



## Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 06:43 pm GMT

PDB ID : 7ASK  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

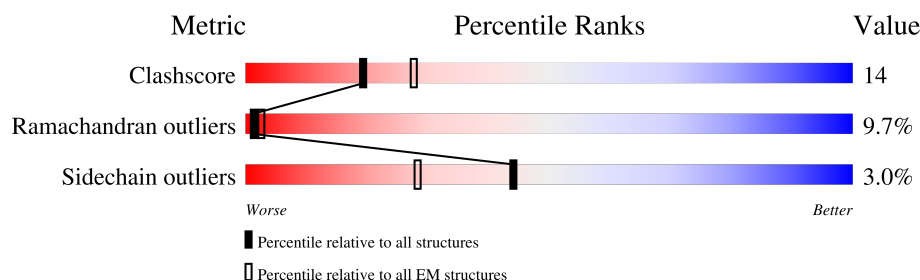
# 1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	<div> <div>29%</div> <div>51%</div> <div>13%</div> <div>.</div> <div>30%</div> </div>

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.

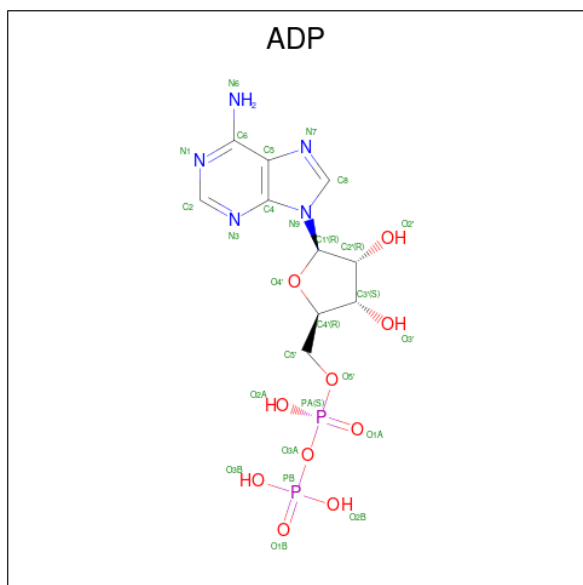
- Molecule 1 is a protein called kDDX60.

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

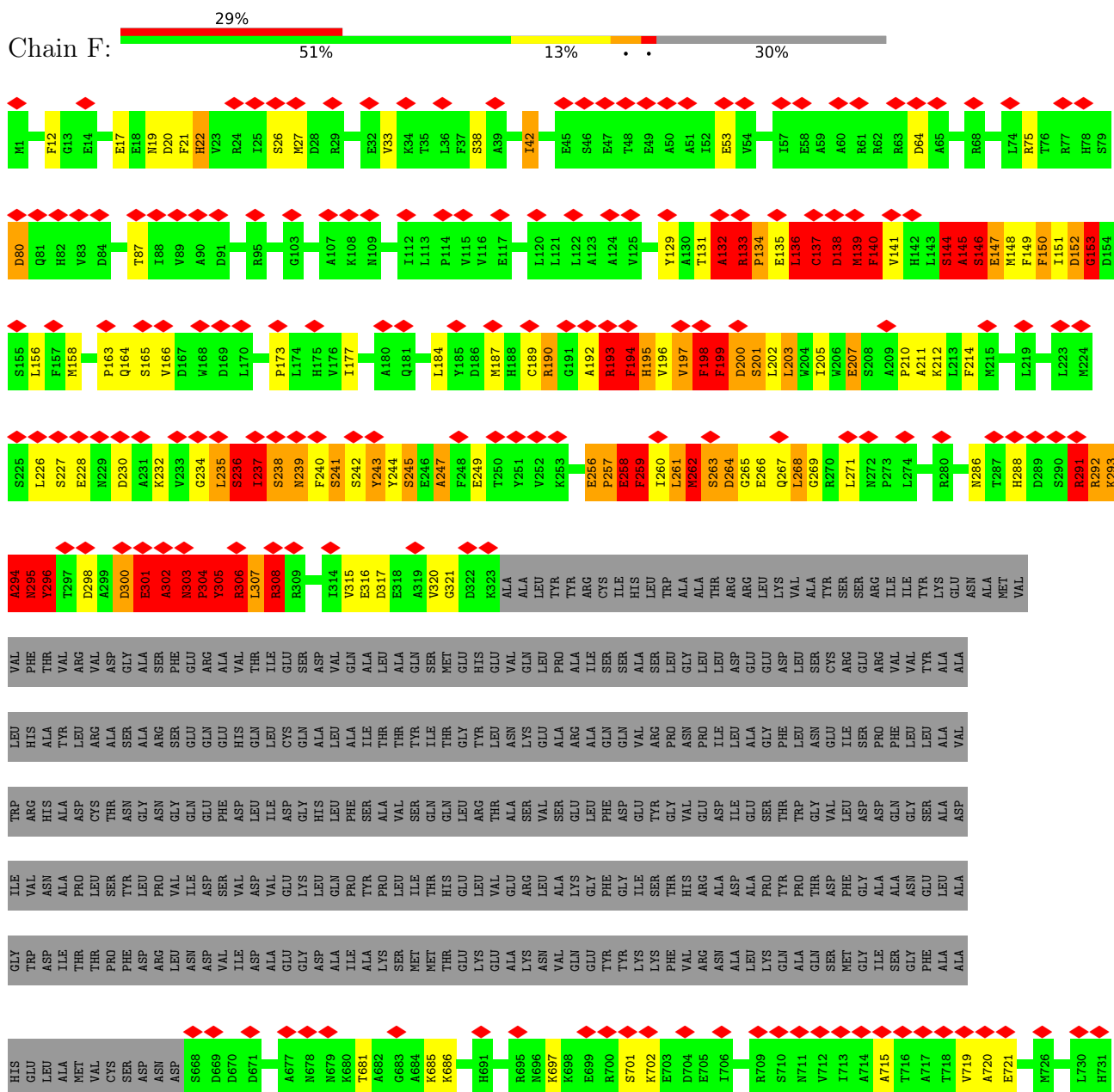


Mol	Chain	Residues	Atoms					AltConf
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

### 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 [i](#)

### 5.1 Standard geometry [i](#)

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	1.19	54/12495 (0.4%)	1.42	170/16839 (1.0%)

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 (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1039	ARG	C-N	18.89	1.67	1.33
1	F	1149	TYR	C-N	16.88	1.72	1.34
1	F	304	PRO	CA-C	-16.65	1.19	1.52
1	F	1221	LEU	C-N	16.65	1.65	1.34
1	F	1076	ALA	C-N	15.57	1.63	1.34
1	F	133	ARG	C-N	13.75	1.60	1.34
1	F	153	GLY	N-CA	-13.49	1.25	1.46
1	F	1183	ALA	N-CA	-13.45	1.19	1.46
1	F	296	TYR	N-CA	-13.41	1.19	1.46
1	F	291	ARG	C-N	-13.23	1.03	1.34
1	F	306	ARG	N-CA	13.21	1.72	1.46
1	F	1152	LEU	C-N	13.14	1.64	1.34
1	F	1215	ASP	C-N	-12.84	1.04	1.34
1	F	1137	SER	N-CA	-12.45	1.21	1.46
1	F	305	TYR	CA-C	-12.43	1.20	1.52
1	F	303	ASN	C-N	11.29	1.55	1.34
1	F	259	PHE	CA-C	11.07	1.81	1.52
1	F	194	PHE	C-N	-10.96	1.08	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	305	TYR	C-O	10.70	1.43	1.23
1	F	1052	LYS	C-N	10.69	1.58	1.34
1	F	265	GLY	N-CA	-10.09	1.30	1.46
1	F	259	PHE	C-N	9.90	1.56	1.34
1	F	1149	TYR	N-CA	-9.52	1.27	1.46
1	F	195	HIS	C-N	-9.17	1.12	1.34
1	F	1044	VAL	C-N	9.10	1.54	1.34
1	F	1122	GLN	C-N	8.88	1.54	1.34
1	F	198	PHE	C-N	-8.52	1.14	1.34
1	F	1155	ILE	N-CA	-8.37	1.29	1.46
1	F	1108	ALA	N-CA	-8.32	1.29	1.46
1	F	304	PRO	C-N	-7.93	1.15	1.34
1	F	197	VAL	N-CA	7.78	1.61	1.46
1	F	1219	HIS	C-N	7.69	1.51	1.34
1	F	1040	GLY	N-CA	-7.39	1.34	1.46
1	F	1176	CYS	C-N	7.08	1.47	1.34
1	F	301	GLU	C-O	-7.05	1.09	1.23
1	F	292	ARG	N-CA	-7.00	1.32	1.46
1	F	307	LEU	CA-C	-6.88	1.35	1.52
1	F	296	TYR	C-N	6.84	1.49	1.34
1	F	301	GLU	C-N	-6.71	1.18	1.34
1	F	234	GLY	C-N	-6.33	1.19	1.34
1	F	147	GLU	C-N	6.12	1.48	1.34
1	F	256	GLU	C-N	6.09	1.45	1.34
1	F	199	PHE	N-CA	6.04	1.58	1.46
1	F	292	ARG	C-N	6.03	1.48	1.34
1	F	134	PRO	CA-C	6.02	1.64	1.52
1	F	305	TYR	N-CA	-5.99	1.34	1.46
1	F	136	LEU	C-N	5.73	1.47	1.34
1	F	303	ASN	C-O	5.71	1.34	1.23
1	F	294	ALA	C-N	-5.68	1.21	1.34
1	F	239	ASN	CA-C	-5.66	1.38	1.52
1	F	305	TYR	C-N	5.65	1.47	1.34
1	F	294	ALA	N-CA	-5.38	1.35	1.46
1	F	146	SER	C-N	5.35	1.46	1.34
1	F	1108	ALA	C-N	5.25	1.46	1.34

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1051	GLY	O-C-N	-23.74	84.72	122.70
1	F	306	ARG	N-CA-CB	20.05	146.69	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	305	TYR	N-CA-CB	19.79	146.22	110.60
1	F	139	MET	O-C-N	-17.39	94.87	122.70
1	F	1155	ILE	N-CA-CB	17.28	150.53	110.80
1	F	1137	SER	N-CA-CB	16.75	135.63	110.50
1	F	296	TYR	N-CA-C	15.98	154.14	111.00
1	F	1136	LEU	O-C-N	15.81	148.00	122.70
1	F	193	ARG	C-N-CA	15.46	160.35	121.70
1	F	152	ASP	O-C-N	-14.86	97.94	123.20
1	F	146	SER	O-C-N	-14.85	98.94	122.70
1	F	1154	GLU	O-C-N	-14.57	99.38	122.70
1	F	1148	ASP	O-C-N	13.96	145.03	122.70
1	F	259	PHE	N-CA-CB	-13.88	85.61	110.60
1	F	238	SER	CB-CA-C	-13.42	84.59	110.10
1	F	234	GLY	O-C-N	12.41	142.56	122.70
1	F	262	MET	O-C-N	-12.35	102.94	122.70
1	F	1136	LEU	CA-C-N	-12.31	90.11	117.20
1	F	1220	LEU	O-C-N	-12.31	103.00	122.70
1	F	147	GLU	O-C-N	-12.31	103.01	122.70
1	F	198	PHE	O-C-N	-12.24	103.11	122.70
1	F	152	ASP	C-N-CA	12.03	147.56	122.30
1	F	1039	ARG	O-C-N	-11.93	102.92	123.20
1	F	1039	ARG	C-N-CA	11.87	147.24	122.30
1	F	258	GLU	O-C-N	-11.77	103.87	122.70
1	F	296	TYR	O-C-N	11.65	141.33	122.70
1	F	1148	ASP	C-N-CA	11.04	149.31	121.70
1	F	1122	GLN	CA-C-O	-10.71	97.60	120.10
1	F	259	PHE	CB-CA-C	-10.68	89.04	110.40
1	F	1125	LEU	CB-CA-C	-10.27	90.68	110.20
1	F	1148	ASP	CA-C-N	-10.26	94.64	117.20
1	F	307	LEU	O-C-N	10.22	139.06	122.70
1	F	1154	GLU	CA-C-N	10.22	139.69	117.20
1	F	262	MET	CA-C-N	10.14	139.51	117.20
1	F	152	ASP	CA-C-N	10.09	136.39	116.20
1	F	301	GLU	CA-C-N	10.06	139.33	117.20
1	F	1127	VAL	O-C-N	9.87	139.85	121.10
1	F	1122	GLN	CA-C-N	9.65	138.43	117.20
1	F	239	ASN	CA-C-O	-9.59	99.96	120.10
1	F	134	PRO	CA-C-O	-9.43	97.56	120.20
1	F	1050	ALA	C-N-CA	-9.43	102.50	122.30
1	F	258	GLU	C-N-CA	9.34	145.04	121.70
1	F	198	PHE	N-CA-C	-9.33	85.80	111.00
1	F	234	GLY	CA-C-N	-9.32	96.70	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	136	LEU	N-CA-CB	-9.22	91.96	110.40
1	F	302	ALA	O-C-N	9.18	137.38	122.70
1	F	132	ALA	C-N-CA	9.16	144.60	121.70
1	F	134	PRO	CA-C-N	9.06	137.14	117.20
1	F	199	PHE	C-N-CA	9.06	144.34	121.70
1	F	137	CYS	O-C-N	-9.05	108.21	122.70
1	F	136	LEU	CA-C-N	9.00	136.99	117.20
1	F	306	ARG	C-N-CA	8.95	144.08	121.70
1	F	139	MET	C-N-CA	-8.81	99.68	121.70
1	F	296	TYR	CA-C-N	-8.69	98.08	117.20
1	F	147	GLU	CA-C-N	8.62	136.16	117.20
1	F	239	ASN	CB-CA-C	8.54	127.48	110.40
1	F	238	SER	C-N-CA	8.53	143.03	121.70
1	F	1039	ARG	CA-C-N	8.41	133.03	116.20
1	F	1121	CYS	O-C-N	-8.36	109.33	122.70
1	F	236	SER	O-C-N	-8.34	109.36	122.70
1	F	1152	LEU	O-C-N	-8.25	109.51	122.70
1	F	263	SER	O-C-N	-8.10	109.75	122.70
1	F	304	PRO	O-C-N	8.10	135.65	122.70
1	F	153	GLY	C-N-CA	-8.05	101.58	121.70
1	F	293	LYS	O-C-N	-7.86	110.13	122.70
1	F	193	ARG	O-C-N	-7.86	110.13	122.70
1	F	1183	ALA	N-CA-CB	7.85	121.08	110.10
1	F	303	ASN	CB-CA-C	7.80	126.00	110.40
1	F	1218	VAL	O-C-N	-7.77	110.27	122.70
1	F	304	PRO	CA-C-O	-7.66	101.82	120.20
1	F	239	ASN	CA-C-N	7.62	133.96	117.20
1	F	138	ASP	C-N-CA	-7.54	102.86	121.70
1	F	1220	LEU	C-N-CA	7.52	140.50	121.70
1	F	194	PHE	CA-C-N	-7.51	100.67	117.20
1	F	1109	LEU	C-N-CA	7.51	138.07	122.30
1	F	1052	LYS	CA-C-N	-7.45	100.82	117.20
1	F	1220	LEU	CA-C-N	7.42	133.53	117.20
1	F	303	ASN	CA-C-O	7.30	135.43	120.10
1	F	234	GLY	N-CA-C	7.27	131.28	113.10
1	F	236	SER	C-N-CA	7.26	139.85	121.70
1	F	1106	TYR	CB-CG-CD2	-7.15	116.71	121.00
1	F	304	PRO	N-CA-C	7.12	130.60	112.10
1	F	199	PHE	N-CA-CB	-7.07	97.88	110.60
1	F	302	ALA	CA-C-N	-7.05	101.69	117.20
1	F	300	ASP	C-N-CA	-7.00	104.20	121.70
1	F	198	PHE	CA-C-N	6.92	132.42	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	295	ASN	N-CA-C	6.91	129.65	111.00
1	F	828	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	F	307	LEU	CA-C-N	-6.90	102.03	117.20
1	F	1108	ALA	C-N-CA	6.87	138.88	121.70
1	F	303	ASN	CA-C-N	-6.84	97.94	117.10
1	F	133	ARG	O-C-N	-6.84	108.10	121.10
1	F	1177	PRO	CB-CA-C	6.81	129.03	112.00
1	F	266	GLU	C-N-CA	6.75	138.58	121.70
1	F	291	ARG	O-C-N	-6.73	111.93	122.70
1	F	259	PHE	CA-C-O	-6.69	106.05	120.10
1	F	1052	LYS	O-C-N	6.66	133.36	122.70
1	F	301	GLU	CA-C-O	-6.54	106.38	120.10
1	F	136	LEU	CA-C-O	-6.47	106.52	120.10
1	F	962	SER	N-CA-CB	6.45	120.18	110.50
1	F	307	LEU	C-N-CA	6.45	137.82	121.70
1	F	1106	TYR	CB-CG-CD1	6.42	124.85	121.00
1	F	137	CYS	N-CA-C	-6.41	93.70	111.00
1	F	292	ARG	C-N-CA	6.40	137.71	121.70
1	F	147	GLU	C-N-CA	6.38	137.65	121.70
1	F	194	PHE	O-C-N	6.29	132.77	122.70
1	F	1219	HIS	O-C-N	-6.21	112.76	122.70
1	F	144	SER	N-CA-CB	6.17	119.75	110.50
1	F	926	TYR	CB-CG-CD1	6.16	124.69	121.00
1	F	1070	LYS	CA-C-N	-6.15	103.66	117.20
1	F	140	PHE	CB-CG-CD1	6.13	125.09	120.80
1	F	1378	PHE	CB-CG-CD1	6.13	125.09	120.80
1	F	293	LYS	C-N-CA	6.11	136.99	121.70
1	F	926	TYR	CB-CG-CD2	-6.11	117.33	121.00
1	F	1051	GLY	CA-C-N	6.09	130.59	117.20
1	F	140	PHE	CB-CG-CD2	-6.08	116.54	120.80
1	F	1378	PHE	N-CA-CB	6.08	121.54	110.60
1	F	1152	LEU	CA-C-N	6.00	130.40	117.20
1	F	1121	CYS	CA-C-N	5.99	130.38	117.20
1	F	294	ALA	O-C-N	5.99	132.29	122.70
1	F	150	PHE	CB-CG-CD1	5.99	124.99	120.80
1	F	234	GLY	C-N-CA	5.97	136.64	121.70
1	F	1103	ARG	O-C-N	-5.94	113.19	122.70
1	F	258	GLU	CA-C-N	5.94	130.27	117.20
1	F	924	PHE	CB-CG-CD1	5.92	124.95	120.80
1	F	153	GLY	CA-C-N	-5.90	104.22	117.20
1	F	1044	VAL	CA-C-N	-5.87	104.29	117.20
1	F	1045	CYS	O-C-N	-5.86	113.32	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	301	GLU	O-C-N	-5.85	113.35	122.70
1	F	840	PHE	CB-CG-CD1	5.79	124.85	120.80
1	F	247	ALA	N-CA-CB	5.78	118.19	110.10
1	F	197	VAL	N-CA-CB	-5.76	98.82	111.50
1	F	133	ARG	C-N-CD	-5.71	108.04	120.60
1	F	307	LEU	CB-CA-C	-5.68	99.41	110.20
1	F	828	TYR	CB-CG-CD1	5.65	124.39	121.00
1	F	12	PHE	CB-CG-CD1	5.64	124.75	120.80
1	F	237	ILE	C-N-CA	5.63	135.77	121.70
1	F	302	ALA	N-CA-CB	-5.59	102.27	110.10
1	F	1837	PHE	N-CA-CB	5.58	120.65	110.60
1	F	924	PHE	CB-CG-CD2	-5.55	116.92	120.80
1	F	1155	ILE	N-CA-C	-5.55	96.02	111.00
1	F	840	PHE	CB-CG-CD2	-5.55	116.92	120.80
1	F	296	TYR	N-CA-CB	-5.53	100.65	110.60
1	F	1474	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	F	1851	ALA	N-CA-CB	5.51	117.82	110.10
1	F	1378	PHE	CB-CG-CD2	-5.50	116.95	120.80
1	F	199	PHE	N-CA-C	-5.49	96.18	111.00
1	F	292	ARG	O-C-N	-5.42	114.04	122.70
1	F	150	PHE	CB-CG-CD2	-5.40	117.02	120.80
1	F	1592	PHE	CB-CG-CD1	5.40	124.58	120.80
1	F	1226	LYS	N-CA-CB	5.38	120.29	110.60
1	F	236	SER	CA-C-N	5.34	128.95	117.20
1	F	1177	PRO	N-CA-C	-5.34	98.22	112.10
1	F	305	TYR	CB-CA-C	-5.26	99.87	110.40
1	F	1076	ALA	O-C-N	5.26	131.10	121.10
1	F	301	GLU	C-N-CA	5.23	134.77	121.70
1	F	803	PHE	N-CA-CB	5.21	119.99	110.60
1	F	1474	PHE	CB-CG-CD1	5.19	124.43	120.80
1	F	145	ALA	N-CA-CB	5.17	117.33	110.10
1	F	1257	ASN	C-N-CA	5.15	134.57	121.70
1	F	12	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	F	245	SER	N-CA-CB	5.12	118.19	110.50
1	F	1108	ALA	N-CA-C	5.12	124.83	111.00
1	F	806	ALA	N-CA-CB	5.09	117.23	110.10
1	F	302	ALA	N-CA-C	5.08	124.70	111.00
1	F	136	LEU	CB-CA-C	-5.05	100.60	110.20
1	F	1214	ARG	C-N-CA	5.05	134.32	121.70
1	F	199	PHE	O-C-N	-5.04	114.64	122.70
1	F	1137	SER	N-CA-C	-5.01	97.47	111.00
1	F	1592	PHE	CB-CG-CD2	-5.01	117.30	120.80

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	296	TYR	CA
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	Mainchain,Peptide
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	Mainchain,Peptide
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

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Mol	Chain	Res	Type	Group
1	F	1175	PRO	Peptide
1	F	1176	CYS	Peptide
1	F	1187	GLU	Peptide
1	F	1188	THR	Mainchain,Peptide
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	Mainchain,Peptide
1	F	1359	LEU	Peptide
1	F	136	LEU	Peptide
1	F	1369	ASN	Peptide
1	F	137	CYS	Mainchain,Peptide
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	Mainchain,Peptide
1	F	1465	SER	Peptide
1	F	1467	SER	Peptide
1	F	1471	SER	Peptide
1	F	152	ASP	Mainchain,Peptide
1	F	153	GLY	Mainchain
1	F	1580	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	F	163	PRO	Peptide
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	Mainchain,Peptide
1	F	194	PHE	Mainchain
1	F	195	HIS	Mainchain
1	F	198	PHE	Mainchain,Peptide
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

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Mol	Chain	Res	Type	Group
1	F	241	SER	Peptide
1	F	242	SER	Peptide
1	F	243	TYR	Peptide
1	F	244	TYR	Sidechain
1	F	257	PRO	Peptide
1	F	258	GLU	Mainchain,Peptide
1	F	259	PHE	Mainchain,Peptide
1	F	26	SER	Peptide
1	F	261	LEU	Peptide
1	F	262	MET	Mainchain
1	F	263	SER	Mainchain
1	F	264	ASP	Mainchain,Peptide
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	Sidechain,Peptide
1	F	294	ALA	Peptide
1	F	295	ASN	Mainchain
1	F	296	TYR	Sidechain,Peptide
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

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Mol	Chain	Res	Type	Group
1	F	827	GLU	Peptide
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	12078	344	0
2	F	1	0	0	0	0
3	F	27	0	12	18	0
All	All	12285	0	12090	344	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 (344) 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	1.48
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	1.43
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:HE2	1:F:301:GLU:OE2	1.35	1.24

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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:187:MET:HE2	1:F:193:ARG:HH11	0.99	1.09
1:F:1041:SER:CB	1:F:1217:GLU:HG3	1.83	1.08
1:F:139:MET:CE	1:F:301:GLU:CG	2.32	1.08
1:F:259:PHE:C	1:F:259:PHE:CG	2.27	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:139:MET:HE2	1:F:301:GLU:CD	1.77	1.05
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:139:MET:HE3	1:F:301:GLU:HG3	1.37	1.04
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:261:LEU:CD2	1:F:294:ALA:HB3	1.89	1.02
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:139:MET:CE	1:F:301:GLU:CD	2.31	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: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:139:MET:HE2	1:F:301:GLU:CG	1.96	0.94
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:187:MET:HE2	1:F:193:ARG:NH1	1.83	0.92
1:F:300:ASP:N	1:F:301:GLU:HA	1.84	0.91
1:F:259:PHE:C	1:F:259:PHE:CB	2.37	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:139:MET:HE3	1:F:301:GLU:CG	1.96	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: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	0.83
1:F:184:LEU:HD13	1:F:235:LEU:CG	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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: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: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: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:1697:ARG:CG	3:F:2202:ADP:O4'	2.37	0.73
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:1195:LEU:C	1:F:1217:GLU:OE1	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1106:TYR:CD2	1:F:1119:ASP:C	2.63	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:1136:LEU:C	1:F:1137:SER:O	2.27	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:306:ARG:N	1:F:306:ARG:C	2.46	0.68
1:F:286:ASN:ND2	1:F:306:ARG:HH12	1.90	0.68
1:F:295:ASN:CG	1:F:303:ASN:HD22	1.97	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:259:PHE:C	1:F:259:PHE:CD1	2.67	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
1:F:144:SER:HA	1:F:145:ALA:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1025:PRO:HG3	1:F:1029:GLN:CD	2.19	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: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: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: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:1025:PRO:CG	1:F:1029:GLN:CD	2.72	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1041:SER:O	1:F:1042:ALA:HB2	2.04	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:140:PHE:CD2	1:F:187:MET:HE1	2.43	0.54
1:F:1155:ILE:HG22	1:F:1182:SER:CA	2.34	0.54
1:F:1106:TYR:CE2	1:F:1119:ASP:C	2.82	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:139:MET:HE3	1:F:301:GLU:CD	2.15	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:1106:TYR:CD2	1:F:1118:HIS:C	2.83	0.52
1:F:1108:ALA:O	1:F:1126:THR:HG22	2.10	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:302:ALA:C	1:F:303:ASN:OD1	2.48	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:262:MET:HG2	1:F:293:LYS:HZ3	1.75	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:1198:VAL:HG13	1:F:1771:VAL:HG21	1.93	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1106:TYR:HD2	1:F:1118:HIS:C	2.16	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:1043:VAL:HG23	1:F:1180:ALA:C	2.35	0.47
1:F:1136:LEU:O	1:F:1137:SER:C	2.41	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: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: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:1041:SER:OG	1:F:1178:PHE:CE2	2.49	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:956:HIS:C	1:F:957:PHE:O	2.53	0.46
1:F:905:ARG:NH2	1:F:956:HIS:CE1	2.80	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1106:TYR:HD2	1:F:1119:ASP:C	2.16	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:140:PHE:CD2	1:F:187:MET:HE2	2.53	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:137:CYS:CA	1:F:138:ASP:CB	2.95	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:1030:ARG:HA	1:F:1030:ARG:HH21	1.86	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%)	<b>0</b> <b>10</b>

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
1	F	295	ASN
1	F	296	TYR

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Mol	Chain	Res	Type
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
1	F	935	ILE
1	F	957	PHE

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Mol	Chain	Res	Type
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
1	F	1751	HIS
1	F	1783	ALA

*Continued on next page...*

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Mol	Chain	Res	Type
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
1	F	1557	ARG
1	F	867	VAL

*Continued on next page...*

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Mol	Chain	Res	Type
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%)	1278 (97%)	40 (3%)	41 64

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	64	ASP
1	F	137	CYS
1	F	138	ASP
1	F	140	PHE
1	F	158	MET
1	F	199	PHE
1	F	207	GLU
1	F	259	PHE
1	F	298	ASP
1	F	301	GLU
1	F	303	ASN
1	F	305	TYR
1	F	308	ARG
1	F	316	GLU
1	F	798	LEU
1	F	840	PHE
1	F	866	ILE
1	F	924	PHE
1	F	941	ARG
1	F	1029	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	F	1030	ARG
1	F	1054	PHE
1	F	1055	ILE
1	F	1122	GLN
1	F	1132	GLU
1	F	1134	MET
1	F	1202	LEU
1	F	1216	PHE
1	F	1240	LEU
1	F	1247	LEU
1	F	1341	ARG
1	F	1378	PHE
1	F	1431	GLN
1	F	1526	ASN
1	F	1558	LEU
1	F	1587	ASP
1	F	1697	ARG
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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	286	ASN
1	F	675	ASN
1	F	850	HIS
1	F	989	GLN
1	F	1122	GLN
1	F	1161	ASN
1	F	1199	GLN
1	F	1632	HIS
1	F	1729	ASN
1	F	1731	GLN
1	F	1808	HIS

### 5.3.3 RNA ⓘ

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 monosaccharides 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	24,29,29	0.83	0	29,45,45	1.37	3 (10%)

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	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2202	ADP	O3'-C3'-C4'	-4.37	98.40	111.05
3	F	2202	ADP	PA-O3A-PB	3.97	146.45	132.83
3	F	2202	ADP	O3B-PB-O2B	2.40	116.82	107.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

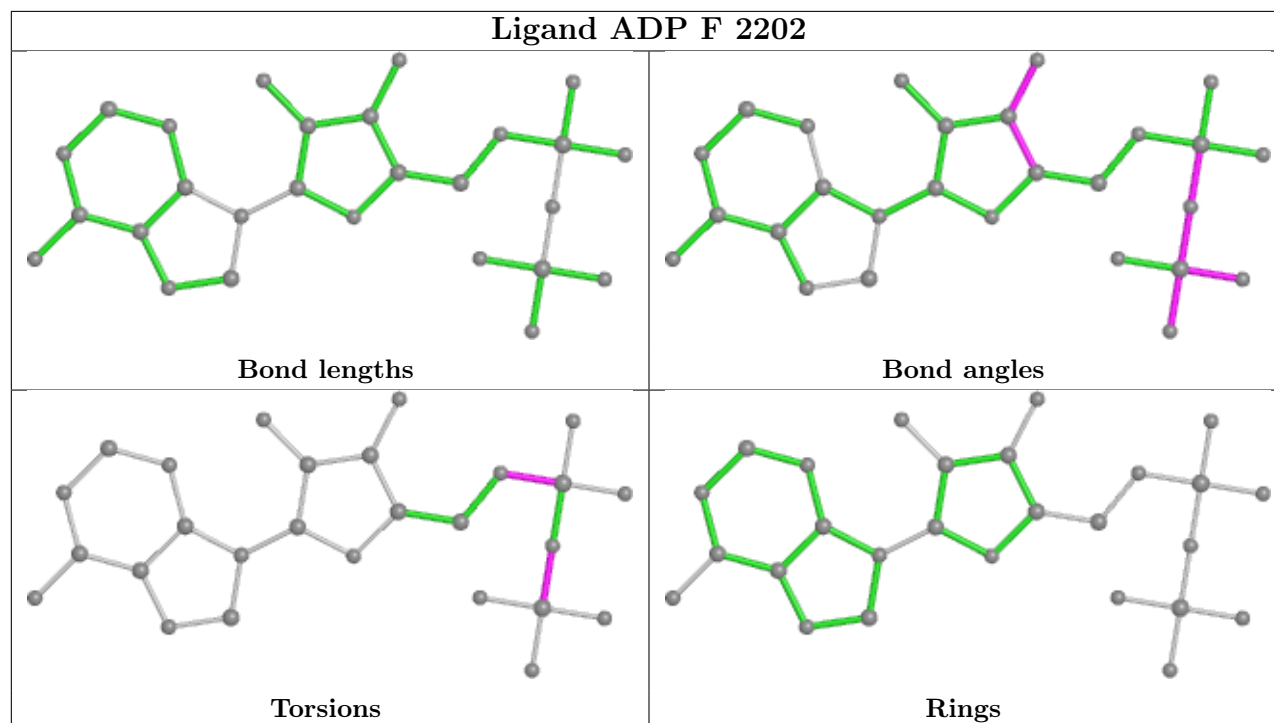
Mol	Chain	Res	Type	Atoms
3	F	2202	ADP	PA-O3A-PB-O3B
3	F	2202	ADP	C5'-O5'-PA-O1A

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
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

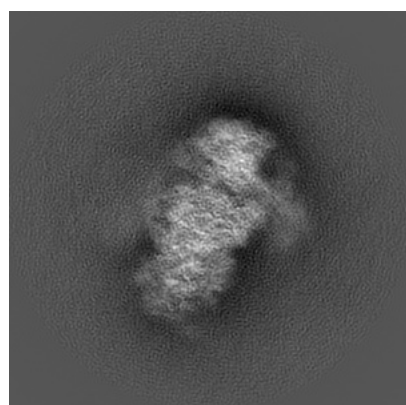
## 6 Map visualisation [i](#)

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.

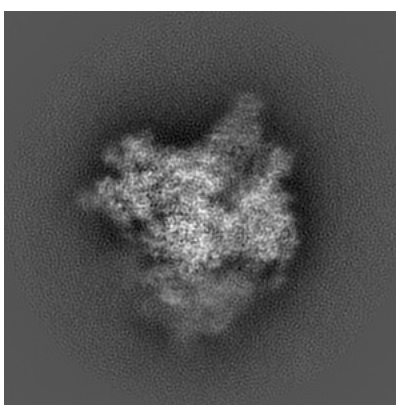
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

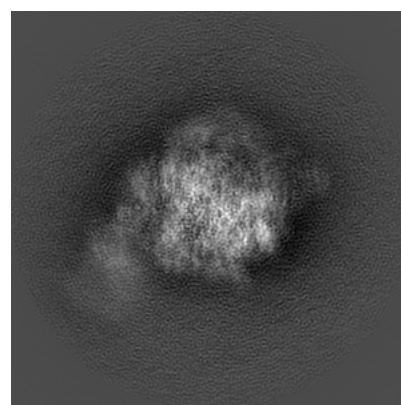
#### 6.1.1 Primary map



X



Y

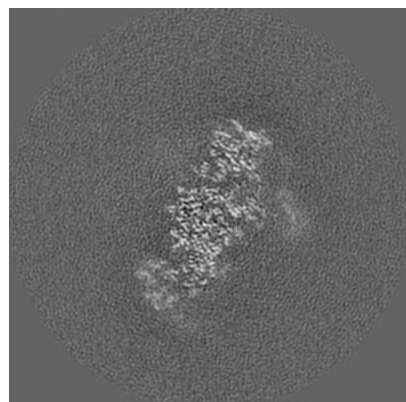


Z

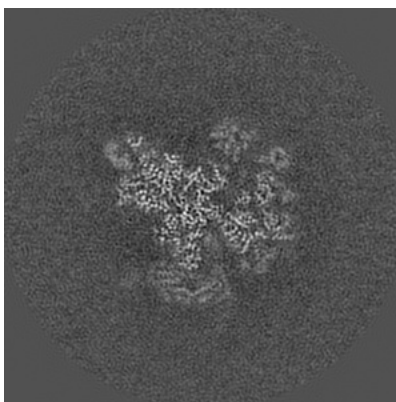
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

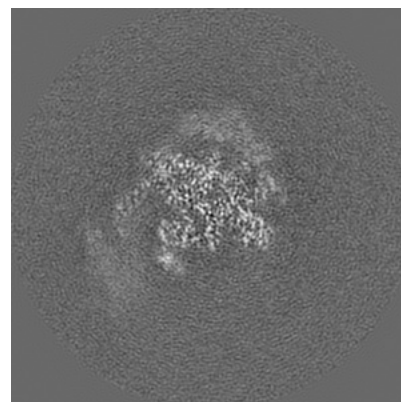
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

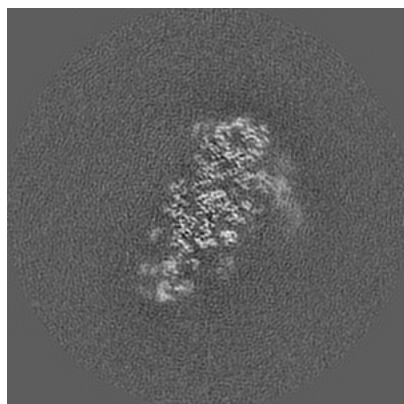


Z Index: 150

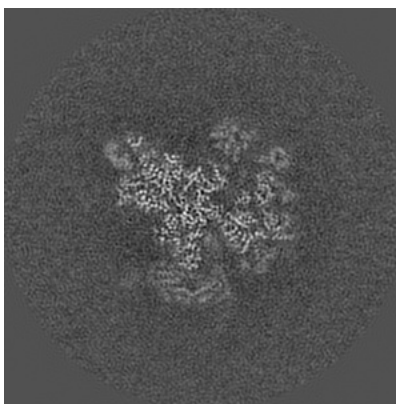
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

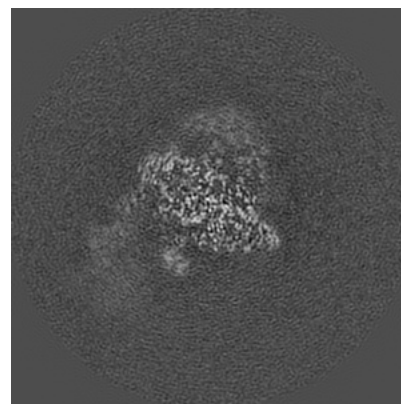
### 6.3.1 Primary map



X Index: 144



Y Index: 150

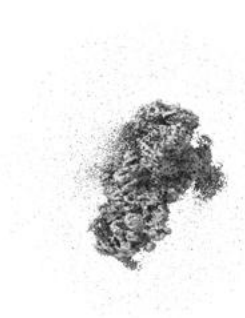


Z Index: 146

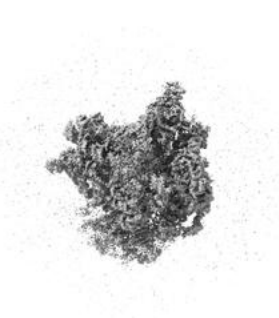
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

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.

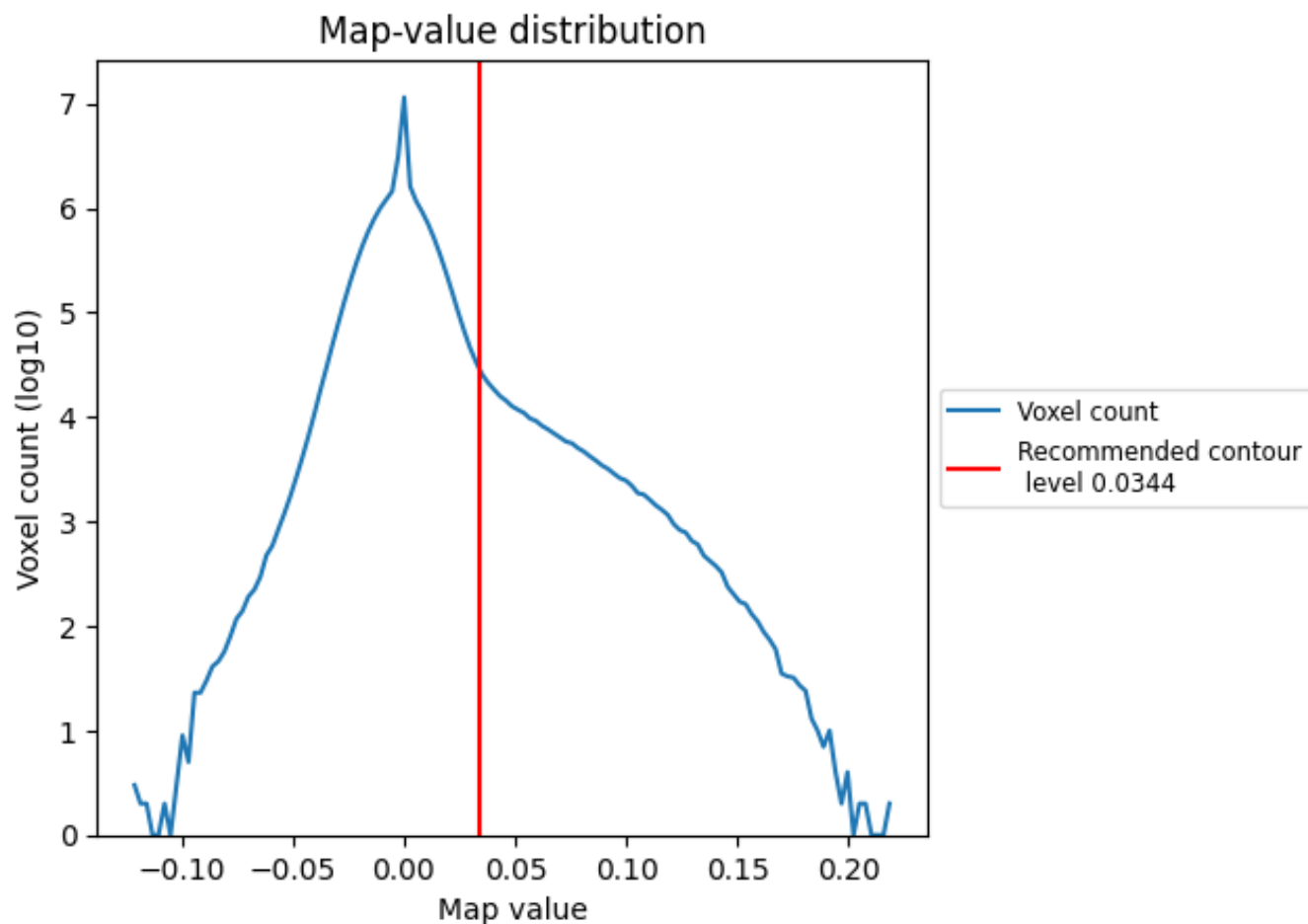
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

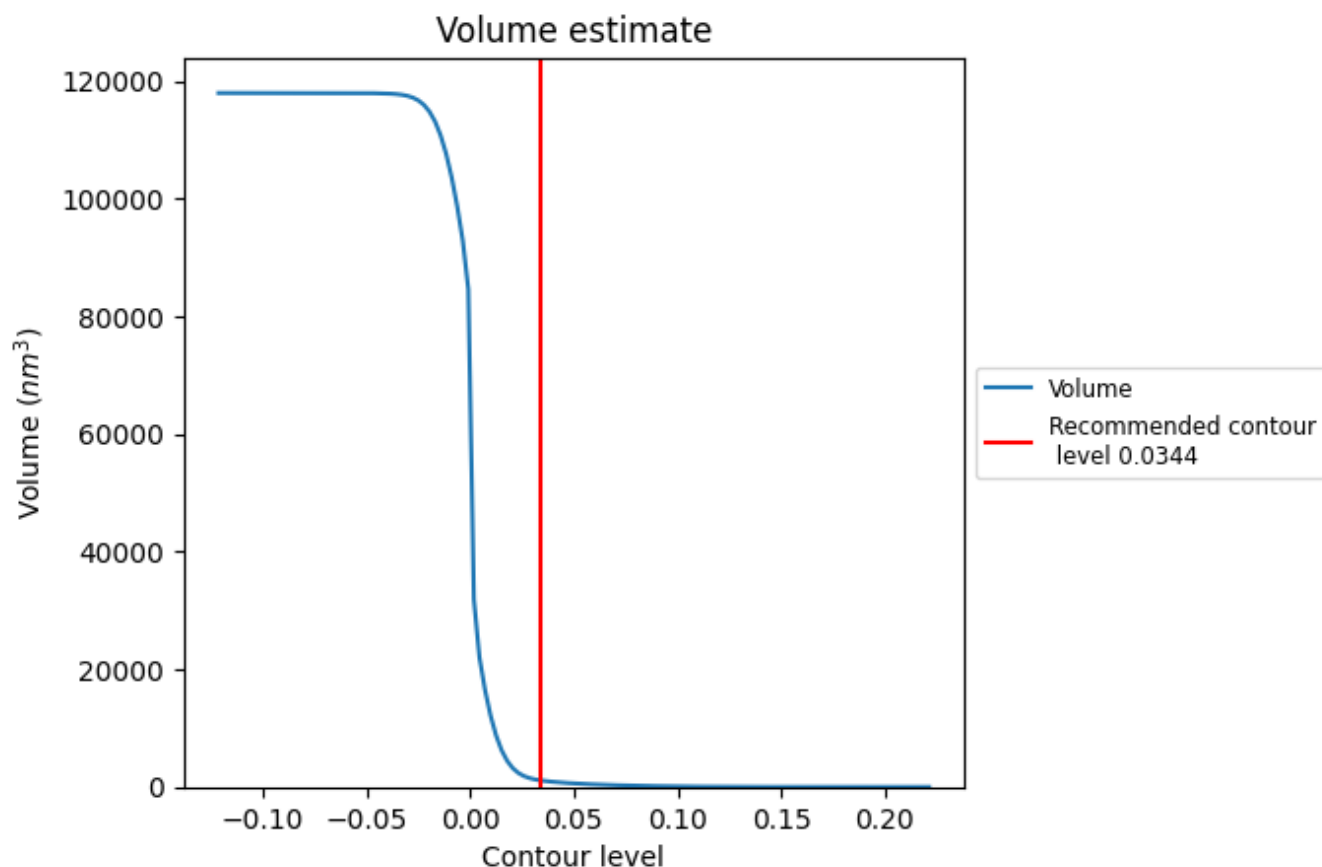
This section contains the results of statistical analysis of the map.

### 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](#)

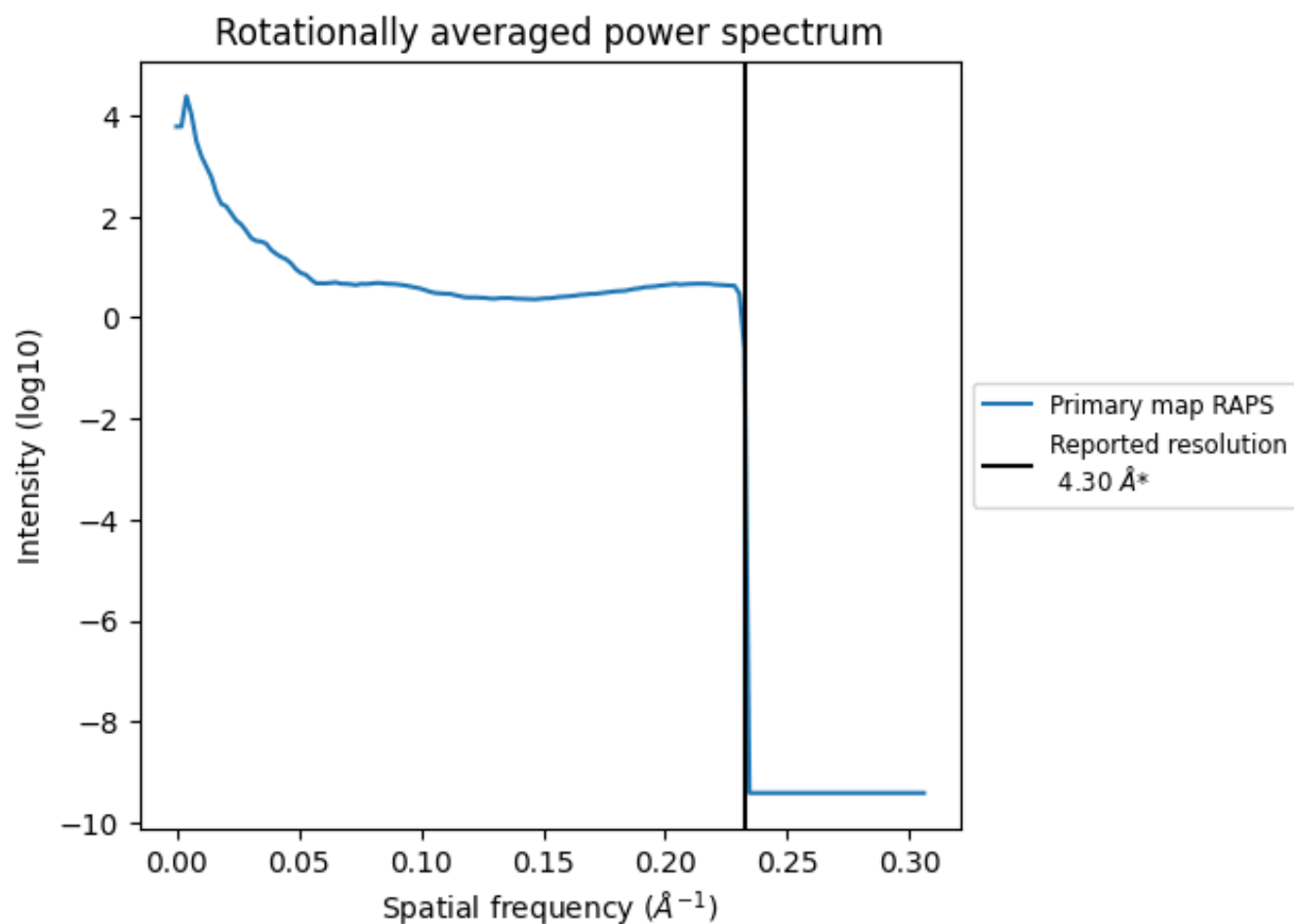


The volume at the recommended contour level is 1092 nm<sup>3</sup>; this corresponds to an approximate mass of 986 kDa.

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<sup>-1</sup>

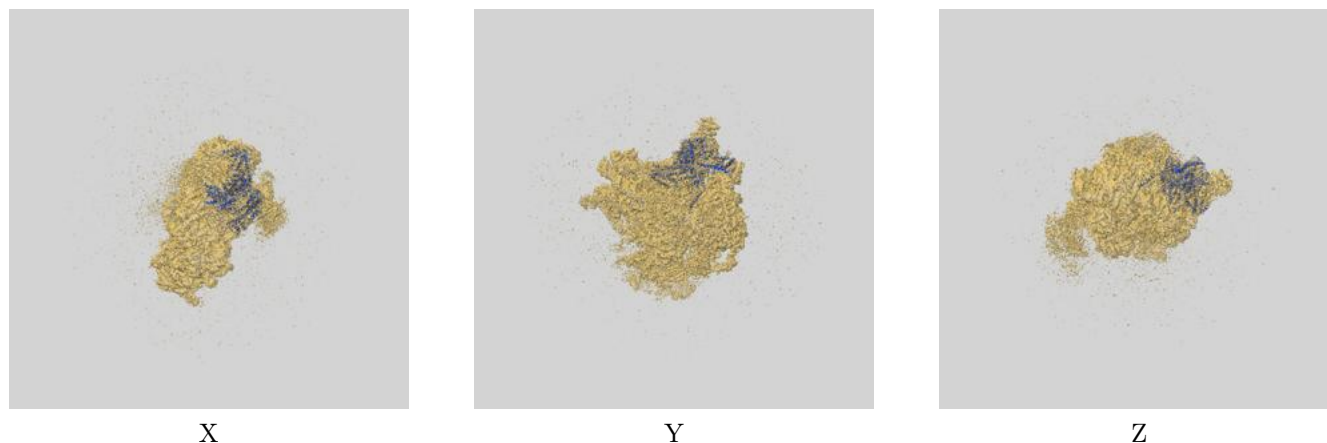
## 8 Fourier-Shell correlation

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 4](#).

### 9.1 Map-model overlay [i](#)



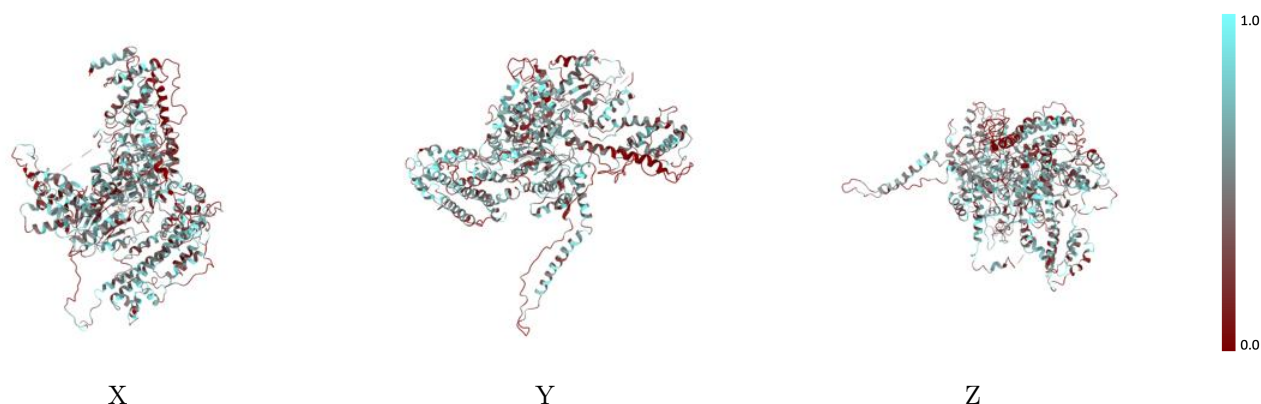
The images above show the 3D surface view of the map at the recommended contour level 0.0344 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



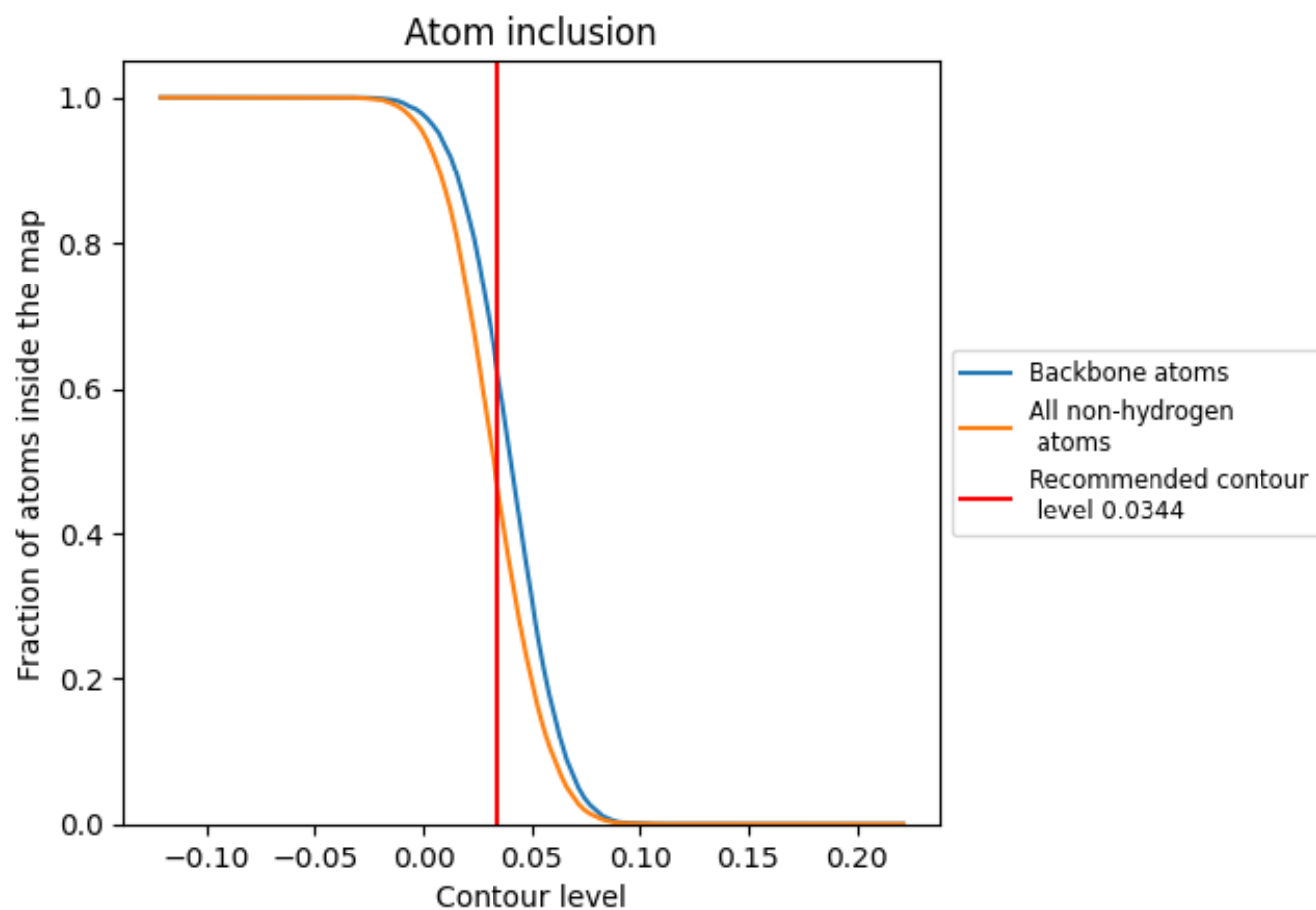
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.4616	<div></div> 0.2720
F	<div></div> 0.4616	<div></div> 0.2720

