARG	Peptide
1	F	1070	LYS	Mainchain
1	F	1080	ALA	Peptide
1	F	1083	ASN	Peptide
1	F	1092	ARG	Peptide
1	F	1100	ASN	Peptide
1	F	1101	PRO	Peptide
1	F	1102	GLY	Peptide
1	F	1103	ARG	Peptide,Mainchain
1	F	1107	GLY	Peptide
1	F	1108	ALA	Mainchain
1	F	1109	LEU	Peptide
1	F	1110	GLY	Peptide
1	F	1116	GLN	Peptide
1	F	1118	HIS	Peptide
1	F	1121	CYS	Peptide
1	F	1122	GLN	Mainchain
1	F	1126	THR	Mainchain
1	F	1148	ASP	Peptide
1	F	1172	ALA	Peptide
1	F	1175	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	F	1176	CYS	Peptide
1	F	1187	GLU	Peptide
1	F	1188	THR	Peptide,Mainchain
1	F	1213	MET	Peptide
1	F	1214	ARG	Peptide
1	F	1215	ASP	Mainchain
1	F	1218	VAL	Mainchain
1	F	1219	HIS	Mainchain
1	F	1220	LEU	Mainchain
1	F	1222	PRO	Peptide
1	F	1223	SER	Peptide
1	F	1224	GLU	Peptide
1	F	1225	GLY	Peptide
1	F	1237	TYR	Peptide
1	F	1250	LYS	Peptide
1	F	1268	SER	Peptide
1	F	1284	SER	Peptide
1	F	1306	TRP	Peptide
1	F	131	THR	Peptide
1	F	132	ALA	Peptide
1	F	133	ARG	Mainchain
1	F	1339	GLN	Peptide
1	F	135	GLU	Peptide,Mainchain
1	F	1359	LEU	Peptide
1	F	136	LEU	Peptide
1	F	1369	ASN	Peptide
1	F	137	CYS	Peptide,Mainchain
1	F	139	MET	Mainchain
1	F	140	PHE	Peptide
1	F	1401	GLU	Peptide
1	F	1402	ALA	Peptide
1	F	144	SER	Peptide
1	F	1458	GLN	Peptide
1	F	1459	GLU	Peptide
1	F	146	SER	Peptide,Mainchain
1	F	1465	SER	Peptide
1	F	1467	SER	Peptide
1	F	1471	SER	Peptide
1	F	152	ASP	Peptide,Mainchain
1	F	153	GLY	Mainchain
1	F	1580	ASP	Peptide
1	F	163	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	F	164	GLN	Peptide
1	F	1707	PHE	Peptide
1	F	1711	THR	Peptide
1	F	1722	SER	Peptide
1	F	1730	VAL	Peptide
1	F	1731	GLN	Peptide
1	F	1744	TYR	Sidechain
1	F	1784	GLY	Peptide
1	F	1786	ASN	Peptide
1	F	1788	GLU	Peptide
1	F	1789	GLY	Peptide
1	F	1804	ARG	Peptide
1	F	1835	GLU	Peptide
1	F	1836	GLY	Peptide
1	F	1837	PHE	Peptide
1	F	1848	PHE	Peptide
1	F	1856	LEU	Peptide
1	F	189	CYS	Peptide
1	F	192	ALA	Peptide
1	F	193	ARG	Peptide,Mainchain
1	F	194	PHE	Mainchain
1	F	195	HIS	Mainchain
1	F	198	PHE	Peptide,Mainchain
1	F	199	PHE	Peptide
1	F	20	ASP	Peptide
1	F	200	ASP	Peptide
1	F	201	SER	Peptide
1	F	202	LEU	Peptide
1	F	205	ILE	Peptide
1	F	207	GLU	Peptide
1	F	21	PHE	Peptide
1	F	211	ALA	Peptide
1	F	212	LYS	Peptide
1	F	22	HIS	Peptide
1	F	226	LEU	Peptide
1	F	227	SER	Peptide
1	F	235	LEU	Peptide
1	F	236	SER	Peptide
1	F	237	ILE	Peptide
1	F	238	SER	Peptide
1	F	239	ASN	Peptide
1	F	241	SER	Peptide

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Mol	Chain	Res	Type	Group
1	F	242	SER	Peptide
1	F	243	TYR	Peptide
1	F	244	TYR	Sidechain
1	F	257	PRO	Peptide
1	F	258	GLU	Peptide,Mainchain
1	F	259	PHE	Peptide,Mainchain
1	F	26	SER	Peptide
1	F	261	LEU	Peptide
1	F	262	MET	Mainchain
1	F	263	SER	Mainchain
1	F	264	ASP	Peptide,Mainchain
1	F	267	GLN	Peptide
1	F	268	LEU	Peptide
1	F	269	GLY	Peptide
1	F	27	MET	Peptide
1	F	288	HIS	Peptide
1	F	291	ARG	Mainchain
1	F	292	ARG	Peptide,Sidechain
1	F	294	ALA	Peptide
1	F	295	ASN	Mainchain
1	F	296	TYR	Peptide,Sidechain
1	F	302	ALA	Peptide
1	F	304	PRO	Peptide
1	F	305	TYR	Peptide
1	F	306	ARG	Peptide
1	F	308	ARG	Mainchain
1	F	321	GLY	Peptide
1	F	38	SER	Peptide
1	F	42	ILE	Peptide
1	F	681	THR	Peptide
1	F	685	LYS	Peptide
1	F	701	SER	Peptide
1	F	702	LYS	Peptide
1	F	720	ALA	Peptide
1	F	736	SER	Peptide
1	F	775	GLY	Peptide
1	F	795	ALA	Peptide
1	F	796	SER	Peptide
1	F	799	ARG	Peptide
1	F	80	ASP	Peptide
1	F	801	VAL	Peptide
1	F	827	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	F	829	LYS	Peptide
1	F	831	LEU	Peptide
1	F	850	HIS	Peptide
1	F	860	ALA	Peptide
1	F	877	TYR	Peptide
1	F	917	ILE	Peptide
1	F	936	ARG	Peptide
1	F	956	HIS	Peptide
1	F	976	ASN	Peptide
1	F	978	THR	Peptide
1	F	994	PHE	Peptide
1	F	996	THR	Peptide

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	F	12257	0	12083	347	0
2	F	1	0	0	0	0
3	F	27	0	12	18	0
All	All	12285	0	12095	347	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 14.

All (347) 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)
1:F:259:PHE:C	1:F:259:PHE:CA	1.81	1.52
1:F:139:MET:HE3	1:F:301:GLU:CG	1.41	1.50
1:F:306:ARG:N	1:F:306:ARG:CA	1.72	1.47
1:F:1149:TYR:C	1:F:1150:VAL:N	1.72	1.46
1:F:199:PHE:HE1	1:F:214:PHE:CE1	1.43	1.35
1:F:956:HIS:CD2	1:F:991:LYS:HG2	1.65	1.29
1:F:1155:ILE:HG21	1:F:1182:SER:CB	1.60	1.29
1:F:139:MET:HE3	1:F:301:GLU:CD	1.58	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:ARG:HE	1:F:308:ARG:CA	1.45	1.23
1:F:199:PHE:CE1	1:F:214:PHE:CE1	2.25	1.23
1:F:139:MET:CE	1:F:301:GLU:HG3	1.69	1.22
1:F:1025:PRO:HG2	1:F:1029:GLN:OE1	1.35	1.21
1:F:308:ARG:NE	1:F:308:ARG:HA	1.34	1.21
1:F:295:ASN:OD1	1:F:303:ASN:ND2	1.73	1.20
1:F:199:PHE:HE1	1:F:214:PHE:CZ	1.62	1.18
1:F:1068:ASN:HB2	1:F:1122:GLN:NE2	1.59	1.18
1:F:140:PHE:CE2	1:F:193:ARG:NH1	2.11	1.18
1:F:1195:LEU:HB3	1:F:1217:GLU:OE1	1.44	1.17
1:F:1025:PRO:CG	1:F:1029:GLN:OE1	1.93	1.16
1:F:184:LEU:HD13	1:F:235:LEU:CD1	1.72	1.16
1:F:1068:ASN:CB	1:F:1122:GLN:HE22	1.58	1.15
1:F:140:PHE:HE2	1:F:193:ARG:NH1	1.44	1.15
1:F:259:PHE:C	1:F:259:PHE:CG	2.27	1.13
1:F:1041:SER:CB	1:F:1217:GLU:HG3	1.83	1.08
1:F:261:LEU:HD23	1:F:294:ALA:HB3	1.09	1.08
1:F:1041:SER:HB2	1:F:1217:GLU:HG3	1.11	1.07
1:F:149:PHE:HE2	1:F:193:ARG:NH2	1.52	1.05
1:F:1044:VAL:CG1	1:F:1220:LEU:HD12	1.85	1.05
1:F:187:MET:HE2	1:F:193:ARG:HH11	1.16	1.05
1:F:1155:ILE:HG21	1:F:1182:SER:HB2	1.08	1.04
1:F:1697:ARG:HE	3:F:2202:ADP:H5'1	1.17	1.04
1:F:1044:VAL:HG12	1:F:1220:LEU:HD12	1.06	1.04
1:F:956:HIS:HD2	1:F:991:LYS:CG	1.72	1.03
1:F:184:LEU:HD13	1:F:235:LEU:HD11	1.02	1.02
1:F:139:MET:CE	1:F:301:GLU:CD	2.31	1.02
1:F:139:MET:HE3	1:F:301:GLU:HG3	1.04	1.02
1:F:261:LEU:CD2	1:F:294:ALA:HB3	1.89	1.02
1:F:139:MET:CE	1:F:301:GLU:CG	2.32	1.01
1:F:1155:ILE:HB	1:F:1181:LEU:O	1.60	1.01
1:F:1059:CYS:SG	1:F:1149:TYR:CD1	2.52	1.01
1:F:139:MET:CE	1:F:301:GLU:OE2	2.09	1.00
1:F:199:PHE:CE1	1:F:214:PHE:CZ	2.48	1.00
1:F:1059:CYS:HG	1:F:1149:TYR:HD1	1.03	0.99
1:F:1127:VAL:HG13	1:F:1128:PRO:HD2	1.45	0.99
1:F:956:HIS:HD2	1:F:991:LYS:HG2	0.85	0.98
1:F:146:SER:HB3	1:F:147:GLU:HB2	1.46	0.98
1:F:1178:PHE:HZ	1:F:1217:GLU:OE2	1.47	0.97
1:F:259:PHE:C	1:F:259:PHE:CB	2.37	0.97
1:F:1155:ILE:CG2	1:F:1182:SER:CB	2.42	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:LEU:HD23	1:F:294:ALA:CB	1.94	0.96
1:F:1045:CYS:SG	1:F:1221:LEU:HG	2.06	0.96
1:F:1195:LEU:CB	1:F:1217:GLU:OE1	2.13	0.95
1:F:1035:ILE:HG12	1:F:1218:VAL:HG11	1.48	0.95
1:F:1044:VAL:HG12	1:F:1220:LEU:CD1	1.97	0.94
1:F:1149:TYR:CD2	1:F:1177:PRO:HG2	2.03	0.93
1:F:1697:ARG:NE	3:F:2202:ADP:H5'1	1.82	0.93
1:F:1074:TYR:HE2	1:F:1083:ASN:ND2	1.66	0.92
1:F:300:ASP:N	1:F:301:GLU:HA	1.84	0.91
1:F:905:ARG:NH2	1:F:956:HIS:NE2	2.17	0.91
1:F:1149:TYR:HD2	1:F:1177:PRO:HG2	1.34	0.91
1:F:149:PHE:CE2	1:F:193:ARG:NH2	2.37	0.91
1:F:129:TYR:CZ	1:F:264:ASP:OD2	2.23	0.91
1:F:184:LEU:CD1	1:F:235:LEU:HD21	2.01	0.90
1:F:235:LEU:O	1:F:236:SER:OG	1.89	0.90
1:F:151:ILE:HG12	1:F:261:LEU:HB2	1.52	0.89
1:F:1133:THR:O	1:F:1137:SER:CB	2.20	0.89
1:F:1106:TYR:CD2	1:F:1119:ASP:N	2.42	0.88
1:F:150:PHE:CZ	1:F:258:GLU:OE2	2.27	0.88
1:F:1068:ASN:HB2	1:F:1122:GLN:HE22	0.76	0.88
1:F:1059:CYS:SG	1:F:1149:TYR:CE1	2.67	0.88
1:F:140:PHE:HE2	1:F:193:ARG:HH12	0.90	0.87
1:F:1127:VAL:CG1	1:F:1128:PRO:HD2	2.03	0.87
1:F:1155:ILE:HG23	1:F:1156:HIS:N	1.88	0.87
1:F:1133:THR:O	1:F:1137:SER:HB2	1.73	0.86
1:F:184:LEU:CD1	1:F:235:LEU:HD11	1.99	0.86
1:F:139:MET:HE3	1:F:301:GLU:OE2	1.69	0.86
1:F:141:VAL:CG2	1:F:301:GLU:OE2	2.23	0.86
1:F:302:ALA:HA	1:F:303:ASN:OD1	1.74	0.85
1:F:1203:LYS:HB2	1:F:1215:ASP:OD1	1.75	0.85
1:F:1155:ILE:HG22	1:F:1182:SER:HA	1.57	0.85
1:F:184:LEU:CD1	1:F:235:LEU:CG	2.54	0.85
1:F:137:CYS:HA	1:F:138:ASP:HB2	1.59	0.84
1:F:1025:PRO:HB2	3:F:2202:ADP:N6	1.92	0.84
1:F:1155:ILE:CG2	1:F:1156:HIS:H	1.89	0.84
1:F:184:LEU:HD11	1:F:235:LEU:HG	1.60	0.84
1:F:187:MET:CE	1:F:193:ARG:HH11	1.90	0.84
1:F:184:LEU:HD13	1:F:235:LEU:CG	2.08	0.83
1:F:136:LEU:O	1:F:136:LEU:HG	1.78	0.83
1:F:1155:ILE:CG2	1:F:1156:HIS:N	2.41	0.83
1:F:304:PRO:HB2	1:F:305:TYR:CD2	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1059:CYS:SG	1:F:1149:TYR:HD1	1.98	0.83
1:F:140:PHE:CE1	1:F:144:SER:OG	2.31	0.82
1:F:1178:PHE:CZ	1:F:1217:GLU:OE2	2.31	0.82
1:F:140:PHE:H	1:F:301:GLU:HB2	1.44	0.82
1:F:1054:PHE:HZ	3:F:2202:ADP:C8	1.97	0.82
1:F:187:MET:HE2	1:F:193:ARG:NH1	1.95	0.82
1:F:303:ASN:CB	1:F:304:PRO:HD2	2.10	0.82
1:F:955:LYS:HD3	1:F:989:GLN:O	1.80	0.81
1:F:294:ALA:O	1:F:295:ASN:HB2	1.79	0.81
1:F:1165:ASP:HB3	1:F:1729:ASN:HD22	1.46	0.81
1:F:140:PHE:CD2	1:F:187:MET:HE2	2.15	0.80
1:F:1054:PHE:CZ	3:F:2202:ADP:C8	2.69	0.80
1:F:150:PHE:CD1	1:F:196:VAL:HB	2.16	0.80
1:F:302:ALA:CA	1:F:303:ASN:OD1	2.30	0.80
1:F:1128:PRO:HB3	1:F:1166:VAL:HG11	1.63	0.80
1:F:150:PHE:CD2	1:F:198:PHE:CZ	2.70	0.79
1:F:129:TYR:CE1	1:F:264:ASP:OD2	2.36	0.79
1:F:955:LYS:NZ	1:F:989:GLN:HE21	1.81	0.79
1:F:139:MET:HE2	1:F:301:GLU:OE2	1.80	0.79
1:F:1025:PRO:HG3	1:F:1029:GLN:OE1	1.81	0.78
1:F:1042:ALA:HB2	1:F:1218:VAL:CG1	2.13	0.77
1:F:1218:VAL:HG22	1:F:1219:HIS:H	1.48	0.77
1:F:1135:LEU:HD21	1:F:1174:LEU:HD12	1.63	0.77
1:F:1195:LEU:C	1:F:1217:GLU:OE1	2.28	0.77
1:F:1059:CYS:SG	1:F:1151:ILE:HD11	2.26	0.76
1:F:1041:SER:HB2	1:F:1217:GLU:CG	2.06	0.76
1:F:1054:PHE:CZ	3:F:2202:ADP:H8	2.04	0.76
1:F:1106:TYR:CD2	1:F:1119:ASP:C	2.63	0.76
1:F:148:MET:O	1:F:258:GLU:HA	1.86	0.75
1:F:1074:TYR:HE2	1:F:1083:ASN:HD21	0.84	0.75
1:F:1155:ILE:CG2	1:F:1182:SER:HB2	2.02	0.75
1:F:1060:MET:HE2	1:F:1123:VAL:HG11	1.68	0.75
1:F:184:LEU:CD1	1:F:235:LEU:CD2	2.63	0.75
1:F:259:PHE:CD1	1:F:260:ILE:N	2.55	0.74
1:F:1160:SER:HB2	1:F:1685:THR:HG21	1.69	0.74
1:F:306:ARG:N	1:F:306:ARG:HA	1.99	0.74
1:F:1042:ALA:HB2	1:F:1218:VAL:HG13	1.70	0.74
1:F:149:PHE:CD2	1:F:193:ARG:HD3	2.24	0.73
1:F:295:ASN:CG	1:F:303:ASN:HD22	1.97	0.73
1:F:306:ARG:N	1:F:306:ARG:C	2.46	0.73
1:F:1697:ARG:CG	3:F:2202:ADP:O4'	2.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1032:LEU:HD13	1:F:1220:LEU:CD1	2.18	0.72
1:F:1156:HIS:CE1	1:F:1183:ALA:HB3	2.24	0.72
1:F:1135:LEU:HD21	1:F:1174:LEU:CD1	2.19	0.72
1:F:199:PHE:CE1	1:F:214:PHE:HE1	2.02	0.72
1:F:1032:LEU:HD13	1:F:1220:LEU:HD11	1.70	0.72
1:F:1697:ARG:HG2	3:F:2202:ADP:O4'	1.89	0.72
1:F:259:PHE:C	1:F:259:PHE:CD1	2.67	0.72
1:F:1697:ARG:HG2	3:F:2202:ADP:C4'	2.20	0.71
1:F:200:ASP:OD1	1:F:203:LEU:HD11	1.90	0.71
1:F:151:ILE:HG12	1:F:261:LEU:CB	2.18	0.71
1:F:1154:GLU:OE1	1:F:1156:HIS:CE1	2.43	0.71
1:F:1128:PRO:HB3	1:F:1166:VAL:CG1	2.20	0.70
1:F:190:ARG:NH1	1:F:301:GLU:OE1	2.24	0.70
1:F:1151:ILE:HG23	1:F:1179:VAL:O	1.90	0.70
1:F:137:CYS:O	1:F:302:ALA:HB1	1.92	0.70
1:F:1106:TYR:CE2	1:F:1119:ASP:N	2.60	0.69
1:F:141:VAL:HG22	1:F:301:GLU:OE2	1.90	0.69
1:F:141:VAL:HG23	1:F:301:GLU:OE2	1.92	0.69
1:F:137:CYS:CA	1:F:138:ASP:HB2	2.19	0.69
1:F:1045:CYS:SG	1:F:1221:LEU:CG	2.79	0.69
1:F:1218:VAL:HG22	1:F:1219:HIS:N	2.08	0.69
1:F:286:ASN:HD21	1:F:306:ARG:HH12	1.39	0.69
1:F:1045:CYS:SG	1:F:1221:LEU:CD1	2.81	0.69
1:F:1106:TYR:HD2	1:F:1119:ASP:N	1.86	0.69
1:F:140:PHE:CD1	1:F:144:SER:OG	2.46	0.68
1:F:149:PHE:HD2	1:F:193:ARG:HD3	1.57	0.68
1:F:184:LEU:HD12	1:F:235:LEU:HD21	1.75	0.68
1:F:286:ASN:ND2	1:F:306:ARG:HH12	1.90	0.68
1:F:1025:PRO:HB2	3:F:2202:ADP:HN62	1.56	0.68
1:F:184:LEU:CD1	1:F:235:LEU:CD1	2.61	0.68
1:F:1052:LYS:N	3:F:2202:ADP:O1B	2.25	0.68
1:F:1215:ASP:O	1:F:1216:PHE:HB3	1.93	0.67
1:F:1025:PRO:HG3	1:F:1029:GLN:CD	2.19	0.67
1:F:1133:THR:HG22	1:F:1739:ARG:HH22	1.59	0.67
1:F:956:HIS:HA	1:F:991:LYS:HB3	1.77	0.66
1:F:1155:ILE:HG21	1:F:1182:SER:OG	1.94	0.66
1:F:1041:SER:HB3	1:F:1178:PHE:CZ	2.30	0.66
1:F:1155:ILE:HG22	1:F:1156:HIS:H	1.60	0.66
1:F:1045:CYS:SG	1:F:1221:LEU:HD12	2.37	0.65
1:F:139:MET:HG2	1:F:140:PHE:H	1.61	0.65
1:F:1155:ILE:CG2	1:F:1182:SER:HA	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:SER:HA	1:F:145:ALA:HB2	1.79	0.64
1:F:955:LYS:CD	1:F:989:GLN:O	2.44	0.64
1:F:1216:PHE:CE1	1:F:1218:VAL:HB	2.32	0.64
1:F:149:PHE:HE2	1:F:193:ARG:CZ	2.10	0.64
1:F:187:MET:HG3	1:F:193:ARG:NH1	2.13	0.64
1:F:1051:GLY:N	3:F:2202:ADP:O2B	2.30	0.64
1:F:1155:ILE:CG2	1:F:1182:SER:CA	2.77	0.63
1:F:1025:PRO:CG	1:F:1029:GLN:CD	2.72	0.63
1:F:1106:TYR:CE2	1:F:1120:SER:N	2.67	0.63
1:F:184:LEU:HD11	1:F:235:LEU:CG	2.22	0.63
1:F:199:PHE:CZ	1:F:214:PHE:CE1	2.85	0.62
1:F:1216:PHE:CZ	1:F:1218:VAL:HB	2.34	0.62
1:F:1042:ALA:CB	1:F:1218:VAL:HG13	2.29	0.62
1:F:1041:SER:OG	1:F:1178:PHE:CE2	2.49	0.62
1:F:148:MET:O	1:F:258:GLU:CA	2.47	0.62
1:F:259:PHE:CA	1:F:259:PHE:O	2.45	0.62
1:F:1135:LEU:HD12	1:F:1144:VAL:CG2	2.29	0.62
1:F:1155:ILE:CG2	1:F:1182:SER:OG	2.48	0.62
1:F:140:PHE:CD2	1:F:187:MET:CE	2.84	0.61
1:F:197:VAL:HG13	1:F:237:ILE:HG13	1.82	0.61
1:F:1128:PRO:CB	1:F:1166:VAL:HG11	2.29	0.61
1:F:148:MET:HG3	1:F:256:GLU:HB3	1.81	0.61
1:F:1257:ASN:HA	1:F:1259:CYS:H	1.66	0.61
1:F:140:PHE:HB2	1:F:301:GLU:CB	2.31	0.61
1:F:151:ILE:HD13	1:F:296:TYR:OH	2.01	0.60
1:F:262:MET:O	1:F:296:TYR:HD2	1.83	0.60
1:F:1050:ALA:N	3:F:2202:ADP:O2B	2.35	0.60
1:F:1136:LEU:C	1:F:1137:SER:O	2.27	0.60
1:F:1025:PRO:CB	3:F:2202:ADP:N6	2.65	0.59
1:F:139:MET:SD	1:F:301:GLU:HG3	2.42	0.59
1:F:261:LEU:CD2	1:F:294:ALA:CB	2.69	0.59
1:F:262:MET:HG2	1:F:293:LYS:HZ3	1.67	0.59
1:F:184:LEU:CD1	1:F:235:LEU:HG	2.21	0.59
1:F:194:PHE:CE2	1:F:1277:ARG:NH2	2.70	0.59
1:F:1127:VAL:CG1	1:F:1128:PRO:CD	2.80	0.58
1:F:308:ARG:HE	1:F:308:ARG:HA	0.54	0.58
1:F:1155:ILE:CB	1:F:1181:LEU:O	2.45	0.58
1:F:1042:ALA:HB2	1:F:1218:VAL:HG12	1.85	0.58
1:F:1106:TYR:CE2	1:F:1119:ASP:C	2.82	0.58
1:F:150:PHE:CE2	1:F:198:PHE:CZ	2.92	0.58
1:F:139:MET:HG2	1:F:140:PHE:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:PHE:N	1:F:301:GLU:HB2	2.18	0.58
1:F:262:MET:O	1:F:296:TYR:CD2	2.57	0.58
1:F:200:ASP:OD1	1:F:200:ASP:O	2.22	0.58
1:F:1169:ARG:CZ	1:F:1731:GLN:HE22	2.16	0.57
1:F:905:ARG:HH21	1:F:956:HIS:CE1	2.21	0.57
1:F:197:VAL:CG1	1:F:237:ILE:HG13	2.35	0.57
1:F:1195:LEU:CA	1:F:1217:GLU:OE1	2.52	0.57
1:F:300:ASP:H	1:F:301:GLU:HA	1.66	0.57
1:F:302:ALA:C	1:F:303:ASN:OD1	2.48	0.57
1:F:1041:SER:O	1:F:1042:ALA:HB2	2.04	0.56
1:F:1106:TYR:CD2	1:F:1118:HIS:C	2.83	0.56
1:F:200:ASP:OD1	1:F:203:LEU:CD1	2.53	0.56
1:F:1072:VAL:O	1:F:1123:VAL:HG13	2.05	0.56
1:F:146:SER:HB3	1:F:147:GLU:CB	2.31	0.56
1:F:1071:VAL:HA	1:F:1122:GLN:O	2.07	0.55
1:F:303:ASN:HB2	1:F:304:PRO:HD2	1.89	0.55
1:F:1149:TYR:CE2	1:F:1177:PRO:HG2	2.42	0.55
1:F:1106:TYR:HD2	1:F:1118:HIS:C	2.16	0.54
1:F:1155:ILE:HG22	1:F:1182:SER:CA	2.34	0.54
1:F:1135:LEU:HD12	1:F:1144:VAL:HG22	1.90	0.53
1:F:1218:VAL:CG2	1:F:1219:HIS:H	2.18	0.53
1:F:148:MET:HB2	1:F:258:GLU:HG2	1.90	0.53
1:F:1203:LYS:HD3	1:F:1215:ASP:OD1	2.09	0.53
1:F:1032:LEU:CD1	1:F:1220:LEU:HD11	2.38	0.52
1:F:1585:VAL:H	1:F:1586:PRO:CD	2.22	0.52
1:F:1042:ALA:CB	1:F:1218:VAL:O	2.57	0.52
1:F:1091:ALA:CB	1:F:1105:ILE:HD11	2.39	0.52
1:F:1133:THR:O	1:F:1137:SER:OG	2.28	0.52
1:F:1160:SER:CB	1:F:1685:THR:HG21	2.39	0.52
1:F:262:MET:HG2	1:F:293:LYS:NZ	2.24	0.52
1:F:1043:VAL:HG23	1:F:1180:ALA:C	2.35	0.52
1:F:1108:ALA:O	1:F:1126:THR:HG22	2.10	0.52
1:F:140:PHE:CE2	1:F:187:MET:HE2	2.44	0.52
1:F:1068:ASN:CB	1:F:1122:GLN:NE2	2.41	0.52
1:F:1041:SER:OG	1:F:1199:GLN:NE2	2.42	0.51
1:F:308:ARG:CA	1:F:308:ARG:NE	2.24	0.51
1:F:133:ARG:HB3	1:F:134:PRO:HD2	1.93	0.51
1:F:1054:PHE:HZ	3:F:2202:ADP:N7	2.08	0.51
1:F:148:MET:CB	1:F:258:GLU:HG2	2.41	0.50
1:F:956:HIS:C	1:F:957:PHE:O	2.53	0.50
1:F:1198:VAL:HG13	1:F:1771:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1218:VAL:CG2	1:F:1219:HIS:N	2.73	0.50
1:F:1697:ARG:HG3	3:F:2202:ADP:O4'	2.10	0.50
1:F:150:PHE:CD2	1:F:198:PHE:CE2	3.00	0.50
1:F:1135:LEU:CD2	1:F:1174:LEU:HD12	2.36	0.49
1:F:956:HIS:CD2	1:F:991:LYS:CG	2.59	0.49
1:F:1156:HIS:CE1	1:F:1183:ALA:CB	2.93	0.49
1:F:1043:VAL:HG23	1:F:1180:ALA:O	2.12	0.49
1:F:1596:GLY:HA3	1:F:1651:ARG:HH22	1.77	0.49
1:F:1050:ALA:HB3	1:F:1052:LYS:CD	2.42	0.49
1:F:1059:CYS:SG	1:F:1149:TYR:HE1	2.30	0.49
1:F:1106:TYR:HD2	1:F:1119:ASP:C	2.16	0.49
1:F:1159:GLU:OE1	1:F:1726:ILE:HG22	2.13	0.49
1:F:303:ASN:OD1	1:F:303:ASN:N	2.45	0.49
1:F:42:ILE:HD12	1:F:42:ILE:H	1.78	0.49
1:F:150:PHE:HE1	1:F:196:VAL:HG21	1.77	0.49
1:F:1135:LEU:CD2	1:F:1174:LEU:CD1	2.90	0.49
1:F:905:ARG:NH2	1:F:956:HIS:CD2	2.80	0.49
1:F:140:PHE:HB2	1:F:301:GLU:HB2	1.94	0.48
1:F:258:GLU:N	1:F:1717:ARG:NH2	2.62	0.48
1:F:150:PHE:CD2	1:F:198:PHE:HZ	2.29	0.48
1:F:1156:HIS:NE2	1:F:1183:ALA:HB3	2.28	0.48
1:F:1840:ILE:HD12	1:F:1840:ILE:H	1.78	0.48
1:F:150:PHE:HD1	1:F:196:VAL:HB	1.75	0.48
1:F:198:PHE:CZ	1:F:249:GLU:OE2	2.67	0.47
1:F:1216:PHE:CD1	1:F:1217:GLU:N	2.83	0.47
1:F:150:PHE:CE2	1:F:198:PHE:HZ	2.32	0.47
1:F:956:HIS:HA	1:F:991:LYS:CB	2.43	0.47
1:F:1053:THR:HG21	1:F:1074:TYR:OH	2.15	0.47
1:F:1106:TYR:N	1:F:1121:CYS:SG	2.87	0.47
1:F:1106:TYR:HB2	1:F:1121:CYS:SG	2.54	0.47
1:F:1134:MET:HE2	1:F:1143:TRP:CB	2.43	0.47
1:F:1041:SER:CB	1:F:1178:PHE:CZ	2.97	0.47
1:F:1045:CYS:SG	1:F:1221:LEU:HA	2.55	0.46
1:F:816:LYS:HG3	1:F:820:LYS:HZ3	1.81	0.46
1:F:1075:LEU:HD13	1:F:1152:LEU:HD21	1.64	0.46
1:F:199:PHE:CE1	1:F:201:SER:HB2	2.51	0.46
1:F:133:ARG:HD3	1:F:133:ARG:N	2.29	0.46
1:F:145:ALA:HB3	1:F:193:ARG:HA	1.97	0.46
1:F:140:PHE:HB2	1:F:301:GLU:HB3	1.97	0.46
1:F:184:LEU:HD11	1:F:235:LEU:CD2	2.43	0.46
1:F:905:ARG:NH2	1:F:956:HIS:CE1	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:915:PRO:HB2	1:F:916:LYS:HA	1.98	0.45
1:F:1852:HIS:CG	1:F:1852:HIS:O	2.69	0.45
1:F:303:ASN:HA	1:F:304:PRO:HD3	1.75	0.45
1:F:956:HIS:N	1:F:957:PHE:O	2.50	0.45
1:F:150:PHE:CZ	1:F:258:GLU:CD	2.93	0.45
1:F:294:ALA:CB	1:F:295:ASN:ND2	2.80	0.44
1:F:1136:LEU:HB3	1:F:1743:LEU:HD11	1.99	0.44
1:F:1041:SER:HB3	1:F:1178:PHE:CE1	2.52	0.44
1:F:1155:ILE:HG23	1:F:1156:HIS:H	1.58	0.44
1:F:150:PHE:CE1	1:F:196:VAL:HG21	2.53	0.44
1:F:286:ASN:HD21	1:F:306:ARG:NH1	2.12	0.44
1:F:1149:TYR:OH	1:F:1179:VAL:HG23	2.18	0.43
1:F:1735:ILE:HD12	1:F:1735:ILE:H	1.83	0.43
1:F:136:LEU:O	1:F:136:LEU:CG	2.43	0.43
1:F:151:ILE:CD1	1:F:296:TYR:OH	2.65	0.43
1:F:259:PHE:HB2	1:F:291:ARG:HH21	1.82	0.43
1:F:1050:ALA:HB3	1:F:1052:LYS:HD2	1.98	0.43
1:F:149:PHE:HD1	1:F:259:PHE:O	2.02	0.43
1:F:1154:GLU:OE1	1:F:1156:HIS:ND1	2.52	0.43
1:F:240:PHE:HA	1:F:241:SER:HB2	2.00	0.43
1:F:1091:ALA:HB1	1:F:1105:ILE:HD11	2.00	0.43
1:F:1135:LEU:CD1	1:F:1144:VAL:CG1	2.96	0.43
1:F:1041:SER:O	1:F:1218:VAL:HG12	2.18	0.43
1:F:75:ARG:HE	1:F:87:THR:H	1.65	0.42
1:F:1108:ALA:HB1	1:F:1109:LEU:H	1.31	0.42
1:F:1134:MET:O	1:F:1140:TYR:HB3	2.20	0.42
1:F:184:LEU:HD13	1:F:235:LEU:CD2	2.40	0.42
1:F:1041:SER:HB3	1:F:1217:GLU:HG3	1.89	0.42
1:F:1042:ALA:HA	1:F:1218:VAL:O	2.19	0.42
1:F:1053:THR:HA	1:F:1181:LEU:HD13	2.01	0.42
1:F:1076:ALA:HB1	1:F:1078:ALA:H	1.84	0.42
1:F:1135:LEU:CD1	1:F:1144:VAL:HG13	2.49	0.42
1:F:1025:PRO:HB2	3:F:2202:ADP:HN61	1.82	0.42
1:F:1168:GLU:OE1	1:F:1776:PHE:HE2	2.03	0.42
1:F:1149:TYR:HE2	1:F:1177:PRO:HB2	1.84	0.42
1:F:1220:LEU:O	1:F:1221:LEU:HD12	2.20	0.42
1:F:300:ASP:HA	1:F:301:GLU:CB	2.50	0.41
1:F:1851:ALA:H	1:F:1852:HIS:HB3	1.84	0.41
1:F:1134:MET:O	1:F:1140:TYR:CB	2.68	0.41
1:F:1697:ARG:CG	3:F:2202:ADP:H5'1	2.51	0.41
1:F:184:LEU:HD13	1:F:235:LEU:HD21	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:787:GLU:HA	1:F:790:ARG:HE	1.86	0.41
1:F:1136:LEU:O	1:F:1137:SER:C	2.41	0.41
1:F:1030:ARG:HA	1:F:1030:ARG:HH21	1.86	0.41
1:F:138:ASP:H	1:F:139:MET:C	2.28	0.41
1:F:1126:THR:HB	1:F:1130:THR:HB	2.03	0.41
1:F:153:GLY:HA2	1:F:156:LEU:CB	2.51	0.41
1:F:955:LYS:HD3	1:F:990:ASP:OD1	2.21	0.41
1:F:1072:VAL:H	1:F:1123:VAL:HG22	1.86	0.40
1:F:1741:LEU:HB3	1:F:1852:HIS:CE1	2.55	0.40
1:F:150:PHE:CE2	1:F:258:GLU:OE1	2.74	0.40
1:F:1106:TYR:CD2	1:F:1119:ASP:CA	3.05	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	F	1489/2174 (68%)	1095 (74%)	250 (17%)	144 (10%)	0 7

All (144) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	22	HIS
1	F	80	ASP
1	F	132	ALA
1	F	138	ASP
1	F	145	ALA
1	F	190	ARG
1	F	203	LEU
1	F	228	GLU
1	F	245	SER
1	F	247	ALA

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Mol	Chain	Res	Type
1	F	295	ASN
1	F	296	TYR
1	F	305	TYR
1	F	686	LYS
1	F	796	SER
1	F	803	PHE
1	F	851	TRP
1	F	989	GLN
1	F	1008	LEU
1	F	1010	GLU
1	F	1013	PHE
1	F	1017	HIS
1	F	1078	ALA
1	F	1108	ALA
1	F	1114	TYR
1	F	1117	PHE
1	F	1121	CYS
1	F	1149	TYR
1	F	1155	ILE
1	F	1189	GLN
1	F	1214	ARG
1	F	1216	PHE
1	F	1226	LYS
1	F	1249	GLN
1	F	1340	GLU
1	F	1378	PHE
1	F	1468	PHE
1	F	1581	GLU
1	F	1585	VAL
1	F	1712	MET
1	F	1837	PHE
1	F	1839	PHE
1	F	1851	ALA
1	F	165	SER
1	F	243	TYR
1	F	302	ALA
1	F	306	ARG
1	F	317	ASP
1	F	320	VAL
1	F	697	LYS
1	F	775	GLY
1	F	912	GLN

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Mol	Chain	Res	Type
1	F	935	ILE
1	F	957	PHE
1	F	962	SER
1	F	987	LEU
1	F	988	PRO
1	F	1042	ALA
1	F	1054	PHE
1	F	1065	ARG
1	F	1081	LEU
1	F	1103	ARG
1	F	1109	LEU
1	F	1223	SER
1	F	1248	THR
1	F	1305	VAL
1	F	1363	GLY
1	F	1475	ILE
1	F	1582	LEU
1	F	1774	LEU
1	F	1820	LEU
1	F	1826	VAL
1	F	17	GLU
1	F	230	ASP
1	F	232	LYS
1	F	268	LEU
1	F	715	ALA
1	F	719	VAL
1	F	721	GLU
1	F	807	MET
1	F	863	ASP
1	F	977	MET
1	F	992	GLN
1	F	1012	PRO
1	F	1122	GLN
1	F	1213	MET
1	F	1268	SER
1	F	1284	SER
1	F	1370	LEU
1	F	1565	ASP
1	F	1583	PHE
1	F	1601	VAL
1	F	1617	GLY
1	F	1727	LYS

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Mol	Chain	Res	Type
1	F	1751	HIS
1	F	1783	ALA
1	F	166	VAL
1	F	173	PRO
1	F	271	LEU
1	F	307	LEU
1	F	315	VAL
1	F	866	ILE
1	F	915	PRO
1	F	919	LEU
1	F	1024	ASN
1	F	1069	LYS
1	F	1115	HIS
1	F	1250	LYS
1	F	1258	ASN
1	F	1265	HIS
1	F	1460	LYS
1	F	1632	HIS
1	F	19	ASN
1	F	802	GLU
1	F	854	LEU
1	F	936	ARG
1	F	940	PRO
1	F	959	LEU
1	F	996	THR
1	F	997	PRO
1	F	1016	GLU
1	F	1066	ARG
1	F	1300	LYS
1	F	1407	HIS
1	F	1567	GLU
1	F	1588	VAL
1	F	1801	TYR
1	F	1803	GLN
1	F	53	GLU
1	F	210	PRO
1	F	828	TYR
1	F	1101	PRO
1	F	1312	LEU
1	F	1368	GLU
1	F	1437	PRO
1	F	1466	VAL

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Mol	Chain	Res	Type
1	F	1557	ARG
1	F	867	VAL
1	F	1100	ASN
1	F	33	VAL
1	F	257	PRO
1	F	1102	GLY
1	F	177	ILE
1	F	1221	LEU

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	F	1318/1862 (71%)	1284 (97%)	34 (3%)	40 60

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	137	CYS
1	F	138	ASP
1	F	158	MET
1	F	262	MET
1	F	298	ASP
1	F	301	GLU
1	F	303	ASN
1	F	305	TYR
1	F	307	LEU
1	F	308	ARG
1	F	316	GLU
1	F	320	VAL
1	F	866	ILE
1	F	1029	GLN
1	F	1030	ARG
1	F	1054	PHE
1	F	1055	ILE
1	F	1081	LEU

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Mol	Chain	Res	Type
1	F	1101	PRO
1	F	1122	GLN
1	F	1128	PRO
1	F	1132	GLU
1	F	1202	LEU
1	F	1216	PHE
1	F	1240	LEU
1	F	1247	LEU
1	F	1378	PHE
1	F	1386	VAL
1	F	1526	ASN
1	F	1558	LEU
1	F	1587	ASP
1	F	1819	ILE
1	F	1820	LEU
1	F	1828	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	172	GLN
1	F	175	HIS
1	F	254	GLN
1	F	286	ASN
1	F	310	GLN
1	F	675	ASN
1	F	691	HIS
1	F	723	HIS
1	F	731	HIS
1	F	737	HIS
1	F	850	HIS
1	F	928	HIS
1	F	965	ASN
1	F	989	GLN
1	F	1007	HIS
1	F	1122	GLN
1	F	1161	ASN
1	F	1199	GLN
1	F	1219	HIS
1	F	1255	GLN
1	F	1258	ASN
1	F	1276	GLN

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Mol	Chain	Res	Type
1	F	1339	GLN
1	F	1478	HIS
1	F	1555	GLN
1	F	1689	GLN
1	F	1704	HIS
1	F	1729	ASN
1	F	1731	GLN
1	F	1761	HIS
1	F	1772	ASN
1	F	1780	ASN
1	F	1808	HIS
1	F	1812	HIS
1	F	1831	HIS
1	F	1852	HIS

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
3	ADP	F	2202	2	28,29,29	1.00	1 (3%)	43,45,45	1.47	5 (11%)

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
3	ADP	F	2202	2	-	2/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2202	ADP	PA-O3A	-4.23	1.54	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2202	ADP	O4'-C1'-N9	5.79	119.20	108.09
3	F	2202	ADP	O3'-C3'-C4'	-4.41	98.40	111.08
3	F	2202	ADP	O2A-PA-O3A	-3.85	96.86	107.27
3	F	2202	ADP	C2'-C1'-N9	3.10	121.00	113.30
3	F	2202	ADP	O3B-PB-O2B	2.41	116.82	107.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2202	ADP	PA-O3A-PB-O3B
3	F	2202	ADP	PB-O3A-PA-O2A

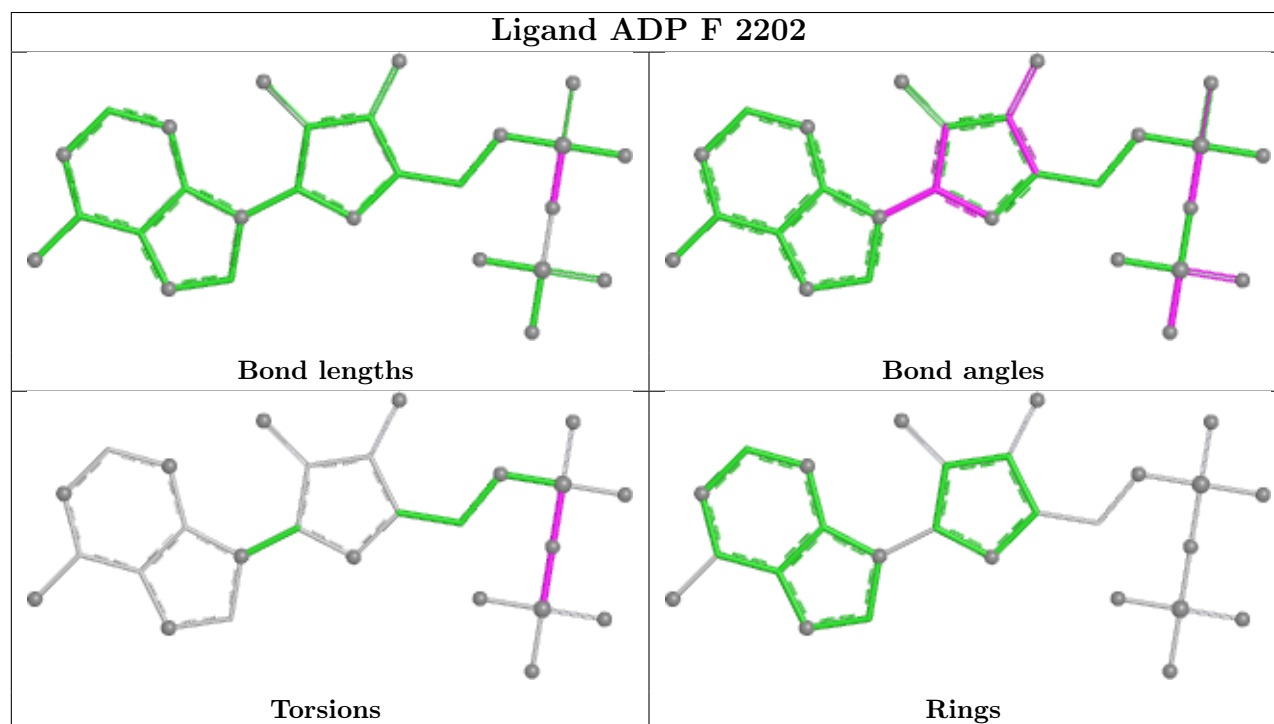
There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2202	ADP	18	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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	28

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	1752:LEU	C	1753:LYS	N	4.20

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	29:ARG	C	30:VAL	N	3.96
1	F	1473:GLN	C	1474:PHE	N	3.84
1	F	1047:PRO	C	1048:THR	N	3.74
1	F	1729:ASN	C	1730:VAL	N	3.69
1	F	944:SER	C	945:GLU	N	3.34
1	F	1057:TYR	C	1058:TYR	N	3.23
1	F	1855:PRO	C	1856:LEU	N	3.20
1	F	1488:ALA	C	1489:ARG	N	3.18
1	F	1026:ASP	C	1027:ASN	N	3.16
1	F	1501:SER	C	1502:GLU	N	3.14
1	F	39:ALA	C	40:LYS	N	3.11
1	F	213:LEU	C	214:PHE	N	3.11
1	F	1164:GLY	C	1165:ASP	N	3.11
1	F	1521:ARG	C	1522:TYR	N	2.98
1	F	1149:TYR	C	1150:VAL	N	1.72
1	F	1039:ARG	C	1040:GLY	N	1.67
1	F	1221:LEU	C	1222:PRO	N	1.65
1	F	1152:LEU	C	1153:ASP	N	1.64
1	F	1076:ALA	C	1077:PRO	N	1.63
1	F	234:GLY	C	235:LEU	N	1.19
1	F	301:GLU	C	302:ALA	N	1.18
1	F	304:PRO	C	305:TYR	N	1.15
1	F	198:PHE	C	199:PHE	N	1.14
1	F	195:HIS	C	196:VAL	N	1.12
1	F	194:PHE	C	195:HIS	N	1.08
1	F	1215:ASP	C	1216:PHE	N	1.04
1	F	291:ARG	C	292:ARG	N	1.03

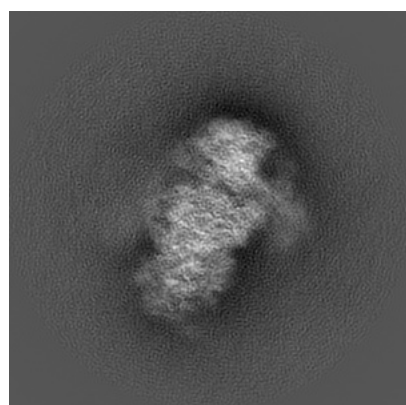
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11895. These allow visual inspection of the internal detail of the map and identification of artifacts.

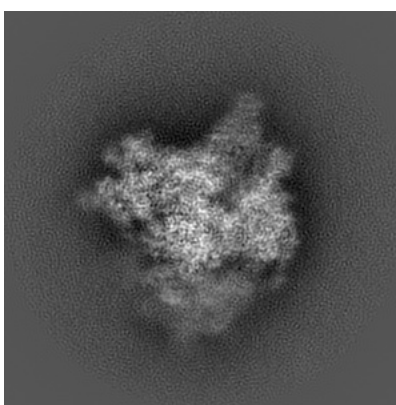
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

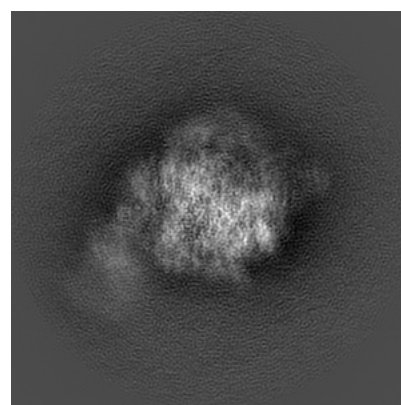
6.1.1 Primary map



X



Y

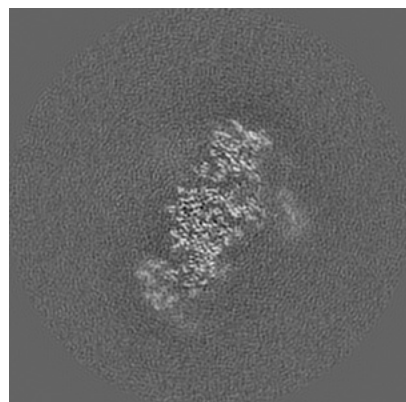


Z

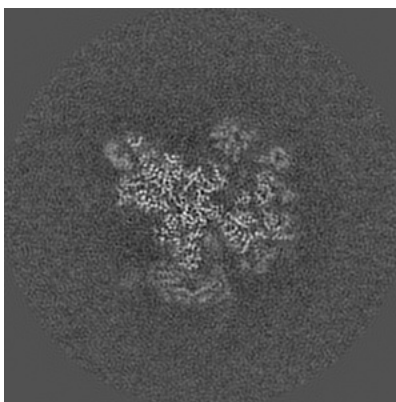
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

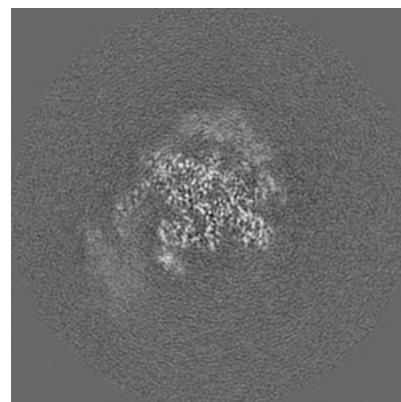
6.2.1 Primary map



X Index: 150



Y Index: 150

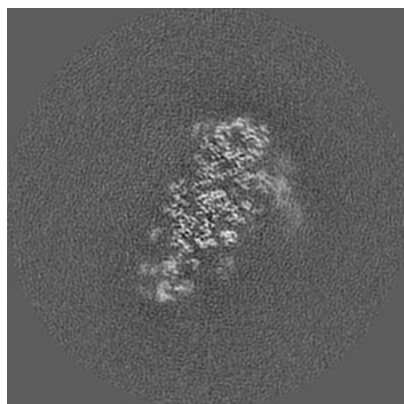


Z Index: 150

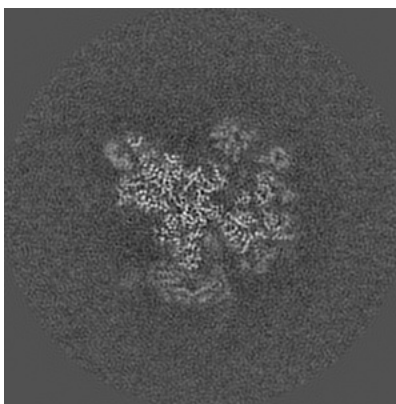
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

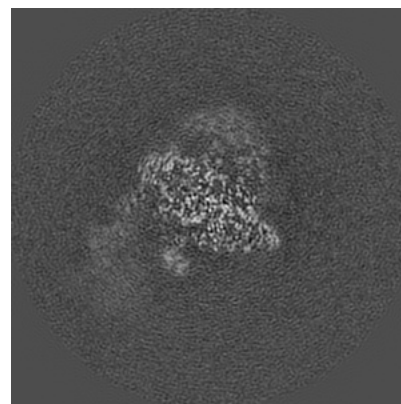
6.3.1 Primary map



X Index: 144



Y Index: 150

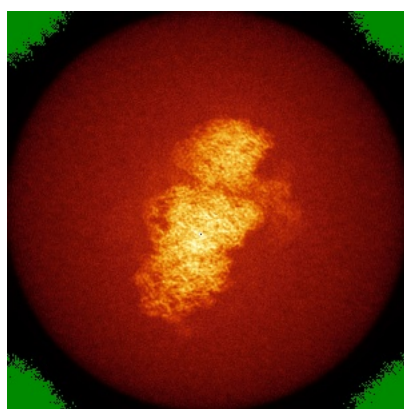


Z Index: 146

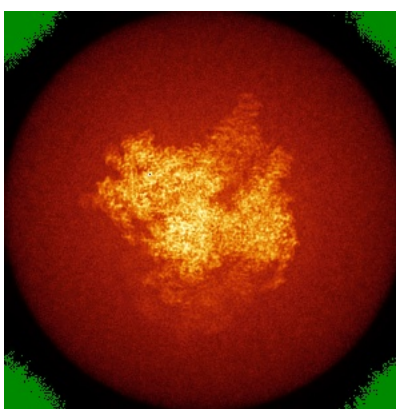
The images above show the largest variance slices of the map in three orthogonal directions.

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

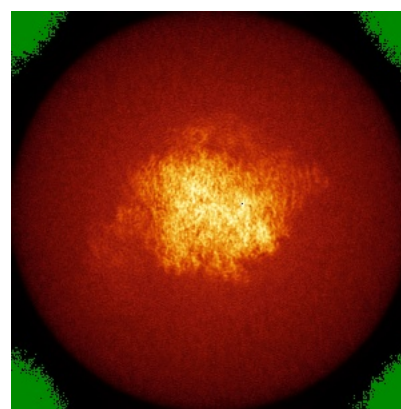
6.4.1 Primary map



X



Y

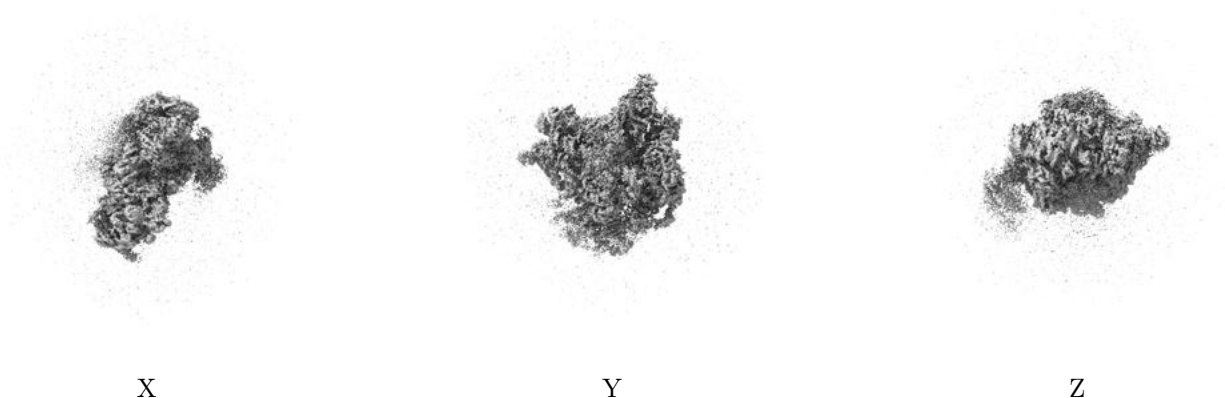


Z

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 0.0344. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

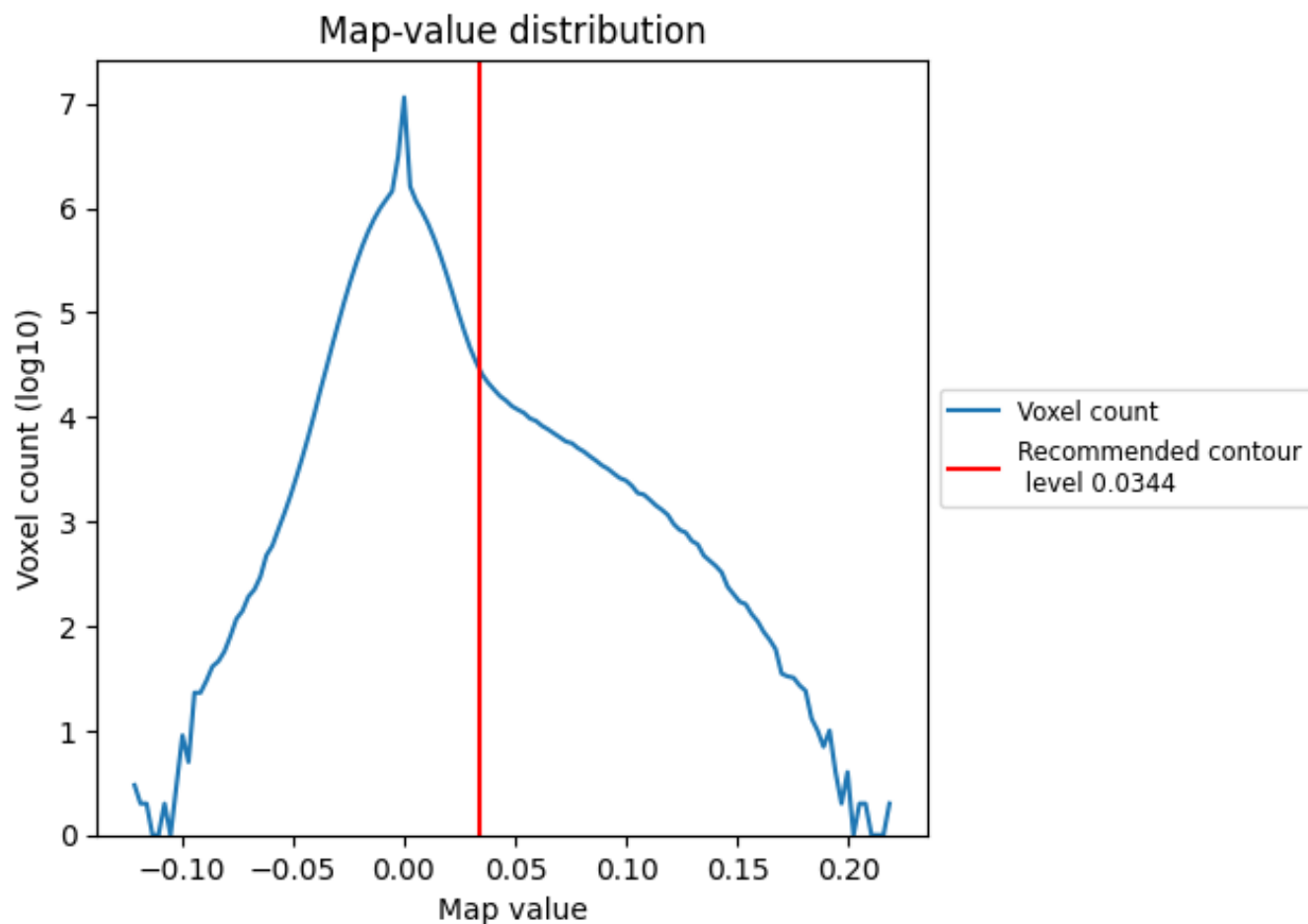
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

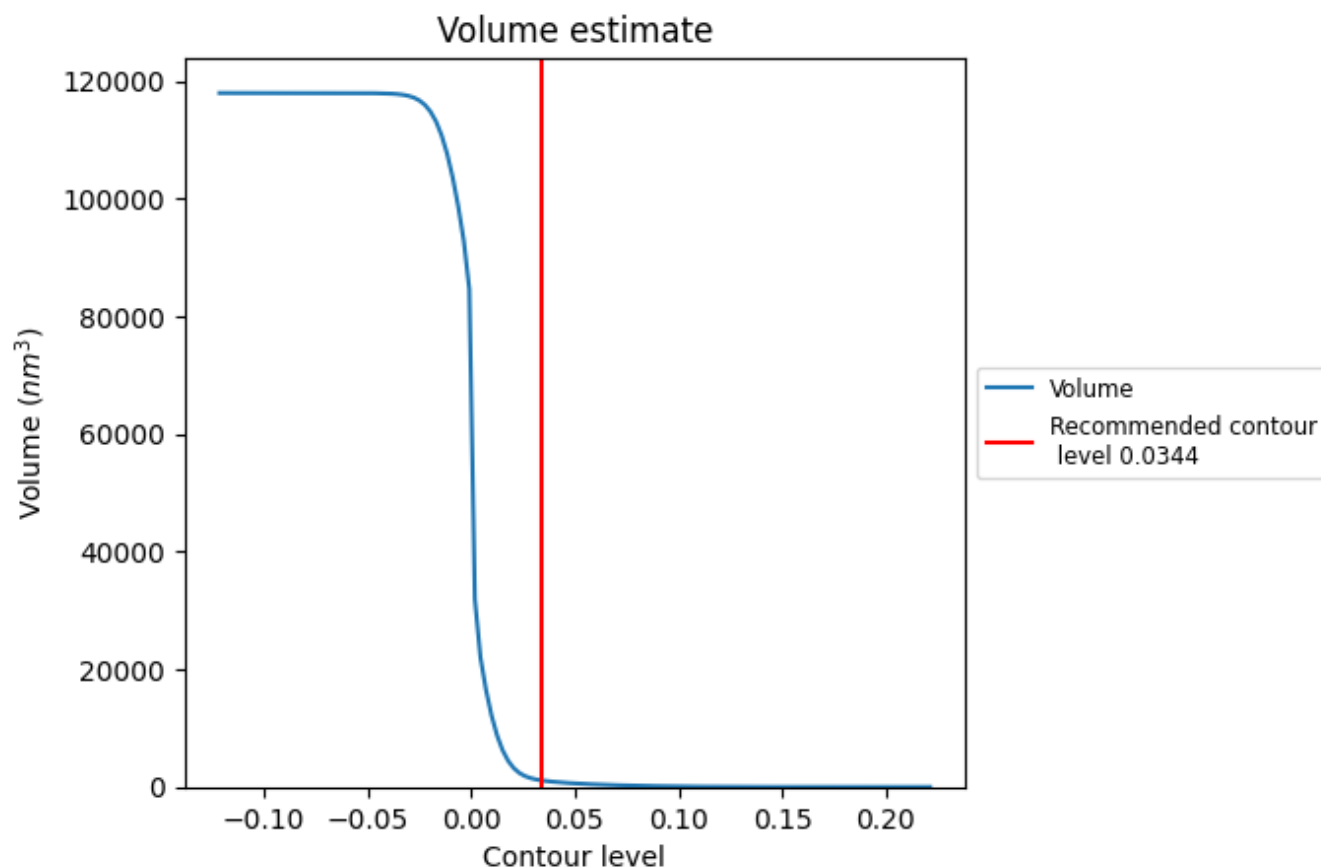
This section contains the results of statistical analysis of the map.

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.

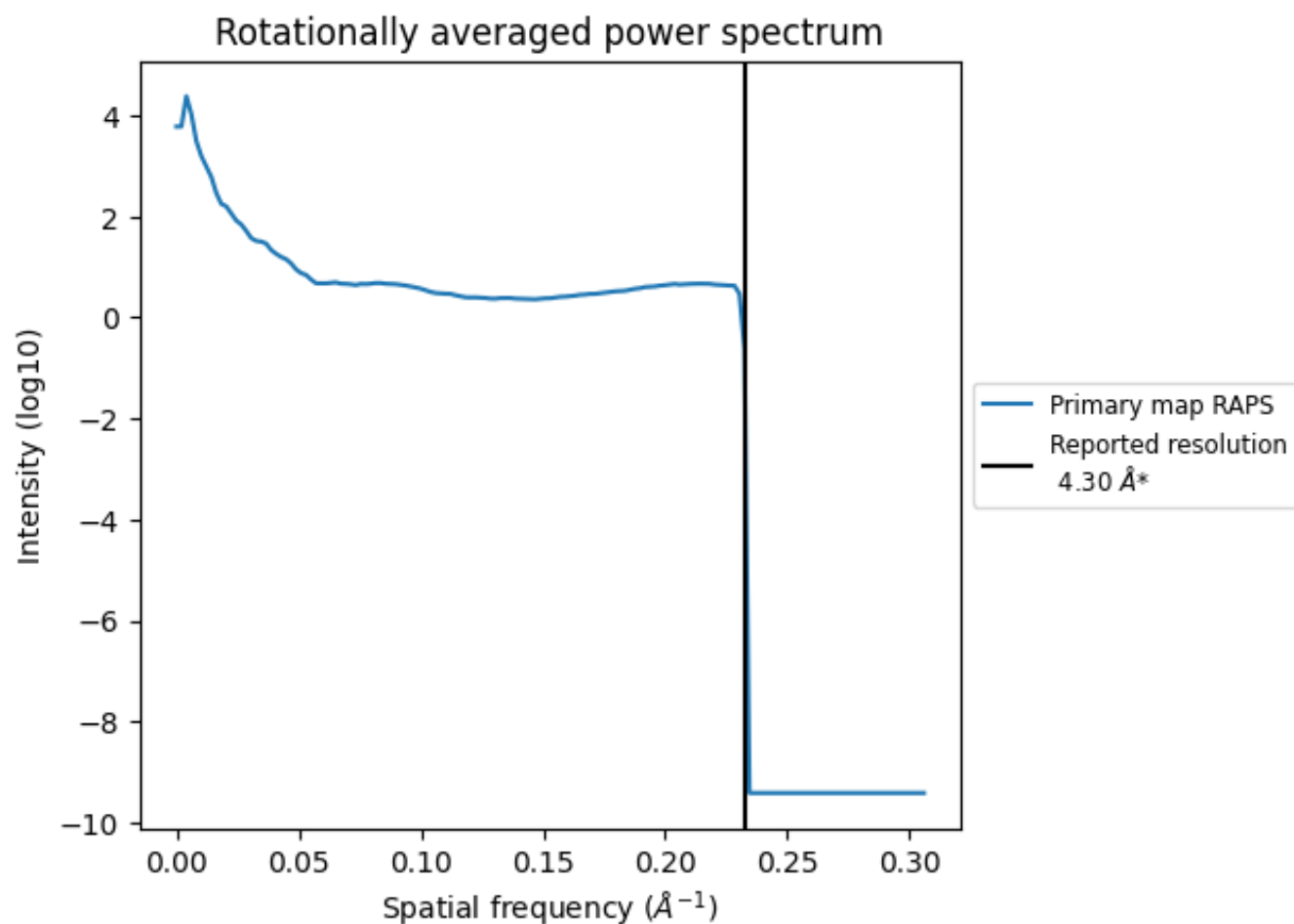
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1092 nm³; this corresponds to an approximate mass of 986 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 0.233 Å⁻¹

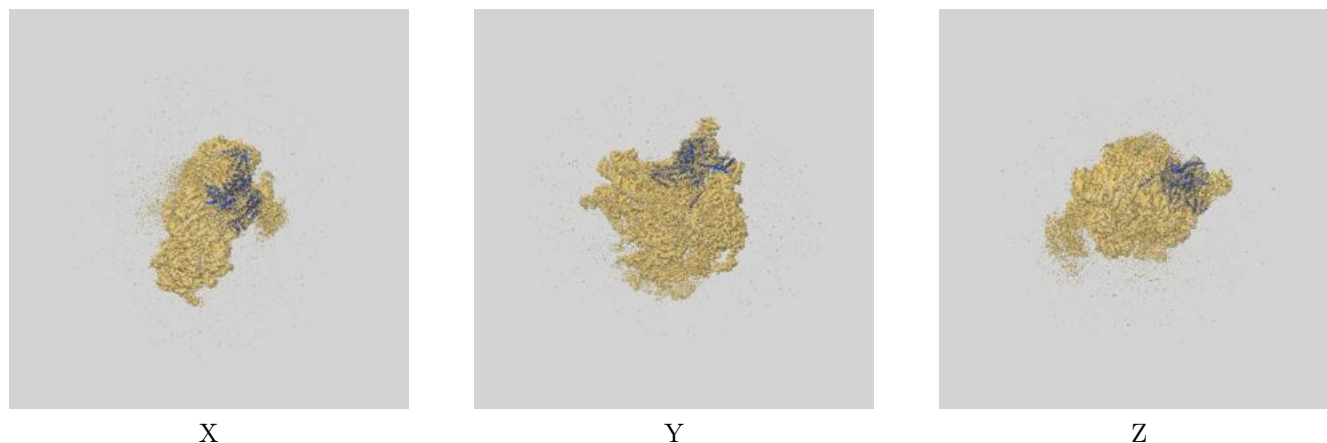
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11895 and PDB model 7ASK. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



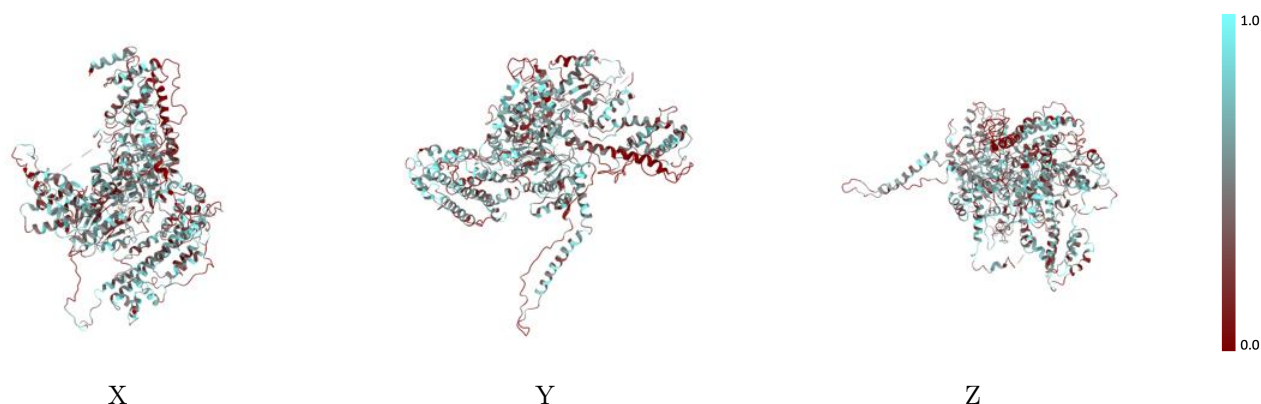
The images above show the 3D surface view of the map at the recommended contour level 0.0344 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



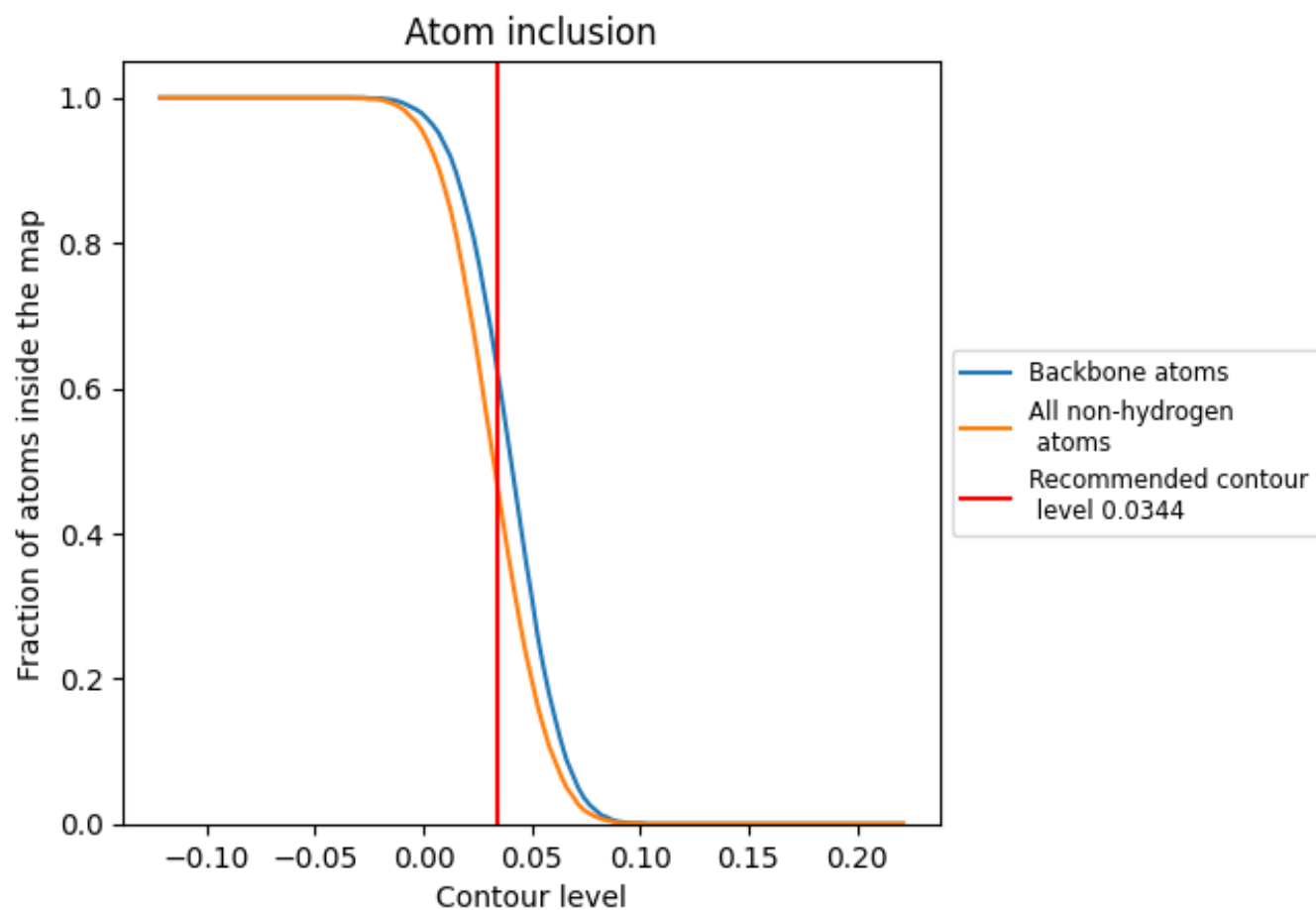
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0344).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 46% 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 (0.0344) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4620	0.2720
F	0.4620	0.2720

