



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 05:35 AM UTC

PDB ID : 6JMA / pdb_00006jma
EMDB ID : EMD-9844
Title : cryo-EM structure of DOT1L bound to H2B ubiquitinated nucleosome
Authors : Jang, S.; Song, J.J.
Deposited on : 2019-03-07
Resolution : 6.80 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:

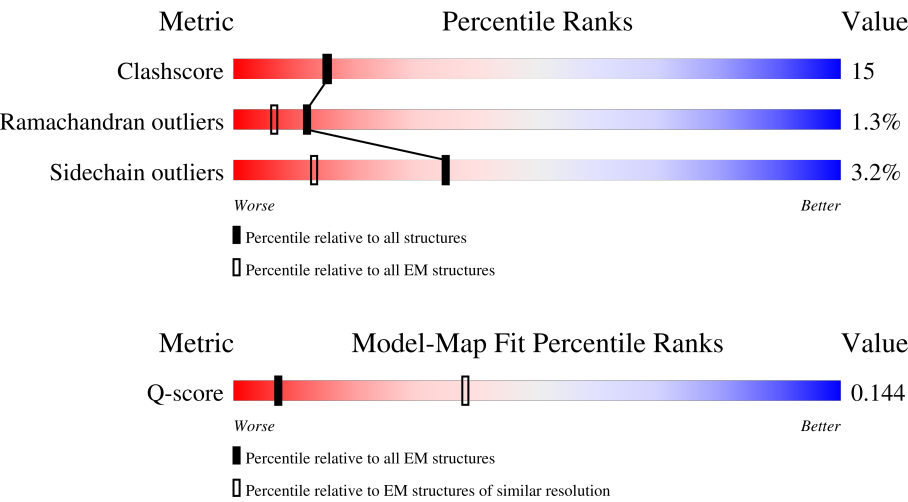
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 6.80 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	503 (6.30 - 7.30)

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	I	114	
1	J	114	
2	A	98	
2	E	98	

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Mol	Chain	Length	Quality of chain
3	B	87	
3	F	87	
4	C	116	
4	G	116	
5	D	94	
5	H	94	
6	X	328	
7	Y	76	

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
8	SAM	X	500	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14060 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 DNA chain called DNA I&J.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	114	Total	C	N	O	P	0	0
			2337	1118	421	684	114		
1	J	114	Total	C	N	O	P	0	0
			2337	1118	421	684	114		

- Molecule 2 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	98	Total	C	N	O	S	0	0
			807	508	156	140	3		
2	E	98	Total	C	N	O	S	0	0
			807	508	156	140	3		

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
3	F	87	Total	C	N	O	S	0	0
			703	442	142	118	1		

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	107	Total	C	N	O	0	0
			825	520	161	144		
4	G	106	Total	C	N	O	0	0
			818	516	160	142		

- Molecule 5 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	94	Total	C	N	O	S	0	0
			736	463	132	139	2		
5	H	94	Total	C	N	O	S	0	0
			736	463	132	139	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	-	expression tag	UNP P02281
H	29	THR	-	expression tag	UNP P02281

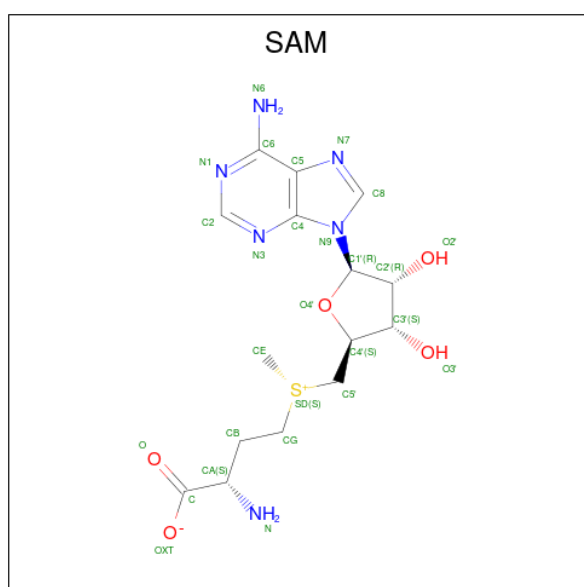
- Molecule 6 is a protein called Histone-lysine N-methyltransferase, H3 lysine-79 specific.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	328	Total	C	N	O	S	0	0
			2672	1706	455	499	12		

- Molecule 7 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	76	Total	C	N	O	S	0	0
			602	378	105	118	1		

- Molecule 8 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).

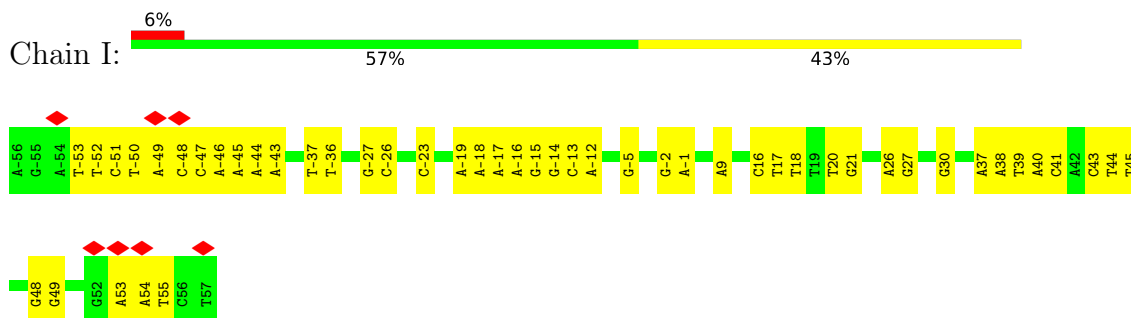


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
8	X	1	27	15	6	5	1	0

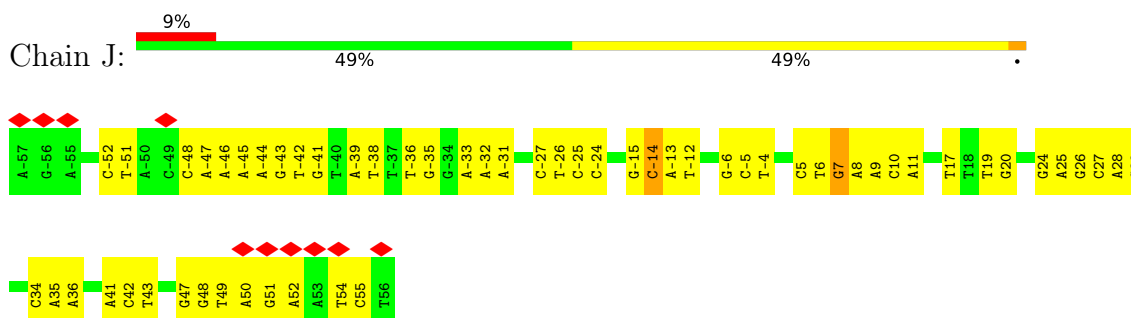
3 Residue-property plots [i](#)

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.

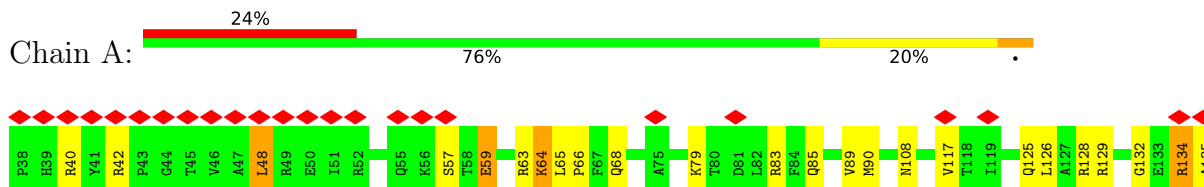
• Molecule 1: DNA I&J



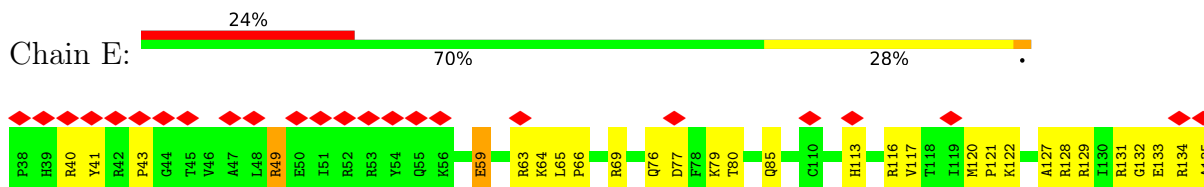
• Molecule 1: DNA I&J



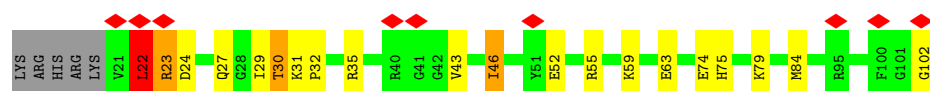
• Molecule 2: Histone H3.2



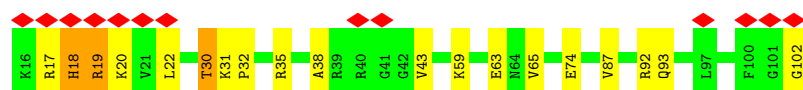
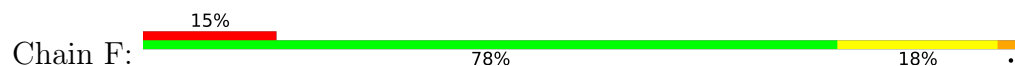
• Molecule 2: Histone H3.2



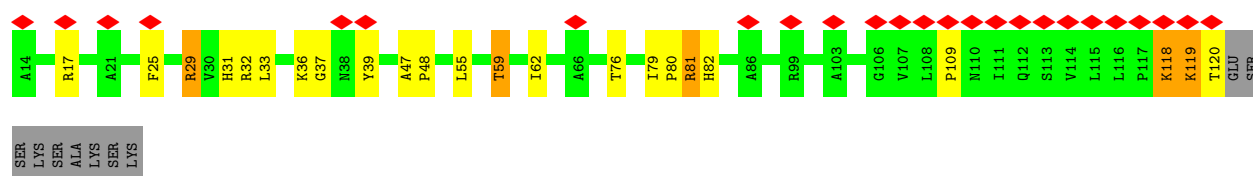
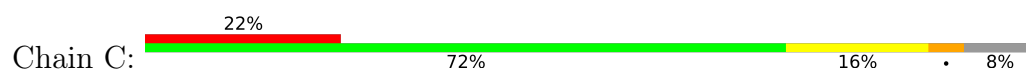
• Molecule 3: Histone H4



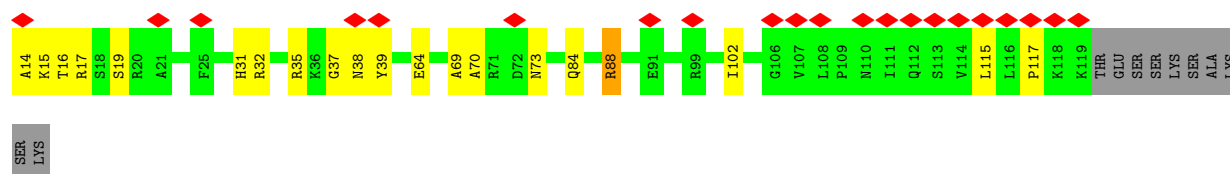
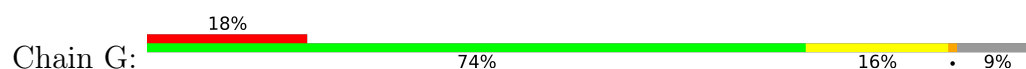
- Molecule 3: Histone H4



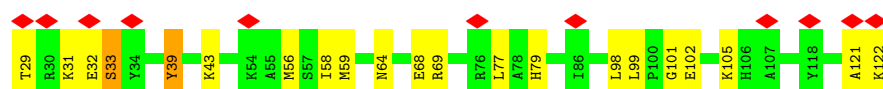
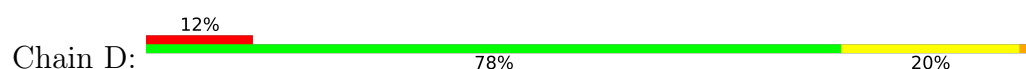
- Molecule 4: Histone H2A



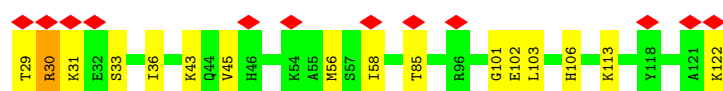
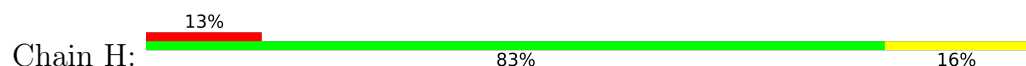
- Molecule 4: Histone H2A



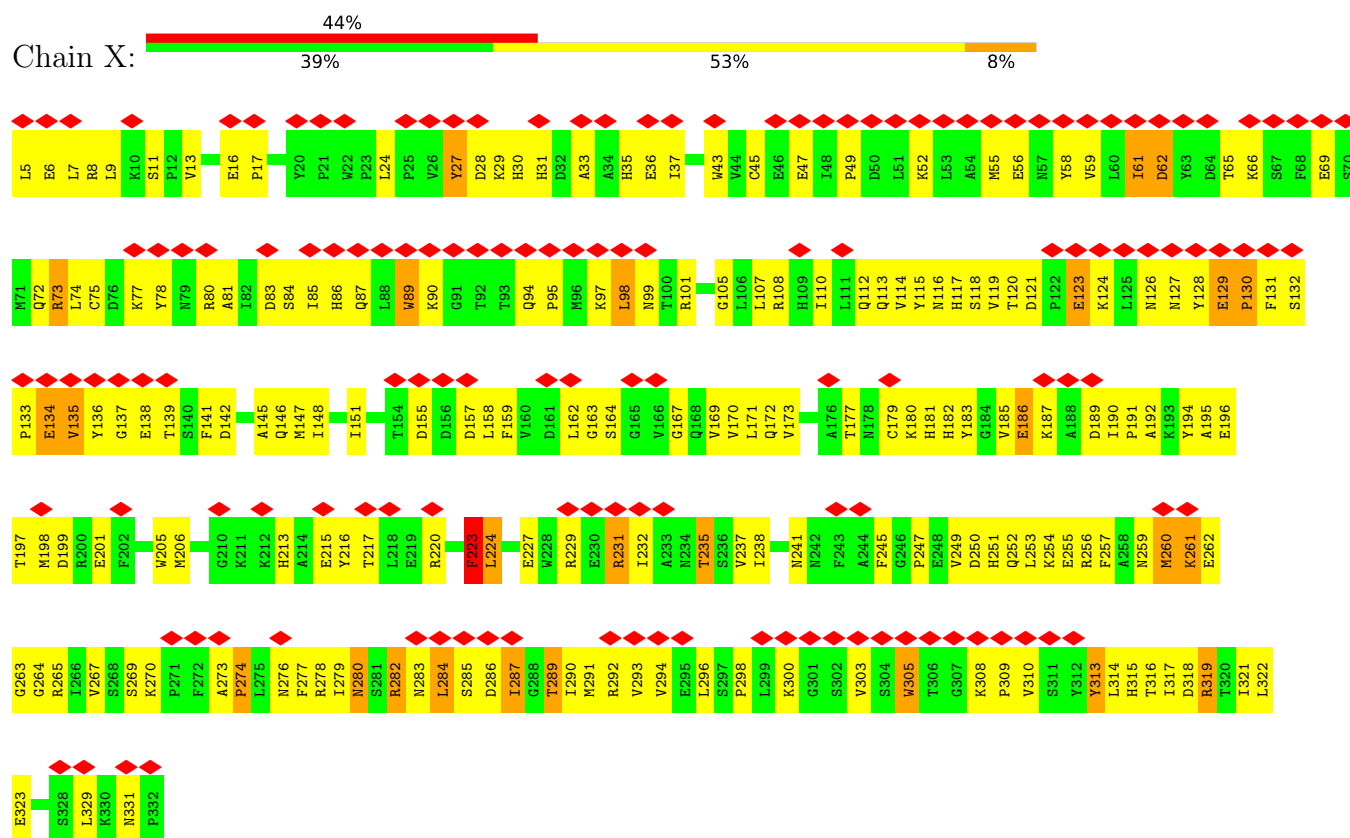
- Molecule 5: Histone H2B 1.1



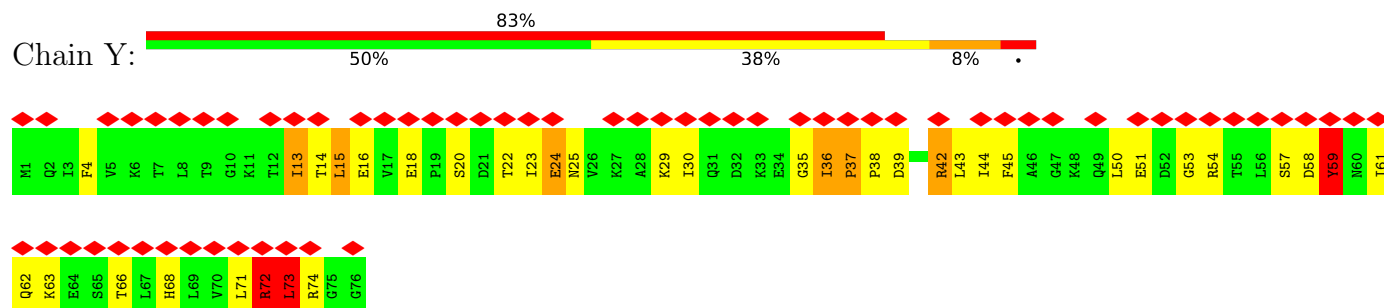
- Molecule 5: Histone H2B 1.1



- Molecule 6: Histone-lysine N-methyltransferase, H3 lysine-79 specific



• Molecule 7: Ubiquitin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	122242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37.28	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	0.105	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0251	Depositor
Map size ($\text{\AA}$)	233.19998, 233.19998, 233.19998	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	I	0.29	0/2621	0.67	0/4043
1	J	0.31	0/2621	0.69	2/4043 (0.0%)
2	A	0.67	0/819	1.04	4/1097 (0.4%)
2	E	0.85	0/819	1.07	4/1097 (0.4%)
3	B	0.72	0/660	1.03	4/883 (0.5%)
3	F	0.87	0/711	1.04	2/948 (0.2%)
4	C	0.82	0/835	1.00	1/1127 (0.1%)
4	G	0.65	0/828	0.91	1/1117 (0.1%)
5	D	0.85	1/747 (0.1%)	1.04	1/1004 (0.1%)
5	H	0.71	1/747 (0.1%)	0.93	1/1004 (0.1%)
6	X	2.28	107/2742 (3.9%)	2.49	217/3718 (5.8%)
7	Y	2.20	21/608 (3.5%)	2.36	33/816 (4.0%)
All	All	1.20	130/14758 (0.9%)	1.38	270/20897 (1.3%)

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	J	0	2
5	D	0	1
6	X	0	6
7	Y	0	6
All	All	0	15

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	118	SER	CA-C	-12.88	1.43	1.52
6	X	159	PHE	CA-C	-8.54	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	74	LEU	C-N	8.37	1.44	1.33
6	X	303	VAL	N-CA	-8.31	1.36	1.46
7	Y	13	ILE	CA-C	-8.12	1.43	1.52
6	X	294	VAL	CA-C	-7.96	1.43	1.52
6	X	276	ASN	C-N	7.70	1.43	1.33
6	X	285	SER	CA-C	-7.69	1.42	1.52
7	Y	68	HIS	CA-C	-7.68	1.43	1.52
6	X	87	GLN	N-CA	7.58	1.55	1.46
6	X	201	GLU	C-N	7.51	1.43	1.33
6	X	215	GLU	N-CA	-7.49	1.36	1.46
7	Y	51	GLU	CA-C	-7.47	1.43	1.52
6	X	292	ARG	CA-CB	7.47	1.64	1.53
6	X	59	VAL	CA-C	-7.44	1.43	1.52
6	X	255	GLU	CA-CB	7.23	1.65	1.53
6	X	229	ARG	CD-NE	7.02	1.56	1.46
6	X	220	ARG	CD-NE	7.00	1.56	1.46
6	X	11	SER	CA-C	7.00	1.61	1.52
6	X	116	ASN	CA-CB	6.98	1.64	1.53
6	X	319	ARG	CZ-NH2	6.98	1.42	1.33
7	Y	57	SER	N-CA	-6.97	1.37	1.46
6	X	7	LEU	C-N	6.95	1.44	1.33
6	X	215	GLU	C-N	6.94	1.42	1.33
6	X	263	GLY	C-N	6.91	1.41	1.33
7	Y	15	LEU	CA-C	-6.90	1.44	1.52
6	X	124	LYS	C-N	6.82	1.43	1.33
6	X	85	ILE	N-CA	-6.80	1.38	1.46
6	X	247	PRO	N-CD	6.76	1.57	1.47
7	Y	15	LEU	N-CA	-6.76	1.37	1.46
6	X	217	THR	CA-C	-6.71	1.44	1.52
6	X	105	GLY	CA-C	-6.68	1.44	1.52
6	X	190	ILE	CA-C	-6.64	1.46	1.52
6	X	263	GLY	CA-C	-6.58	1.42	1.51
6	X	75	CYS	C-N	6.54	1.42	1.33
6	X	291	MET	N-CA	-6.52	1.38	1.46
6	X	257	PHE	CA-C	-6.49	1.43	1.52
6	X	132	SER	CA-C	-6.42	1.46	1.52
6	X	249	VAL	CA-CB	-6.41	1.46	1.54
6	X	108	ARG	NE-CZ	6.40	1.40	1.33
6	X	192	ALA	N-CA	-6.38	1.38	1.46
6	X	30	HIS	CE1-NE2	-6.34	1.26	1.32
6	X	313	TYR	N-CA	-6.30	1.38	1.46
6	X	77	LYS	C-N	6.30	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	293	VAL	N-CA	-6.25	1.39	1.46
6	X	298	PRO	C-N	6.20	1.42	1.33
6	X	309	PRO	CA-C	-6.15	1.45	1.52
6	X	56	GLU	N-CA	-6.13	1.38	1.46
6	X	197	THR	CA-CB	6.09	1.62	1.53
6	X	186	GLU	C-N	6.06	1.42	1.33
6	X	279	ILE	N-CA	-6.05	1.39	1.46
6	X	7	LEU	CA-C	6.03	1.59	1.52
6	X	167	GLY	C-O	-6.03	1.16	1.24
6	X	181	HIS	CA-C	-6.01	1.45	1.52
6	X	251	HIS	C-N	5.99	1.42	1.33
7	Y	44	ILE	N-CA	-5.96	1.39	1.46
6	X	5	LEU	N-CA	5.96	1.57	1.46
6	X	251	HIS	CE1-NE2	5.96	1.38	1.32
6	X	181	HIS	ND1-CE1	5.95	1.38	1.32
6	X	99	ASN	CA-C	5.94	1.60	1.52
6	X	171	LEU	CA-CB	5.93	1.62	1.53
7	Y	68	HIS	ND1-CE1	5.92	1.38	1.32
6	X	115	TYR	CA-CB	5.88	1.62	1.53
6	X	52	LYS	CA-CB	5.87	1.62	1.53
6	X	172	GLN	C-N	5.87	1.41	1.33
7	Y	68	HIS	CB-CG	5.86	1.58	1.50
6	X	284	LEU	CA-CB	5.85	1.62	1.53
6	X	141	PHE	N-CA	-5.84	1.39	1.46
6	X	162	LEU	C-N	5.83	1.40	1.33
6	X	72	GLN	C-O	5.79	1.31	1.24
6	X	296	LEU	CA-C	-5.79	1.45	1.52
6	X	187	LYS	N-CA	-5.79	1.39	1.46
6	X	134	GLU	CA-C	-5.76	1.45	1.52
7	Y	24	GLU	CA-CB	5.76	1.62	1.53
6	X	113	GLN	CA-CB	5.72	1.62	1.53
6	X	138	GLU	CA-C	-5.72	1.45	1.52
7	Y	62	GLN	N-CA	-5.71	1.38	1.46
5	H	56	MET	SD-CE	5.67	1.93	1.79
6	X	66	LYS	N-CA	-5.66	1.38	1.46
6	X	117	HIS	ND1-CE1	5.64	1.38	1.32
6	X	286	ASP	C-N	5.62	1.40	1.33
6	X	250	ASP	C-N	5.59	1.41	1.33
6	X	119	VAL	CA-C	5.58	1.59	1.52
6	X	33	ALA	N-CA	-5.52	1.39	1.46
6	X	232	ILE	CA-CB	-5.52	1.47	1.54
6	X	251	HIS	ND1-CE1	5.52	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	260	MET	N-CA	5.49	1.52	1.46
7	Y	13	ILE	N-CA	-5.49	1.39	1.46
6	X	151	ILE	CA-C	-5.46	1.46	1.52
6	X	314	LEU	CA-C	-5.42	1.46	1.52
6	X	157	ASP	CA-CB	5.39	1.62	1.53
6	X	130	PRO	N-CA	-5.38	1.41	1.46
6	X	185	VAL	N-CA	-5.34	1.40	1.46
6	X	292	ARG	CZ-NH1	5.34	1.40	1.32
6	X	181	HIS	CA-CB	5.33	1.62	1.53
6	X	317	ILE	CA-CB	-5.32	1.47	1.53
6	X	116	ASN	C-N	5.31	1.41	1.33
6	X	89	TRP	CA-CB	-5.31	1.44	1.53
6	X	162	LEU	CA-C	5.30	1.59	1.52
7	Y	42	ARG	CD-NE	5.26	1.53	1.46
5	D	56	MET	SD-CE	5.26	1.92	1.79
6	X	148	ILE	N-CA	-5.24	1.40	1.46
6	X	47	GLU	CA-CB	5.22	1.61	1.53
6	X	238	ILE	CA-C	-5.21	1.46	1.52
6	X	78	TYR	CA-C	-5.21	1.46	1.52
6	X	179	CYS	N-CA	-5.21	1.39	1.45
6	X	127	ASN	CA-CB	5.20	1.59	1.53
6	X	269	SER	C-N	5.20	1.38	1.33
7	Y	39	ASP	CA-CB	5.20	1.61	1.53
7	Y	35	GLY	C-N	5.20	1.37	1.33
6	X	255	GLU	N-CA	-5.20	1.39	1.46
6	X	259	ASN	C-N	5.18	1.40	1.33
6	X	8	ARG	CZ-NH2	5.18	1.40	1.33
6	X	145	ALA	N-CA	-5.17	1.40	1.46
6	X	145	ALA	C-N	5.16	1.41	1.33
6	X	124	LYS	CA-CB	5.15	1.62	1.53
7	Y	25	ASN	CA-CB	5.15	1.61	1.53
6	X	305	TRP	C-N	5.14	1.41	1.33
6	X	147	MET	N-CA	-5.13	1.40	1.46
7	Y	72	ARG	N-CA	-5.11	1.39	1.46
6	X	196	GLU	N-CA	-5.09	1.40	1.46
6	X	86	HIS	CB-CG	5.08	1.57	1.50
6	X	206	MET	C-N	5.06	1.40	1.33
7	Y	58	ASP	C-N	5.05	1.40	1.33
7	Y	43	LEU	N-CA	-5.04	1.39	1.46
7	Y	29	LYS	CA-C	-5.04	1.46	1.52
6	X	24	LEU	C-N	-5.03	1.29	1.33
6	X	285	SER	CA-CB	5.03	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	110	ILE	CA-C	5.01	1.59	1.52
7	Y	36	ILE	CA-CB	5.00	1.60	1.54

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	16	GLU	CA-C-N	11.08	133.69	119.84
6	X	16	GLU	C-N-CA	11.08	133.69	119.84
6	X	287	ILE	N-CA-C	-9.66	102.99	112.17
6	X	173	VAL	CA-C-O	-9.25	111.05	120.85
6	X	146	GLN	N-CA-C	-9.19	101.35	111.36
6	X	132	SER	O-C-N	-8.89	116.02	121.71
2	A	64	LYS	N-CA-C	8.56	120.30	110.97
2	A	117	VAL	N-CA-C	-8.49	105.05	113.20
6	X	231	ARG	CA-C-N	8.23	131.74	120.46
6	X	231	ARG	C-N-CA	8.23	131.74	120.46
6	X	33	ALA	CB-CA-C	-8.13	97.30	110.79
2	E	117	VAL	N-CA-C	-8.12	105.23	113.10
2	A	85	GLN	N-CA-C	-8.07	99.88	110.53
6	X	182	HIS	CA-CB-CG	8.04	121.84	113.80
6	X	173	VAL	O-C-N	8.00	130.07	121.83
6	X	30	HIS	ND1-CE1-NE2	7.80	116.20	108.40
6	X	201	GLU	CA-C-N	7.79	130.94	120.65
6	X	201	GLU	C-N-CA	7.79	130.94	120.65
6	X	205	TRP	N-CA-C	7.69	119.75	111.36
6	X	142	ASP	CA-CB-CG	-7.67	104.93	112.60
6	X	170	VAL	CA-C-N	7.67	130.55	120.28
6	X	170	VAL	C-N-CA	7.67	130.55	120.28
6	X	33	ALA	N-CA-C	7.63	119.60	111.28
6	X	29	LYS	CA-C-N	7.62	133.63	121.98
6	X	29	LYS	C-N-CA	7.62	133.63	121.98
6	X	267	VAL	N-CA-C	-7.61	97.51	108.17
6	X	237	VAL	CA-C-O	7.50	126.90	120.22
6	X	315	HIS	CA-C-O	-7.42	112.68	120.70
7	Y	25	ASN	CA-C-N	7.34	129.81	120.56
7	Y	25	ASN	C-N-CA	7.34	129.81	120.56
6	X	315	HIS	CA-CB-CG	7.27	121.07	113.80
6	X	62	ASP	CA-CB-CG	-7.17	105.42	112.60
2	E	64	LYS	N-CA-C	7.15	118.86	111.14
6	X	98	LEU	N-CA-C	-7.13	104.52	112.57
6	X	117	HIS	CA-CB-CG	7.08	120.88	113.80
6	X	113	GLN	OE1-CD-NE2	7.08	129.68	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	147	MET	N-CA-C	7.06	118.63	111.07
6	X	274	PRO	CA-C-N	7.06	129.74	120.28
6	X	274	PRO	C-N-CA	7.06	129.74	120.28
6	X	182	HIS	O-C-N	-6.96	115.02	123.30
6	X	171	LEU	CA-C-N	6.92	129.44	120.44
6	X	171	LEU	C-N-CA	6.92	129.44	120.44
3	B	29	ILE	N-CA-C	-6.91	96.57	107.15
6	X	114	VAL	O-C-N	-6.90	115.18	121.87
6	X	69	GLU	CA-C-N	6.85	130.72	120.31
6	X	69	GLU	C-N-CA	6.85	130.72	120.31
6	X	189	ASP	N-CA-CB	6.83	119.92	110.01
6	X	289	THR	N-CA-C	-6.80	104.31	114.64
6	X	280	ASN	OD1-CG-ND2	-6.79	115.81	122.60
6	X	182	HIS	CA-C-O	6.77	127.67	120.36
6	X	28	ASP	N-CA-C	-6.73	99.36	108.24
6	X	164	SER	N-CA-C	6.68	125.03	110.80
6	X	117	HIS	CE1-NE2-CD2	-6.68	102.32	109.00
6	X	107	LEU	CA-C-N	6.68	129.23	120.28
6	X	107	LEU	C-N-CA	6.68	129.23	120.28
5	D	99	LEU	N-CA-C	6.64	118.44	110.07
6	X	65	THR	CA-C-O	-6.63	112.34	119.97
7	Y	44	ILE	CB-CA-C	6.61	120.42	110.63
5	H	85	THR	N-CA-C	6.60	119.69	109.07
6	X	192	ALA	N-CA-C	6.60	118.47	111.28
6	X	276	ASN	OD1-CG-ND2	6.58	129.18	122.60
6	X	84	SER	CA-C-O	-6.57	113.58	120.55
6	X	273	ALA	CA-C-N	6.56	128.04	119.84
6	X	273	ALA	C-N-CA	6.56	128.04	119.84
6	X	171	LEU	O-C-N	6.54	129.05	122.12
1	J	-14	DC	C5'-C4'-C3'	-6.52	105.12	114.90
6	X	296	LEU	N-CA-CB	6.47	120.12	110.29
6	X	321	ILE	N-CA-C	6.46	116.62	110.42
6	X	135	VAL	N-CA-CB	6.43	117.89	110.49
6	X	280	ASN	CA-CB-CG	-6.43	106.17	112.60
6	X	80	ARG	N-CA-C	-6.42	104.36	111.36
6	X	190	ILE	O-C-N	-6.41	113.79	121.10
6	X	181	HIS	CA-CB-CG	6.40	120.20	113.80
6	X	251	HIS	CE1-NE2-CD2	-6.40	102.60	109.00
6	X	331	ASN	CA-C-O	-6.40	114.84	120.60
6	X	97	LYS	O-C-N	6.38	130.44	123.10
6	X	308	LYS	N-CA-CB	6.37	121.99	111.17
6	X	198	MET	CA-C-N	6.35	128.78	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	198	MET	C-N-CA	6.35	128.78	120.28
6	X	280	ASN	N-CA-CB	6.34	121.21	110.49
6	X	155	ASP	CB-CA-C	6.34	122.09	110.36
6	X	190	ILE	CA-C-N	6.33	126.24	119.28
6	X	190	ILE	C-N-CA	6.33	126.24	119.28
6	X	181	HIS	CE1-NE2-CD2	-6.32	102.68	109.00
6	X	94	GLN	CA-C-O	-6.32	114.88	120.19
7	Y	20	SER	N-CA-CB	6.31	120.37	110.46
6	X	158	LEU	N-CA-C	-6.29	97.99	108.75
6	X	322	LEU	O-C-N	6.20	128.46	122.07
6	X	247	PRO	CA-C-N	6.20	128.50	120.44
6	X	247	PRO	C-N-CA	6.20	128.50	120.44
6	X	290	ILE	N-CA-C	-6.18	106.75	112.43
6	X	187	LYS	CA-C-O	-6.17	114.34	120.70
6	X	195	ALA	N-CA-C	6.17	118.00	111.28
6	X	145	ALA	CA-C-N	6.15	129.02	120.29
6	X	145	ALA	C-N-CA	6.15	129.02	120.29
6	X	116	ASN	CB-CA-C	-6.15	99.25	110.63
6	X	180	LYS	N-CA-CB	6.14	118.92	110.01
4	C	118	LYS	CB-CA-C	-6.14	108.49	115.79
6	X	27	TYR	CB-CG-CD1	6.14	130.01	120.80
7	Y	16	GLU	O-C-N	6.13	130.86	123.13
6	X	305	TRP	CA-CB-CG	6.11	125.21	113.60
6	X	59	VAL	N-CA-C	-6.11	99.32	108.12
6	X	186	GLU	CA-C-O	6.09	127.77	120.28
6	X	315	HIS	CG-CD2-NE2	6.06	113.26	107.20
6	X	293	VAL	N-CA-C	-6.03	99.80	108.48
6	X	323	GLU	CA-C-O	-6.02	114.17	120.55
6	X	128	TYR	N-CA-CB	6.01	120.70	111.56
6	X	329	LEU	CB-CA-C	-6.00	97.45	109.99
7	Y	36	ILE	CA-C-O	-6.00	114.82	119.20
6	X	127	ASN	CB-CA-C	-5.96	101.60	110.67
6	X	130	PRO	CA-C-O	-5.96	114.80	122.13
6	X	37	ILE	CA-C-N	5.95	128.62	120.46
6	X	37	ILE	C-N-CA	5.95	128.62	120.46
6	X	7	LEU	N-CA-C	-5.89	98.26	108.69
6	X	31	HIS	CA-CB-CG	-5.89	107.91	113.80
6	X	87	GLN	N-CA-C	-5.86	104.97	111.36
3	F	92	ARG	CB-CA-C	-5.86	101.06	110.79
6	X	270	LYS	CB-CA-C	-5.85	99.31	109.32
6	X	183	TYR	CA-C-O	5.84	128.27	121.44
2	E	85	GLN	N-CA-C	-5.83	101.65	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	75	CYS	CA-CB-SG	-5.82	101.01	114.40
3	B	30	THR	N-CA-C	5.82	118.40	110.55
6	X	98	LEU	N-CA-CB	5.81	120.09	110.91
6	X	319	ARG	N-CA-CB	5.81	119.83	110.42
6	X	216	TYR	O-C-N	-5.78	116.66	123.25
6	X	62	ASP	N-CA-C	-5.78	104.79	112.94
6	X	253	LEU	CA-C-N	5.76	128.00	120.28
6	X	253	LEU	C-N-CA	5.76	128.00	120.28
6	X	278	ARG	O-C-N	-5.76	116.30	123.04
7	Y	29	LYS	CA-C-O	-5.76	114.45	120.55
6	X	254	LYS	CA-C-O	-5.76	114.45	120.55
6	X	276	ASN	CA-C-N	5.74	129.26	121.05
6	X	276	ASN	C-N-CA	5.74	129.26	121.05
6	X	85	ILE	N-CA-C	5.74	116.47	110.62
6	X	31	HIS	CB-CG-CD2	-5.73	123.75	131.20
6	X	145	ALA	O-C-N	-5.73	116.04	122.12
6	X	227	GLU	CA-C-N	5.73	130.29	120.72
6	X	227	GLU	C-N-CA	5.73	130.29	120.72
6	X	86	HIS	CE1-NE2-CD2	-5.72	103.28	109.00
7	Y	23	ILE	CA-C-N	5.72	127.94	120.28
7	Y	23	ILE	C-N-CA	5.72	127.94	120.28
3	B	46	ILE	N-CA-C	5.71	116.34	108.12
7	Y	73	LEU	N-CA-C	-5.68	98.70	110.80
2	A	134	ARG	N-CA-C	-5.67	106.90	113.88
6	X	24	LEU	CA-C-O	-5.67	114.12	120.25
6	X	120	THR	CA-CB-OG1	5.67	118.10	109.60
7	Y	62	GLN	OE1-CD-NE2	-5.66	116.94	122.60
7	Y	59	TYR	N-CA-C	-5.65	106.05	113.17
3	F	30	THR	N-CA-C	5.64	118.17	110.55
6	X	315	HIS	CE1-NE2-CD2	-5.63	103.37	109.00
6	X	81	ALA	CA-C-N	5.63	128.17	120.46
6	X	81	ALA	C-N-CA	5.63	128.17	120.46
7	Y	54	ARG	NE-CZ-NH1	5.63	127.13	121.50
6	X	264	GLY	CA-C-O	-5.62	115.30	121.71
6	X	283	ASN	CA-C-O	-5.62	115.43	121.56
6	X	45	CYS	CA-C-N	5.61	128.84	120.31
6	X	45	CYS	C-N-CA	5.61	128.84	120.31
6	X	35	HIS	CA-CB-CG	5.60	119.40	113.80
6	X	252	GLN	O-C-N	5.59	128.52	122.15
6	X	303	VAL	N-CA-C	-5.58	99.46	107.78
6	X	296	LEU	CA-C-N	5.58	128.81	120.83
6	X	296	LEU	C-N-CA	5.58	128.81	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	121	ASP	CA-CB-CG	5.58	118.18	112.60
6	X	123	GLU	CA-CB-CG	5.58	125.25	114.10
6	X	126	ASN	CA-C-N	5.58	130.36	121.66
6	X	126	ASN	C-N-CA	5.58	130.36	121.66
6	X	310	VAL	N-CA-C	-5.58	100.39	108.36
6	X	321	ILE	N-CA-CB	5.57	117.07	110.55
6	X	135	VAL	O-C-N	-5.57	116.70	122.66
7	Y	68	HIS	ND1-CG-CD2	5.56	111.66	106.10
6	X	114	VAL	CA-C-N	5.54	127.97	120.65
6	X	114	VAL	C-N-CA	5.54	127.97	120.65
6	X	252	GLN	N-CA-CB	5.53	118.35	110.16
6	X	101	ARG	CA-C-N	5.53	126.00	120.14
6	X	101	ARG	C-N-CA	5.53	126.00	120.14
6	X	253	LEU	CA-C-O	-5.52	114.70	120.55
6	X	241	ASN	CA-CB-CG	5.51	118.11	112.60
6	X	101	ARG	NE-CZ-NH2	-5.50	114.25	119.20
6	X	223	PHE	CA-CB-CG	5.49	119.29	113.80
6	X	235	THR	CA-CB-CG2	5.49	119.83	110.50
6	X	182	HIS	ND1-CE1-NE2	5.48	113.88	108.40
6	X	77	LYS	CA-C-O	5.47	126.35	120.55
7	Y	15	LEU	N-CA-CB	5.47	120.91	111.00
6	X	265	ARG	NH1-CZ-NH2	-5.45	112.21	119.30
6	X	282	ARG	N-CA-C	-5.45	108.41	114.62
6	X	293	VAL	CA-C-N	5.44	130.42	122.69
6	X	293	VAL	C-N-CA	5.44	130.42	122.69
7	Y	22	THR	CA-CB-OG1	5.44	117.76	109.60
6	X	112	GLN	CA-CB-CG	5.43	124.97	114.10
6	X	256	ARG	NE-CZ-NH1	5.43	126.94	121.50
6	X	33	ALA	CA-C-N	5.43	127.55	120.28
6	X	33	ALA	C-N-CA	5.43	127.55	120.28
6	X	72	GLN	CB-CG-CD	5.39	121.77	112.60
6	X	169	VAL	CA-C-N	5.38	127.34	120.56
6	X	169	VAL	C-N-CA	5.38	127.34	120.56
6	X	192	ALA	CB-CA-C	-5.38	101.85	110.79
6	X	117	HIS	CG-CD2-NE2	5.38	112.58	107.20
6	X	83	ASP	CA-CB-CG	-5.37	107.23	112.60
7	Y	18	GLU	O-C-N	-5.36	117.37	121.55
6	X	120	THR	N-CA-C	-5.36	105.45	112.41
7	Y	57	SER	CA-C-N	5.35	127.99	120.28
7	Y	57	SER	C-N-CA	5.35	127.99	120.28
6	X	36	GLU	N-CA-CB	5.33	117.96	110.12
6	X	303	VAL	CA-C-O	5.32	125.52	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	74	LEU	N-CA-C	-5.32	104.91	111.40
6	X	80	ARG	CA-C-N	5.31	127.40	120.28
6	X	80	ARG	C-N-CA	5.31	127.40	120.28
6	X	191	PRO	N-CA-C	5.31	120.82	113.65
6	X	52	LYS	O-C-N	5.30	127.74	122.12
6	X	199	ASP	O-C-N	5.30	127.74	122.12
6	X	9	LEU	CA-C-O	5.30	125.97	120.40
6	X	213	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
6	X	129	GLU	N-CA-C	-5.29	102.32	110.32
7	Y	66	THR	CA-C-O	-5.29	114.50	120.32
6	X	279	ILE	CA-C-N	5.27	131.61	121.54
6	X	279	ILE	C-N-CA	5.27	131.61	121.54
6	X	213	HIS	CG-CD2-NE2	5.27	112.47	107.20
6	X	131	PHE	CA-CB-CG	-5.25	108.55	113.80
6	X	172	GLN	OE1-CD-NE2	5.25	127.85	122.60
3	B	43	VAL	N-CA-C	5.25	115.81	108.89
4	G	70	ALA	N-CA-C	-5.24	105.56	111.28
6	X	43	TRP	N-CA-C	5.24	117.08	111.36
2	E	41	TYR	N-CA-C	-5.24	102.73	110.48
6	X	159	PHE	O-C-N	-5.24	117.11	123.29
6	X	181	HIS	ND1-CE1-NE2	5.23	113.63	108.40
6	X	8	ARG	CA-C-N	-5.23	115.43	123.07
6	X	8	ARG	C-N-CA	-5.23	115.43	123.07
6	X	61	ILE	CA-CB-CG1	-5.22	101.53	110.40
6	X	148	ILE	N-CA-C	5.22	115.94	110.62
6	X	27	TYR	N-CA-C	-5.21	106.60	113.12
7	Y	45	PHE	CA-C-N	5.21	129.95	122.40
7	Y	45	PHE	C-N-CA	5.21	129.95	122.40
6	X	110	ILE	N-CA-CB	5.19	117.59	110.54
7	Y	36	ILE	CA-CB-CG2	-5.19	101.68	110.50
6	X	318	ASP	CA-CB-CG	5.18	117.78	112.60
6	X	129	GLU	CA-C-O	-5.17	114.10	120.05
6	X	291	MET	O-C-N	5.17	129.45	123.41
6	X	55	MET	CA-C-N	5.15	127.69	120.28
6	X	55	MET	C-N-CA	5.15	127.69	120.28
6	X	187	LYS	N-CA-C	5.13	116.69	111.14
6	X	251	HIS	CG-CD2-NE2	5.13	112.33	107.20
6	X	107	LEU	CA-C-O	-5.12	115.12	120.55
6	X	296	LEU	N-CA-C	-5.11	102.92	110.48
6	X	224	LEU	CA-C-N	5.10	128.45	120.75
6	X	224	LEU	C-N-CA	5.10	128.45	120.75
7	Y	63	LYS	N-CA-CB	5.09	117.48	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	86	HIS	ND1-CE1-NE2	5.08	113.48	108.40
6	X	6	GLU	CA-C-O	-5.07	114.09	120.84
6	X	308	LYS	CA-C-O	-5.07	114.74	119.91
6	X	58	TYR	O-C-N	5.07	127.30	121.88
7	Y	63	LYS	CA-C-N	5.07	129.38	122.34
7	Y	63	LYS	C-N-CA	5.07	129.38	122.34
7	Y	36	ILE	N-CA-C	5.06	113.44	107.77
7	Y	73	LEU	CA-C-N	5.05	130.79	121.70
7	Y	73	LEU	C-N-CA	5.05	130.79	121.70
1	J	7	DG	C5'-C4'-C3'	-5.05	107.33	114.90
6	X	134	GLU	CB-CA-C	-5.04	100.39	110.42
7	Y	61	ILE	CB-CG1-CD1	5.04	124.39	113.80
6	X	231	ARG	O-C-N	-5.04	116.78	122.12
6	X	171	LEU	CA-C-O	-5.03	115.22	120.55
6	X	45	CYS	CB-CA-C	-5.03	102.30	110.85
6	X	24	LEU	CA-C-N	5.02	127.84	120.46
6	X	24	LEU	C-N-CA	5.02	127.84	120.46
6	X	49	PRO	N-CD-CG	5.02	110.74	103.20
6	X	182	HIS	CE1-NE2-CD2	-5.02	103.98	109.00
7	Y	37	PRO	N-CA-C	5.02	116.83	110.70
7	Y	43	LEU	CA-C-N	5.02	129.72	123.14
7	Y	43	LEU	C-N-CA	5.02	129.72	123.14
6	X	197	THR	CA-C-N	5.02	127.01	120.28
6	X	197	THR	C-N-CA	5.02	127.01	120.28

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	D	39	TYR	Sidechain
1	J	-12	DT	Sidechain
1	J	-6	DG	Sidechain
6	X	194	TYR	Sidechain
6	X	231	ARG	Sidechain
6	X	27	TYR	Sidechain
6	X	282	ARG	Sidechain
6	X	313	TYR	Sidechain
6	X	319	ARG	Sidechain
7	Y	4	PHE	Sidechain
7	Y	42	ARG	Sidechain
7	Y	59	TYR	Sidechain
7	Y	71	LEU	Peptide

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Mol	Chain	Res	Type	Group
7	Y	72	ARG	Peptide
7	Y	74	ARG	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	I	2337	0	1290	55	0
1	J	2337	0	1290	63	0
2	A	807	0	844	37	0
2	E	807	0	844	42	0
3	B	653	0	696	16	0
3	F	703	0	755	20	0
4	C	825	0	884	22	0
4	G	818	0	877	22	0
5	D	736	0	760	18	0
5	H	736	0	758	32	0
6	X	2672	0	2614	139	0
7	Y	602	0	629	4	0
8	X	27	0	21	86	0
All	All	14060	0	12262	386	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 15.

All (386) 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)
5:H:113:LYS:CD	6:X:284:LEU:CB	1.81	1.56
6:X:245:PHE:HZ	8:X:500:SAM:C5'	1.24	1.50
6:X:224:LEU:HG	8:X:500:SAM:N6	1.23	1.44
6:X:245:PHE:CZ	8:X:500:SAM:H5'1	1.52	1.43
6:X:224:LEU:CG	8:X:500:SAM:N6	1.81	1.42
6:X:224:LEU:CD1	8:X:500:SAM:HN61	1.31	1.40
6:X:223:PHE:CZ	8:X:500:SAM:C5	2.06	1.36
6:X:223:PHE:CE2	8:X:500:SAM:C4	2.09	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:224:LEU:CD1	8:X:500:SAM:N6	1.87	1.33
6:X:223:PHE:CD1	8:X:500:SAM:C6	2.15	1.30
6:X:223:PHE:CE1	8:X:500:SAM:C6	2.14	1.29
6:X:223:PHE:CE1	8:X:500:SAM:C5	2.17	1.25
6:X:139:THR:HG21	8:X:500:SAM:O	1.37	1.23
6:X:223:PHE:CG	8:X:500:SAM:C2	2.22	1.23
6:X:245:PHE:CZ	8:X:500:SAM:C5'	2.17	1.21
5:H:113:LYS:HD2	6:X:284:LEU:CB	1.54	1.19
5:H:113:LYS:CE	6:X:284:LEU:HB2	1.56	1.18
5:H:113:LYS:HD3	6:X:284:LEU:CB	1.69	1.17
5:H:113:LYS:CD	6:X:284:LEU:HB2	1.52	1.15
6:X:186:GLU:OE2	8:X:500:SAM:O2'	1.59	1.15
5:H:113:LYS:HD2	6:X:284:LEU:CD2	1.76	1.15
6:X:223:PHE:CD2	8:X:500:SAM:N3	2.17	1.12
6:X:224:LEU:HD11	8:X:500:SAM:HN61	1.14	1.11
1:J:-46:DA:H2''	1:J:-45:DA:H5''	1.27	1.11
5:H:113:LYS:CD	6:X:284:LEU:HB3	1.57	1.10
6:X:223:PHE:CZ	8:X:500:SAM:N7	2.21	1.08
6:X:186:GLU:OE1	8:X:500:SAM:H1'	1.54	1.06
6:X:137:GLY:H	8:X:500:SAM:CE	1.69	1.06
6:X:139:THR:HG21	8:X:500:SAM:C	1.84	1.05
5:H:113:LYS:HD2	6:X:284:LEU:HB3	1.14	1.03
5:H:113:LYS:HD2	6:X:284:LEU:CG	1.86	1.03
6:X:223:PHE:CG	8:X:500:SAM:N1	2.27	1.03
2:A:128:ARG:HD3	2:A:134:ARG:HH12	1.22	1.02
6:X:223:PHE:CD1	8:X:500:SAM:N1	2.28	1.01
4:C:33:LEU:HD23	4:C:36:LYS:HD3	1.42	1.00
1:I:26:DA:H2''	1:I:27:DG:H5'	1.41	0.98
2:E:49:ARG:HG3	2:E:49:ARG:HH11	1.27	0.98
6:X:224:LEU:HD12	8:X:500:SAM:N6	1.75	0.98
6:X:133:PRO:C	8:X:500:SAM:C8	2.35	0.98
6:X:223:PHE:CD2	8:X:500:SAM:C2	2.46	0.98
6:X:223:PHE:CZ	8:X:500:SAM:C4	2.40	0.97
4:C:17:ARG:HH12	4:C:31:HIS:CD2	1.83	0.96
6:X:223:PHE:CD2	8:X:500:SAM:C4	2.46	0.96
4:G:17:ARG:HH12	4:G:31:HIS:HD2	0.98	0.95
3:F:87:VAL:HG11	3:F:102:GLY:HA3	1.45	0.94
2:A:128:ARG:HH11	2:A:134:ARG:NH1	1.64	0.94
6:X:163:GLY:N	6:X:223:PHE:HD2	1.66	0.93
1:J:26:DG:H2''	1:J:27:DC:C5	2.03	0.93
6:X:245:PHE:HZ	8:X:500:SAM:H5'2	1.28	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:223:PHE:CE2	8:X:500:SAM:N9	2.37	0.93
6:X:223:PHE:CZ	8:X:500:SAM:C8	2.52	0.93
6:X:245:PHE:HZ	8:X:500:SAM:H5'1	0.81	0.92
2:A:128:ARG:HH11	2:A:134:ARG:HH12	1.11	0.92
5:H:113:LYS:CD	6:X:284:LEU:CG	2.46	0.92
6:X:224:LEU:CG	8:X:500:SAM:HN62	1.59	0.91
1:J:41:DA:H2''	1:J:42:DC:H5''	1.49	0.91
2:E:116:ARG:CZ	2:E:120:MET:HE2	2.01	0.89
4:C:55:LEU:O	4:C:59:THR:HG23	1.72	0.89
5:H:113:LYS:HD2	6:X:284:LEU:HD22	1.52	0.89
6:X:223:PHE:H	8:X:500:SAM:C2	1.85	0.89
1:J:-46:DA:C2'	1:J:-45:DA:H5''	2.03	0.89
4:G:17:ARG:HH12	4:G:31:HIS:CD2	1.89	0.89
4:C:17:ARG:HH12	4:C:31:HIS:HD2	0.94	0.89
6:X:163:GLY:N	6:X:223:PHE:CD2	2.42	0.87
2:A:128:ARG:HD3	2:A:134:ARG:NH1	1.89	0.87
6:X:223:PHE:CD1	6:X:224:LEU:HG	2.11	0.86
5:H:113:LYS:CE	6:X:284:LEU:CB	2.24	0.86
6:X:137:GLY:H	8:X:500:SAM:HE1	1.37	0.85
6:X:134:GLU:HA	8:X:500:SAM:H2'	1.57	0.84
6:X:186:GLU:OE1	8:X:500:SAM:C1'	2.24	0.84
6:X:223:PHE:CE1	8:X:500:SAM:N6	2.46	0.84
5:H:113:LYS:HD3	6:X:284:LEU:HB2	1.34	0.83
6:X:224:LEU:HG	8:X:500:SAM:HN62	1.18	0.83
2:E:120:MET:CE	2:E:122:LYS:HD3	2.08	0.83
4:C:17:ARG:NH1	4:C:31:HIS:HD2	1.76	0.82
2:E:120:MET:HE3	2:E:122:LYS:HD3	1.61	0.82
5:H:113:LYS:CD	6:X:284:LEU:CD2	2.57	0.82
5:H:113:LYS:CD	6:X:284:LEU:HD22	2.08	0.81
2:A:128:ARG:NH1	2:A:134:ARG:NH1	2.28	0.81
6:X:224:LEU:HG	8:X:500:SAM:C6	2.11	0.80
6:X:139:THR:CG2	8:X:500:SAM:C	2.59	0.80
2:A:129:ARG:HD2	2:A:135:ALA:HB2	1.62	0.80
1:J:42:DC:H2'	1:J:43:DT:H71	1.64	0.80
2:A:125:GLN:HG2	2:A:134:ARG:HH21	1.48	0.79
1:J:5:DC:H2''	1:J:6:DT:C7	2.14	0.78
6:X:223:PHE:CE1	6:X:224:LEU:HG	2.20	0.77
1:J:41:DA:C2'	1:J:42:DC:H5''	2.15	0.76
1:J:49:DT:OP1	5:D:31:LYS:HG2	1.84	0.76
6:X:245:PHE:CZ	8:X:500:SAM:H5'2	2.09	0.76
5:H:113:LYS:HD3	6:X:284:LEU:HB3	1.39	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:134:GLU:CA	8:X:500:SAM:H2'	2.17	0.75
6:X:223:PHE:N	8:X:500:SAM:N1	2.34	0.74
1:I:17:DT:OP2	2:E:69:ARG:NH2	2.20	0.74
4:G:17:ARG:NH1	4:G:31:HIS:HD2	1.82	0.74
6:X:133:PRO:C	8:X:500:SAM:H8	1.99	0.74
6:X:223:PHE:CB	8:X:500:SAM:C2	2.65	0.74
1:J:17:DT:OP1	2:A:66:PRO:HG3	1.89	0.73
6:X:186:GLU:CD	8:X:500:SAM:HO2'	1.91	0.73
1:I:26:DA:C2'	1:I:27:DG:H5'	2.17	0.73
6:X:133:PRO:O	8:X:500:SAM:C8	2.36	0.73
1:J:28:DA:H2''	1:J:29:DG:C8	2.25	0.72
6:X:186:GLU:CD	8:X:500:SAM:H1'	2.14	0.72
1:J:-46:DA:H4'	5:H:30:ARG:HD3	1.72	0.71
1:J:-46:DA:H2''	1:J:-45:DA:C5'	2.13	0.71
1:I:-45:DA:H2''	1:I:-44:DA:H5''	1.73	0.70
1:I:17:DT:P	2:E:69:ARG:HH22	2.14	0.70
1:I:-48:DC:H2''	1:I:-47:DC:H5'	1.74	0.69
6:X:245:PHE:CE1	8:X:500:SAM:H5'1	2.25	0.69
6:X:163:GLY:CA	6:X:223:PHE:CD2	2.75	0.69
6:X:223:PHE:CD1	8:X:500:SAM:N6	2.58	0.69
1:J:5:DC:H2''	1:J:6:DT:H71	1.74	0.69
6:X:137:GLY:N	8:X:500:SAM:CE	2.51	0.69
2:E:80:THR:HG21	6:X:130:PRO:HD3	1.75	0.69
1:J:-39:DA:H2''	1:J:-38:DT:OP2	1.92	0.68
6:X:137:GLY:H	8:X:500:SAM:HE2	1.56	0.68
4:G:84:GLN:OE1	4:G:88:ARG:HD2	1.94	0.68
6:X:223:PHE:H	8:X:500:SAM:H2	1.60	0.67
1:I:-45:DA:C2'	1:I:-44:DA:H5''	2.25	0.67
1:J:24:DG:H2''	1:J:25:DA:N7	2.09	0.67
1:J:-48:DC:H1'	1:J:-47:DA:C5	2.29	0.66
4:C:32:ARG:HH22	5:D:32:GLU:CD	2.03	0.66
6:X:223:PHE:CG	8:X:500:SAM:C6	2.73	0.66
6:X:134:GLU:HA	8:X:500:SAM:C2'	2.26	0.66
3:F:87:VAL:CG1	3:F:102:GLY:HA3	2.24	0.66
4:C:118:LYS:C	4:C:119:LYS:HD3	2.21	0.65
2:E:49:ARG:HG3	2:E:49:ARG:NH1	2.06	0.65
2:A:128:ARG:NH1	2:A:134:ARG:HH12	1.88	0.65
2:E:80:THR:HG23	6:X:130:PRO:HG3	1.79	0.65
4:G:15:LYS:HG3	4:G:19:SER:OG	1.96	0.65
1:I:20:DT:H2''	1:I:21:DG:H5'	1.78	0.64
1:J:-14:DC:H2''	1:J:-13:DA:C8	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:223:PHE:HE1	6:X:224:LEU:HD21	1.63	0.64
2:E:49:ARG:HH11	2:E:49:ARG:CG	2.03	0.64
1:J:-43:DG:O3'	4:G:14:ALA:HB1	1.98	0.63
2:E:76:GLN:HE22	3:F:19:ARG:NH1	1.96	0.63
2:E:76:GLN:NE2	3:F:19:ARG:NH1	2.47	0.63
2:A:129:ARG:HA	2:A:134:ARG:HB2	1.79	0.63
1:I:-13:DC:H5''	2:A:63:ARG:NH1	2.13	0.62
1:J:54:DT:H2''	1:J:55:DC:OP2	1.98	0.62
6:X:163:GLY:O	8:X:500:SAM:H4'	1.99	0.62
6:X:245:PHE:CE2	8:X:500:SAM:O4'	2.52	0.62
1:I:39:DT:OP2	4:G:35:ARG:NH2	2.31	0.62
6:X:163:GLY:CA	6:X:223:PHE:HD2	2.12	0.62
2:E:134:ARG:O	2:E:135:ALA:OXT	2.18	0.62
6:X:137:GLY:N	8:X:500:SAM:HE1	2.12	0.62
1:I:-13:DC:H5''	2:A:63:ARG:CZ	2.29	0.62
6:X:223:PHE:CE1	8:X:500:SAM:N7	2.62	0.62
1:J:10:DC:H2''	1:J:11:DA:C8	2.34	0.61
1:J:41:DA:H2''	1:J:42:DC:C5'	2.25	0.61
2:E:80:THR:CG2	6:X:130:PRO:HD3	2.31	0.61
6:X:133:PRO:C	8:X:500:SAM:H2'	2.26	0.61
1:J:-27:DC:H2''	1:J:-26:DT:H71	1.81	0.60
6:X:134:GLU:HA	8:X:500:SAM:O2'	2.01	0.60
1:J:34:DC:H2''	1:J:35:DA:N7	2.15	0.60
6:X:223:PHE:CZ	8:X:500:SAM:N9	2.67	0.60
6:X:163:GLY:O	8:X:500:SAM:HG2	2.02	0.60
6:X:186:GLU:OE2	8:X:500:SAM:C2'	2.47	0.59
6:X:224:LEU:CB	8:X:500:SAM:HN62	2.15	0.59
2:A:134:ARG:HH11	2:A:134:ARG:HG3	1.68	0.59
6:X:134:GLU:N	8:X:500:SAM:H2'	2.18	0.59
1:I:-14:DG:H2''	1:I:-13:DC:C6	2.38	0.58
1:J:-32:DA:H1'	1:J:-31:DA:O5'	2.03	0.58
1:J:-5:DC:H5'	2:E:43:PRO:HG2	1.85	0.58
4:C:119:LYS:HD3	4:C:119:LYS:N	2.19	0.58
4:G:84:GLN:CD	4:G:88:ARG:HD2	2.29	0.58
2:E:120:MET:HE1	2:E:122:LYS:HD3	1.83	0.58
1:I:-16:DA:H2''	1:I:-15:DG:C8	2.39	0.58
5:H:122:LYS:HG3	5:H:122:LYS:OXT	2.04	0.57
6:X:223:PHE:HZ	8:X:500:SAM:C8	2.14	0.57
1:I:-37:DT:H2''	1:I:-36:DT:OP2	2.03	0.57
2:E:129:ARG:HG3	2:E:135:ALA:HA	1.86	0.57
2:A:125:GLN:HG2	2:A:134:ARG:NH2	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:-23:DC:H1'	2:A:83:ARG:HH21	1.69	0.57
6:X:163:GLY:CA	6:X:223:PHE:CE2	2.87	0.57
2:E:128:ARG:HE	2:E:134:ARG:HH21	1.52	0.57
1:J:25:DA:H1'	2:A:83:ARG:NH1	2.21	0.56
2:E:132:GLY:HA2	2:E:135:ALA:HB2	1.86	0.56
6:X:223:PHE:N	8:X:500:SAM:C2	2.62	0.56
4:C:29:ARG:NH2	5:D:33:SER:O	2.38	0.56
6:X:223:PHE:N	8:X:500:SAM:H2	2.19	0.56
5:D:121:ALA:O	5:D:122:LYS:HB2	2.05	0.56
6:X:223:PHE:HZ	8:X:500:SAM:N7	1.98	0.56
2:E:116:ARG:NH2	2:E:120:MET:HE2	2.20	0.55
1:I:-45:DA:H2''	1:I:-44:DA:C5'	2.37	0.55
6:X:261:LYS:HB3	6:X:261:LYS:HZ2	1.71	0.55
5:D:39:TYR:CZ	5:D:43:LYS:HE2	2.41	0.55
1:J:19:DT:H2''	1:J:20:DG:C8	2.41	0.55
6:X:245:PHE:HE2	8:X:500:SAM:O4'	1.90	0.55
6:X:223:PHE:HE1	6:X:224:LEU:CD2	2.19	0.55
6:X:223:PHE:CE1	6:X:224:LEU:CD2	2.90	0.55
2:A:126:LEU:HD22	2:E:113:HIS:CG	2.41	0.54
2:A:57:SER:HB2	2:A:59:GLU:OE2	2.07	0.54
1:I:18:DT:H5''	2:E:63:ARG:HH12	1.70	0.54
1:J:5:DC:H2''	1:J:6:DT:C5	2.42	0.54
4:G:102:ILE:HG23	5:H:58:ILE:HD13	1.89	0.54
1:I:-53:DT:H2''	1:I:-52:DT:OP2	2.08	0.54
1:I:-46:DA:H2	1:J:47:DG:N2	2.05	0.54
1:I:41:DC:H4'	1:I:41:DC:OP1	2.08	0.54
1:J:-44:DA:OP2	4:G:32:ARG:HD3	2.08	0.53
1:J:-42:DT:H5'	4:G:14:ALA:HB2	1.90	0.53
2:A:68:GLN:HE21	2:A:89:VAL:HG21	1.74	0.53
3:B:75:HIS:CE1	5:D:77:LEU:HD21	2.44	0.53
6:X:135:VAL:O	8:X:500:SAM:SD	2.66	0.53
4:C:62:ILE:CG2	5:D:59:MET:HE1	2.38	0.53
3:B:31:LYS:HB3	3:B:32:PRO:HD3	1.90	0.53
6:X:163:GLY:HA3	6:X:223:PHE:CE2	2.44	0.53
4:C:62:ILE:HG21	5:D:59:MET:HE1	1.90	0.53
2:E:49:ARG:NH1	2:E:49:ARG:CG	2.66	0.53
1:J:29:DG:OP1	5:H:29:THR:HG22	2.09	0.53
6:X:137:GLY:N	8:X:500:SAM:HE2	2.20	0.53
4:G:69:ALA:O	4:G:73:ASN:ND2	2.37	0.52
1:I:40:DA:H2''	1:I:41:DC:O5'	2.10	0.52
3:F:87:VAL:HG11	3:F:102:GLY:CA	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:163:GLY:H	6:X:223:PHE:HD2	1.50	0.52
4:C:37:GLY:HA3	4:C:39:TYR:CE1	2.45	0.52
6:X:223:PHE:CE1	6:X:224:LEU:CG	2.91	0.51
1:I:54:DA:H2''	1:I:55:DT:OP2	2.09	0.51
1:J:6:DT:H2''	1:J:7:DG:C8	2.46	0.51
3:B:84:MET:HE1	3:B:102:GLY:CA	2.40	0.51
1:I:49:DG:H5'	5:H:30:ARG:NH2	2.26	0.51
6:X:223:PHE:CE2	8:X:500:SAM:C5	2.57	0.51
2:A:79:LYS:HD2	3:B:74:GLU:CG	2.41	0.50
4:G:35:ARG:HG2	4:G:35:ARG:HH11	1.76	0.50
2:A:79:LYS:HD2	3:B:74:GLU:CD	2.36	0.50
2:E:116:ARG:NH1	2:E:120:MET:HE2	2.25	0.50
1:J:9:DA:N3	2:A:40:ARG:NH2	2.56	0.50
3:F:17:ARG:HB3	3:F:18:HIS:CD2	2.47	0.50
3:F:59:LYS:O	3:F:63:GLU:HG3	2.12	0.50
1:I:52:DT:H2''	1:I:51:DC:O5'	2.11	0.50
1:I:45:DA:H1'	1:I:44:DA:H5''	1.94	0.50
2:E:76:GLN:HE22	3:F:19:ARG:HH11	1.58	0.50
1:J:51:DG:H2''	1:J:52:DA:OP2	2.12	0.49
6:X:163:GLY:HA3	6:X:223:PHE:HE2	1.78	0.49
1:I:12:DA:OP1	3:B:23:ARG:NH2	2.45	0.49
4:C:25:PHE:CZ	4:C:59:THR:HG21	2.46	0.49
6:X:223:PHE:HD1	6:X:224:LEU:HG	1.73	0.49
2:A:63:ARG:O	2:A:66:PRO:HD2	2.13	0.49
2:E:77:ASP:OD2	6:X:305:TRP:CD2	2.66	0.49
1:I:48:DG:H3'	5:H:36:ILE:HD11	1.95	0.49
1:J:8:DA:OP2	3:B:35:ARG:NH2	2.44	0.49
1:J:48:DG:H2''	1:J:49:DT:H5'	1.94	0.49
2:E:77:ASP:HB3	6:X:305:TRP:NE1	2.27	0.48
1:J:36:DT:H2''	1:J:35:DG:N7	2.28	0.48
1:J:7:DG:H2''	1:J:8:DA:C8	2.48	0.48
2:E:128:ARG:HD2	2:E:133:GLU:OE1	2.13	0.48
2:E:128:ARG:HH21	2:E:134:ARG:NH2	2.11	0.48
1:I:41:DC:H42	1:J:41:DG:H1	1.61	0.48
2:A:57:SER:CB	2:A:59:GLU:OE2	2.62	0.48
3:B:22:LEU:O	3:B:23:ARG:HB2	2.13	0.48
1:I:5:DG:OP1	2:A:42:ARG:CZ	2.61	0.48
2:A:132:GLY:HA2	2:A:135:ALA:HB3	1.95	0.48
5:D:64:ASN:O	5:D:68:GLU:HG3	2.13	0.48
4:C:80:PRO:HG3	5:D:58:ILE:HD12	1.96	0.48
6:X:133:PRO:HA	8:X:500:SAM:H8	1.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:28:DA:H2''	1:J:29:DG:H8	1.77	0.48
2:A:65:LEU:HB3	2:A:66:PRO:HD3	1.95	0.48
4:C:32:ARG:NH1	5:D:32:GLU:OE2	2.44	0.48
5:H:43:LYS:HA	5:H:43:LYS:HD3	1.61	0.48
2:A:79:LYS:HD2	3:B:74:GLU:HG2	1.95	0.47
1:I:-47:DC:H1'	1:I:-46:DA:C5	2.49	0.47
5:D:39:TYR:CE2	5:D:43:LYS:HE2	2.50	0.47
2:E:59:GLU:H	2:E:59:GLU:HG3	1.53	0.47
4:G:84:GLN:O	4:G:88:ARG:HG2	2.15	0.47
1:J:-15:DG:H2''	1:J:-14:DC:O5'	2.15	0.47
6:X:235:THR:O	6:X:260:MET:HE3	2.15	0.47
2:E:80:THR:OG1	6:X:130:PRO:HD2	2.15	0.47
1:I:9:DA:N3	2:E:40:ARG:NH2	2.61	0.47
6:X:186:GLU:CD	8:X:500:SAM:C2'	2.87	0.47
1:I:-13:DC:OP1	2:A:63:ARG:HD2	2.14	0.47
2:A:48:LEU:CD2	4:G:117:PRO:HD3	2.45	0.47
3:B:30:THR:HB	3:B:32:PRO:HD2	1.95	0.47
2:E:65:LEU:HB3	2:E:66:PRO:HD3	1.95	0.47
6:X:186:GLU:OE1	8:X:500:SAM:C4'	2.62	0.47
5:H:113:LYS:NZ	6:X:284:LEU:N	2.63	0.47
2:A:128:ARG:CD	2:A:134:ARG:NH1	2.71	0.46
6:X:223:PHE:HD1	6:X:224:LEU:N	2.13	0.46
1:I:53:DA:H1'	1:I:54:DA:H5'	1.96	0.46
1:J:-46:DA:H4'	5:H:30:ARG:CD	2.44	0.46
3:F:30:THR:CB	3:F:32:PRO:HD2	2.45	0.46
1:I:-46:DA:C2	1:J:47:DG:N2	2.83	0.46
1:J:-43:DG:H5''	4:G:16:THR:HA	1.98	0.46
1:I:-44:DA:H5'	1:I:-44:DA:H8	1.80	0.46
1:I:-47:DC:H1'	1:I:-46:DA:C4	2.51	0.46
6:X:223:PHE:CB	8:X:500:SAM:H2	2.45	0.46
1:J:42:DC:H2''	1:J:43:DT:O5'	2.15	0.46
6:X:62:ASP:H	6:X:73:ARG:HH22	1.63	0.46
1:I:18:DT:OP1	2:E:63:ARG:NH1	2.48	0.46
5:D:79:HIS:CE1	4:G:38:ASN:OD1	2.69	0.46
2:E:120:MET:HE3	2:E:122:LYS:CD	2.40	0.46
6:X:223:PHE:CE1	6:X:224:LEU:HD21	2.45	0.46
1:I:44:DT:C6	1:I:45:DT:H72	2.50	0.45
6:X:186:GLU:CD	8:X:500:SAM:C1'	2.85	0.45
4:G:35:ARG:HG2	4:G:35:ARG:NH1	2.32	0.45
3:F:30:THR:OG1	3:F:32:PRO:HD2	2.16	0.45
1:I:43:DC:C2'	1:I:44:DT:H72	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:136:TYR:HA	8:X:500:SAM:SD	2.56	0.45
1:J:-33:DA:C6	1:J:-32:DA:N6	2.84	0.45
4:G:37:GLY:HA3	4:G:39:TYR:CE1	2.52	0.45
1:J:35:DA:C6	1:J:36:DA:C6	3.03	0.45
2:E:128:ARG:HB2	2:E:134:ARG:HE	1.81	0.45
6:X:223:PHE:CD1	6:X:223:PHE:C	2.94	0.45
1:I:-19:DA:H2''	1:I:-18:DA:C8	2.52	0.45
1:I:30:DG:OP1	5:D:29:THR:HG22	2.17	0.45
3:F:59:LYS:NZ	3:F:63:GLU:OE2	2.34	0.44
5:H:29:THR:HG23	5:H:29:THR:O	2.16	0.44
1:J:-27:DC:H2''	1:J:-26:DT:C7	2.45	0.44
2:E:80:THR:OG1	6:X:130:PRO:CD	2.65	0.44
3:F:19:ARG:NH2	3:F:22:LEU:HD11	2.33	0.44
5:H:102:GLU:OE1	5:H:106:HIS:CE1	2.71	0.44
1:I:-43:DA:OP2	4:C:32:ARG:HD3	2.17	0.44
1:J:-45:DA:H2''	1:J:-44:DA:C8	2.53	0.44
4:C:119:LYS:O	4:C:120:THR:HB	2.17	0.44
6:X:186:GLU:OE1	8:X:500:SAM:C2'	2.65	0.44
6:X:223:PHE:HB3	8:X:500:SAM:C2	2.46	0.44
6:X:89:TRP:CD2	6:X:95:PRO:HB3	2.53	0.44
2:A:129:ARG:CD	2:A:135:ALA:HB2	2.41	0.44
5:D:102:GLU:OE2	5:D:105:LYS:HD2	2.18	0.44
2:E:79:LYS:HG3	3:F:74:GLU:OE2	2.18	0.44
1:I:37:DA:H2''	1:I:38:DA:OP2	2.18	0.44
1:I:39:DT:H2''	1:I:40:DA:O5'	2.17	0.43
2:A:128:ARG:CD	2:A:134:ARG:HH12	2.11	0.43
3:B:24:ASP:O	3:B:27:GLN:HB2	2.17	0.43
5:D:69:ARG:HD2	5:D:98:LEU:HD11	1.99	0.43
1:I:-18:DA:H2''	1:I:-17:DA:C8	2.53	0.43
1:J:-32:DA:H4'	1:J:-31:DA:OP1	2.18	0.43
4:C:25:PHE:HZ	4:C:59:THR:HG21	1.83	0.43
4:C:33:LEU:HA	4:C:36:LYS:HG2	2.00	0.43
7:Y:50:LEU:HD22	7:Y:59:TYR:CD2	2.54	0.43
1:J:24:DG:H2''	1:J:25:DA:C8	2.53	0.43
1:I:-18:DA:H2''	1:I:-17:DA:N7	2.34	0.43
4:C:47:ALA:N	4:C:48:PRO:HD2	2.33	0.43
4:C:79:ILE:HG12	4:C:82:HIS:CE1	2.54	0.43
6:X:223:PHE:HB3	8:X:500:SAM:H2	2.01	0.43
3:B:59:LYS:O	3:B:63:GLU:HG3	2.18	0.43
1:I:-2:DG:H1'	1:I:-1:DA:C8	2.54	0.43
2:A:128:ARG:HB2	2:A:134:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:18:HIS:O	3:F:19:ARG:HB2	2.19	0.43
7:Y:15:LEU:HD11	7:Y:30:ILE:HG13	2.01	0.43
5:H:113:LYS:CE	6:X:284:LEU:HD22	2.48	0.42
1:J:-47:DA:H2''	1:J:-46:DA:OP2	2.19	0.42
4:C:81:ARG:O	4:C:81:ARG:HG3	2.16	0.42
1:I:16:DC:H2''	1:I:17:DT:H71	2.00	0.42
4:G:64:GLU:OE1	5:H:45:VAL:HG13	2.19	0.42
5:H:102:GLU:HG3	5:H:106:HIS:CE1	2.54	0.42
6:X:163:GLY:HA2	6:X:223:PHE:CD2	2.53	0.42
3:F:19:ARG:HH22	3:F:22:LEU:HD11	1.83	0.42
3:B:84:MET:HE1	3:B:102:GLY:HA3	2.01	0.42
6:X:223:PHE:HE1	6:X:224:LEU:CG	2.33	0.42
7:Y:24:GLU:HG3	7:Y:53:GLY:H	1.84	0.42
1:J:-5:DC:C5'	2:E:43:PRO:HG2	2.48	0.42
1:J:26:DG:H5'	3:B:79:LYS:HD2	2.01	0.42
1:J:7:DG:H5'	3:B:46:ILE:O	2.19	0.42
6:X:277:PHE:CE2	6:X:289:THR:HA	2.55	0.42
1:J:-32:DA:C1'	1:J:-31:DA:O5'	2.66	0.42
1:J:-5:DC:H2''	1:J:-4:DT:H71	2.02	0.42
3:B:52:GLU:OE2	3:B:55:ARG:NH1	2.49	0.42
5:D:29:THR:O	5:D:29:THR:HG23	2.19	0.42
5:H:113:LYS:CG	6:X:284:LEU:HD22	2.50	0.42
1:J:-52:DC:H2''	1:J:-51:DT:OP2	2.19	0.41
1:J:-25:DC:H1'	1:J:-24:DC:C6	2.56	0.41
3:F:31:LYS:HE3	3:F:35:ARG:HH22	1.84	0.41
1:I:-45:DA:C1'	1:I:-44:DA:H5''	2.50	0.41
2:A:48:LEU:HD21	4:G:117:PRO:HD3	2.01	0.41
2:E:79:LYS:HD3	2:E:80:THR:N	2.35	0.41
1:J:-32:DA:H1'	1:J:-31:DA:C5'	2.50	0.41
2:E:127:ALA:O	2:E:131:ARG:HG3	2.20	0.41
3:F:30:THR:HB	3:F:32:PRO:HD2	2.02	0.41
6:X:223:PHE:HD1	6:X:223:PHE:C	2.28	0.41
2:A:108:ASN:HD21	4:G:115:LEU:HD11	1.85	0.41
6:X:135:VAL:O	8:X:500:SAM:H5'1	2.21	0.41
1:I:44:DT:H2''	1:I:45:DT:OP2	2.20	0.41
3:F:65:VAL:HG22	3:F:93:GLN:OE1	2.19	0.41
1:I:18:DT:H5''	2:E:63:ARG:NH1	2.36	0.41
5:H:29:THR:O	5:H:30:ARG:C	2.64	0.41
3:F:31:LYS:HE3	3:F:35:ARG:NH2	2.35	0.41
1:I:-50:DT:H71	1:I:-49:DA:N6	2.36	0.41
1:I:-27:DG:H2''	1:I:-26:DC:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:30:DG:OP1	5:D:29:THR:CG2	2.69	0.41
1:I:-47:DC:H6	1:I:-47:DC:H2'	1.77	0.40
3:F:38:ALA:HB1	3:F:43:VAL:HB	2.03	0.40
1:J:49:DT:H1'	1:J:50:DA:C8	2.56	0.40
2:A:64:LYS:HE2	2:A:90:MET:HE1	2.03	0.40
6:X:300:LYS:H	6:X:300:LYS:HD3	1.85	0.40
7:Y:37:PRO:HA	7:Y:38:PRO:HD3	2.02	0.40
1:J:-39:DA:C2'	1:J:-38:DT:OP2	2.67	0.40
6:X:137:GLY:CA	8:X:500:SAM:HE2	2.52	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	
2	A	96/98 (98%)	96 (100%)	0	0	100	100
2	E	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
3	B	80/87 (92%)	78 (98%)	0	2 (2%)	4	26
3	F	85/87 (98%)	81 (95%)	1 (1%)	3 (4%)	3	20
4	C	105/116 (90%)	101 (96%)	4 (4%)	0	100	100
4	G	104/116 (90%)	102 (98%)	2 (2%)	0	100	100
5	D	92/94 (98%)	90 (98%)	1 (1%)	1 (1%)	11	46
5	H	92/94 (98%)	88 (96%)	2 (2%)	2 (2%)	5	29
6	X	326/328 (99%)	303 (93%)	18 (6%)	5 (2%)	8	40
7	Y	74/76 (97%)	70 (95%)	2 (3%)	2 (3%)	4	25
All	All	1150/1194 (96%)	1104 (96%)	31 (3%)	15 (1%)	12	42

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	19	ARG
6	X	280	ASN
7	Y	72	ARG
7	Y	73	LEU
3	B	22	LEU
5	D	101	GLY
5	H	101	GLY
6	X	262	GLU
3	F	20	LYS
3	B	23	ARG
3	F	18	HIS
6	X	61	ILE
5	H	30	ARG
6	X	13	VAL
6	X	274	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	85/85 (100%)	83 (98%)	2 (2%)	43	64
2	E	85/85 (100%)	82 (96%)	3 (4%)	32	53
3	B	67/72 (93%)	66 (98%)	1 (2%)	57	72
3	F	72/72 (100%)	72 (100%)	0	100	100
4	C	85/93 (91%)	79 (93%)	6 (7%)	13	35
4	G	84/93 (90%)	83 (99%)	1 (1%)	63	75
5	D	80/80 (100%)	79 (99%)	1 (1%)	61	74
5	H	80/80 (100%)	77 (96%)	3 (4%)	29	50
6	X	294/294 (100%)	283 (96%)	11 (4%)	30	51
7	Y	68/68 (100%)	64 (94%)	4 (6%)	18	39
All	All	1000/1022 (98%)	968 (97%)	32 (3%)	35	56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	48	LEU
2	A	59	GLU
3	B	22	LEU
4	C	29	ARG
4	C	59	THR
4	C	76	THR
4	C	81	ARG
4	C	109	PRO
4	C	119	LYS
5	D	33	SER
2	E	49	ARG
2	E	59	GLU
2	E	121	PRO
4	G	88	ARG
5	H	31	LYS
5	H	33	SER
5	H	103	LEU
6	X	17	PRO
6	X	73	ARG
6	X	90	LYS
6	X	98	LEU
6	X	123	GLU
6	X	129	GLU
6	X	177	THR
6	X	223	PHE
6	X	261	LYS
6	X	287	ILE
6	X	316	THR
7	Y	13	ILE
7	Y	14	THR
7	Y	36	ILE
7	Y	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	68	GLN
2	A	108	ASN
3	B	27	GLN
4	C	24	GLN
4	C	31	HIS
2	E	68	GLN
2	E	76	GLN

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Mol	Chain	Res	Type
3	F	18	HIS
4	G	31	HIS
5	H	44	GLN
5	H	79	HIS
5	H	106	HIS
6	X	31	HIS
6	X	72	GLN
6	X	99	ASN
6	X	109	HIS
6	X	112	GLN
6	X	113	GLN
6	X	126	ASN
6	X	127	ASN
6	X	168	GLN
6	X	182	HIS
6	X	251	HIS
6	X	276	ASN
6	X	280	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
8	SAM	X	500	-	27,29,29	0.72	0	34,42,42	1.07	2 (5%)

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
8	SAM	X	500	-	-	2/17/33/33	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	X	500	SAM	O2'-C2'-C3'	3.14	121.88	111.82
8	X	500	SAM	O3'-C3'-C4'	-2.01	105.30	111.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	X	500	SAM	N-CA-CB-CG
8	X	500	SAM	C-CA-CB-CG

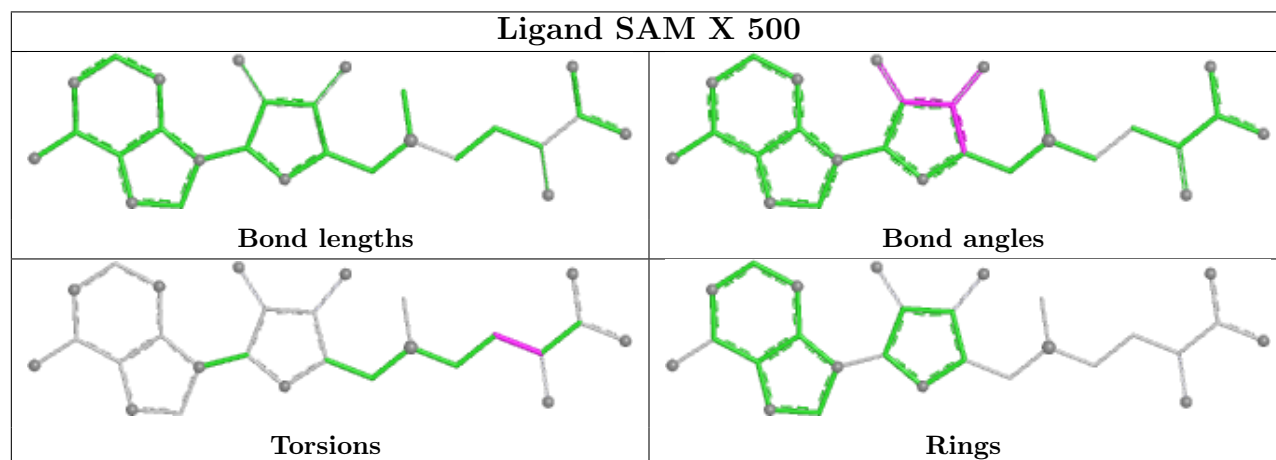
There are no ring outliers.

1 monomer is involved in 86 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	X	500	SAM	86	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](#)

There are no chain breaks in this entry.

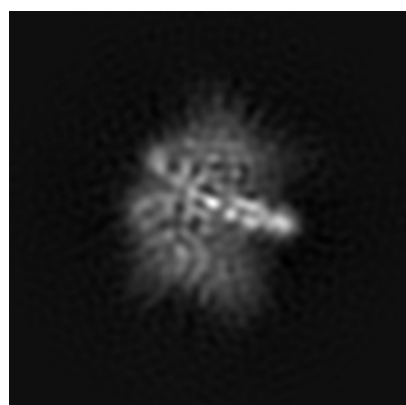
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9844. These allow visual inspection of the internal detail of the map and identification of artifacts.

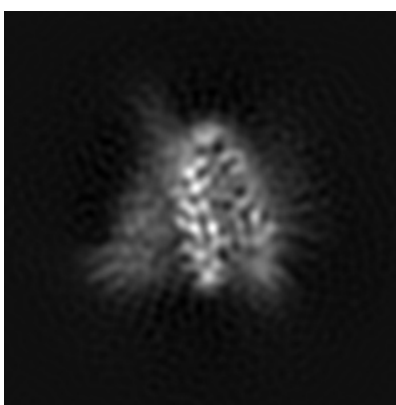
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

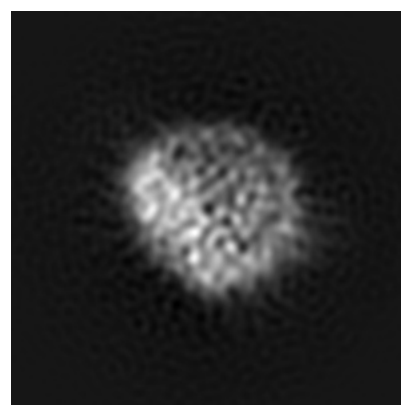
6.1.1 Primary map



X



Y

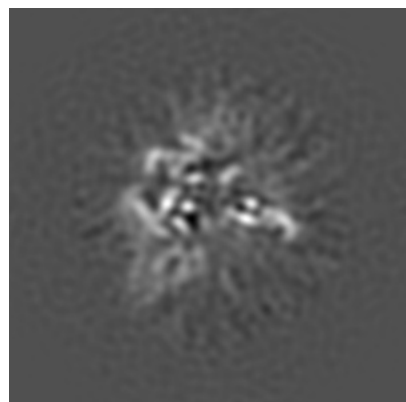


Z

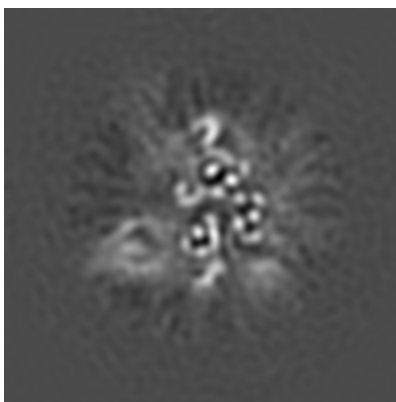
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

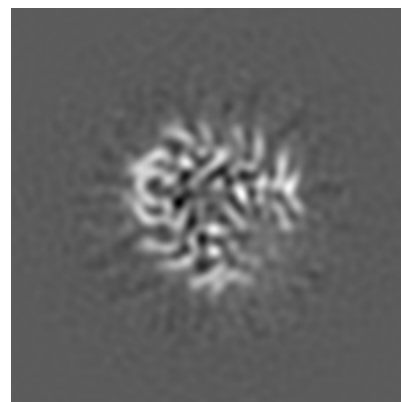
6.2.1 Primary map



X Index: 110



Y Index: 110

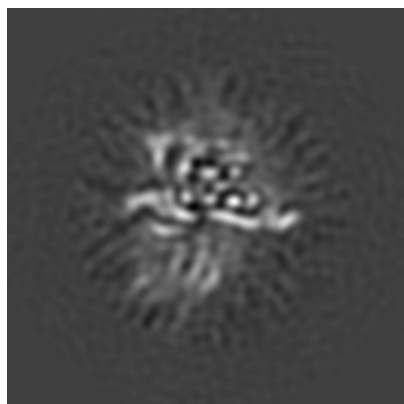


Z Index: 110

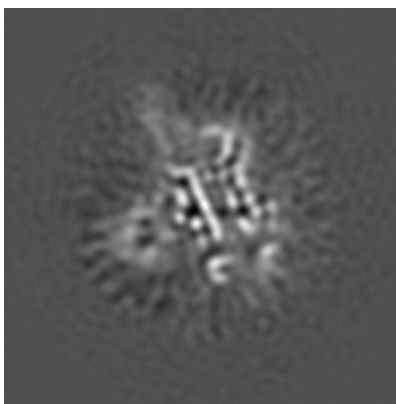
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

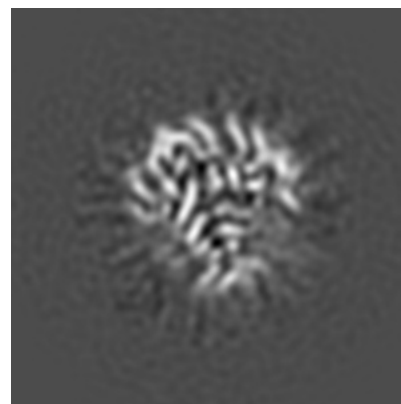
6.3.1 Primary map



X Index: 100



Y Index: 98

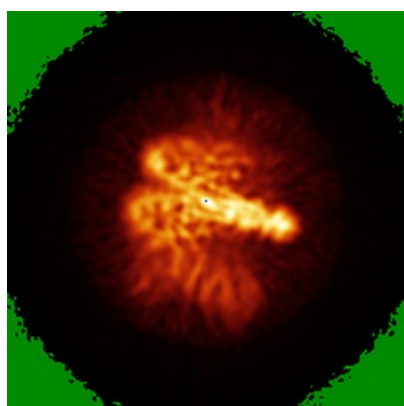


Z Index: 106

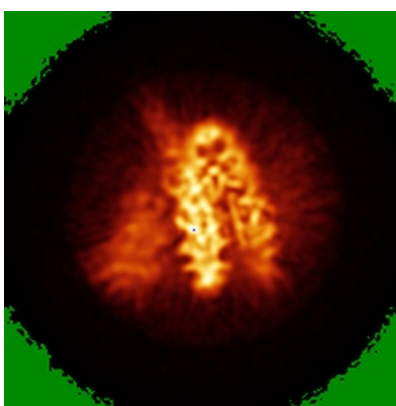
The images above show the largest variance slices of the map in three orthogonal directions.

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

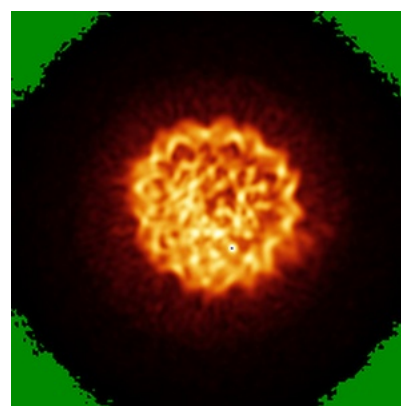
6.4.1 Primary map



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 0.0251. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

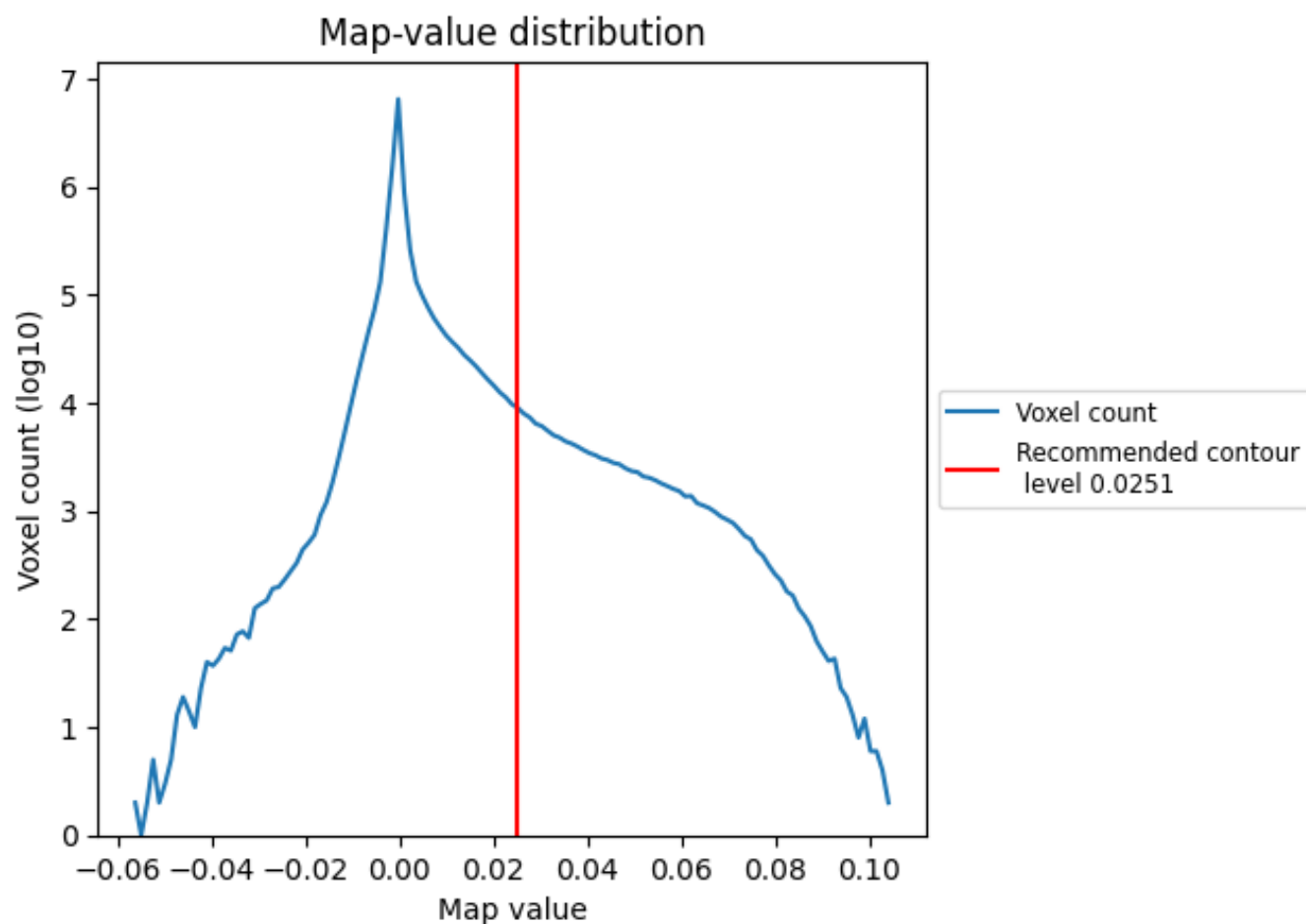
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

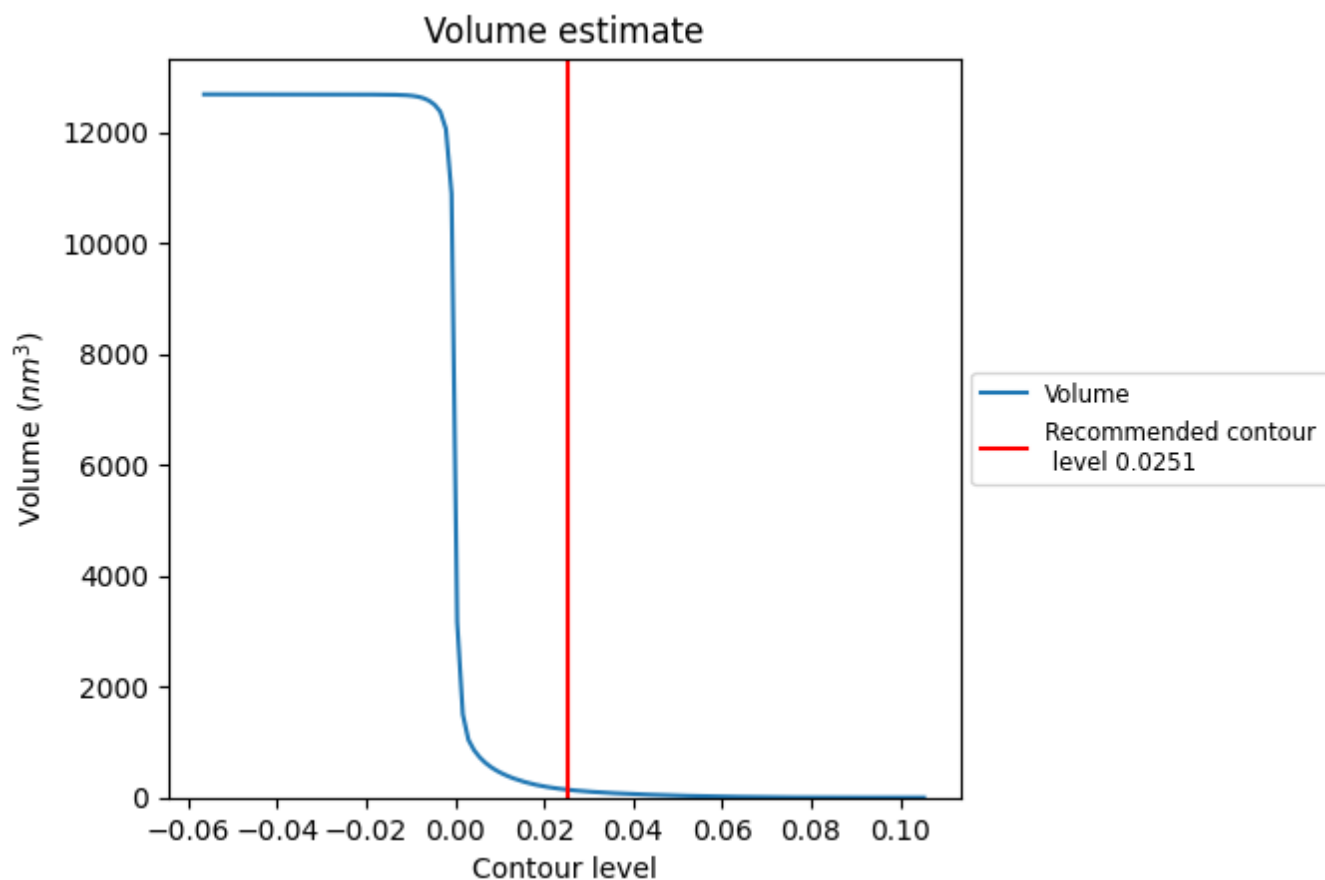
This section contains the results of statistical analysis of the map.

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.

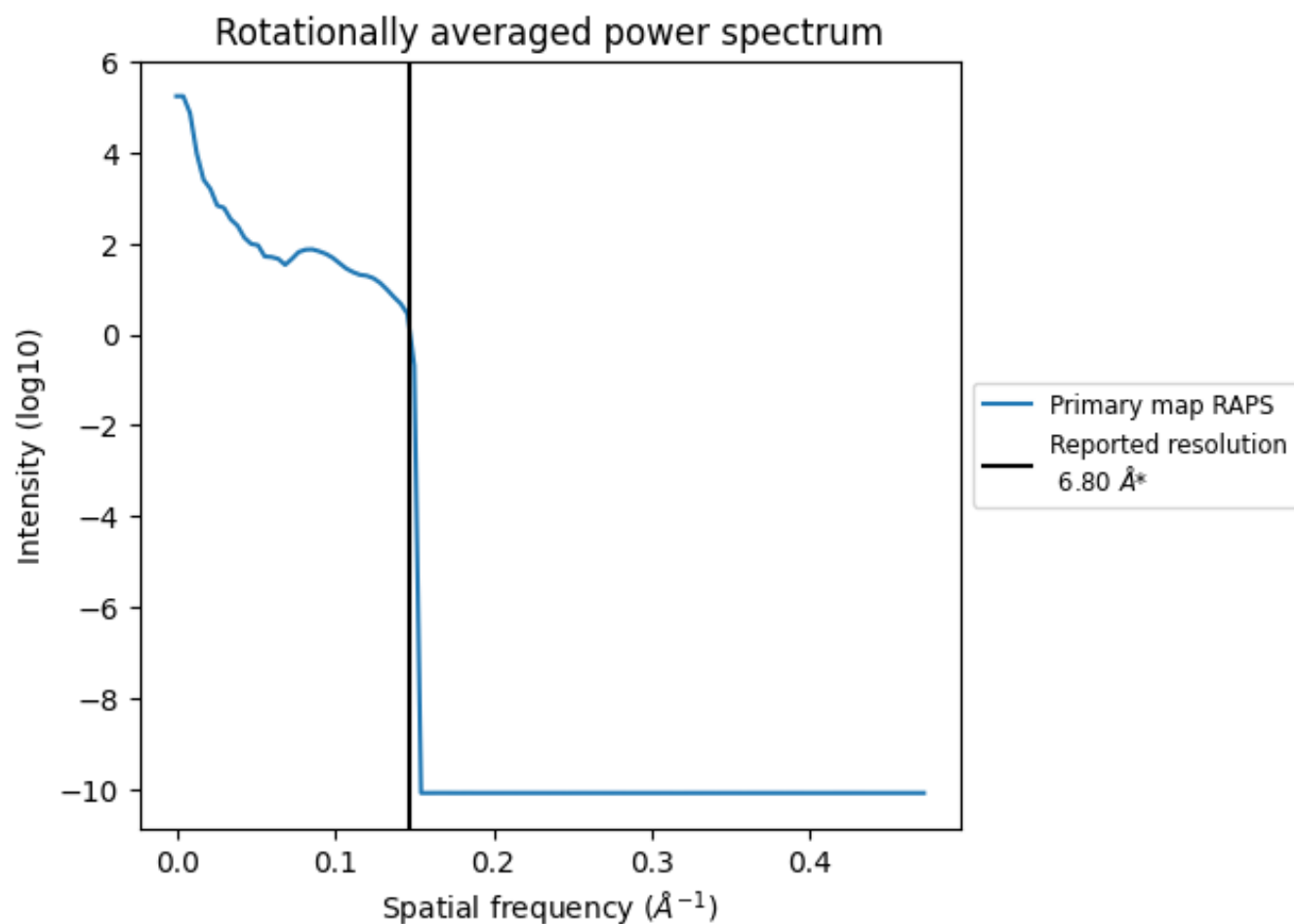
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm³; this corresponds to an approximate mass of 130 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 ⓘ

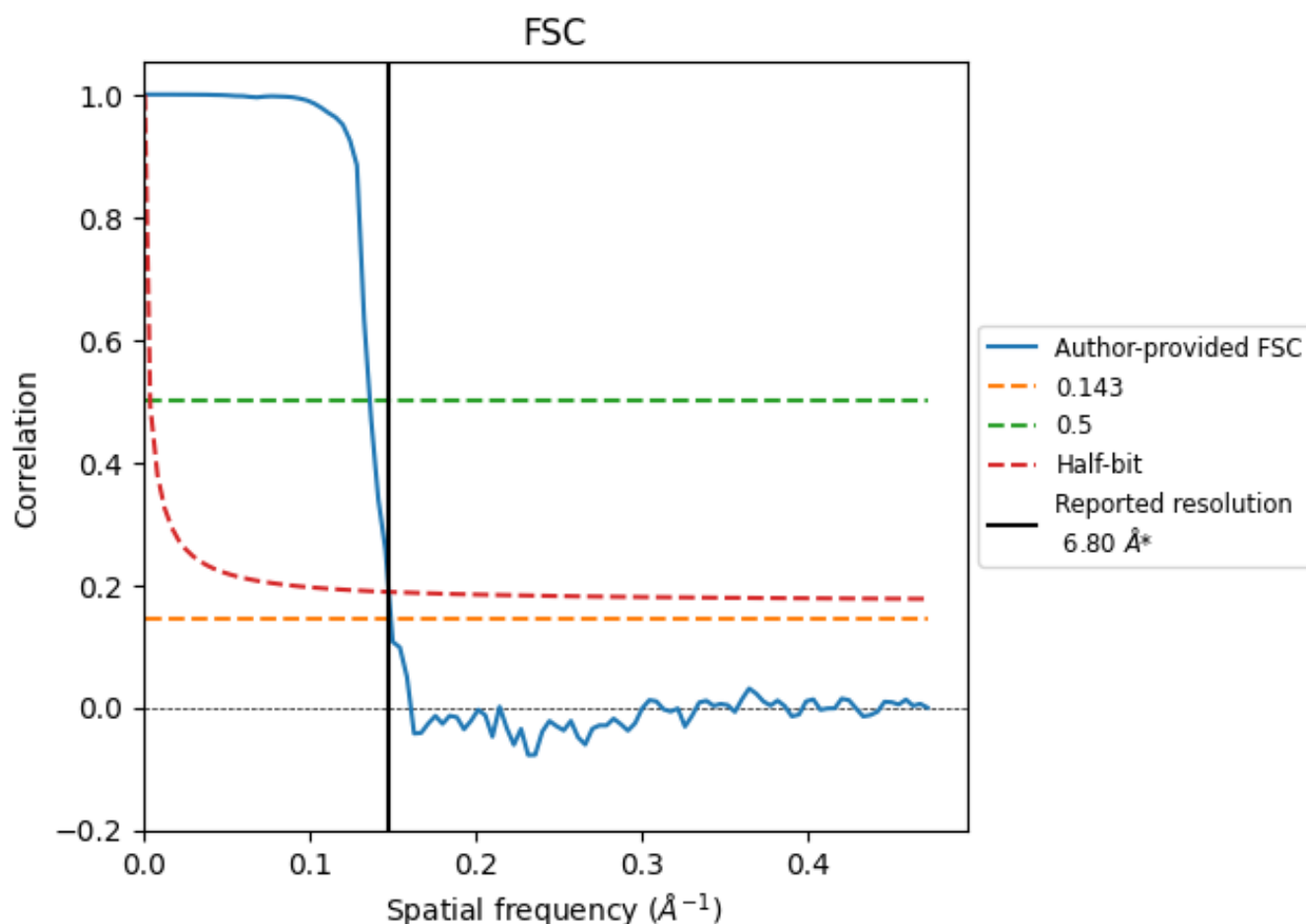


*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8.2 Resolution estimates [i](#)

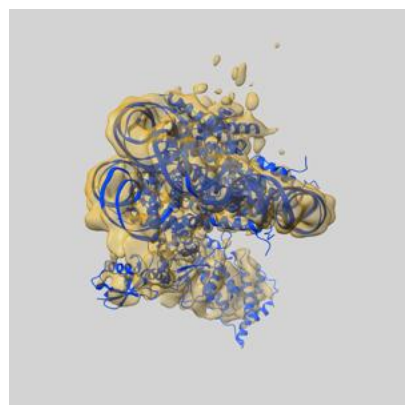
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.71	7.33	6.77
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

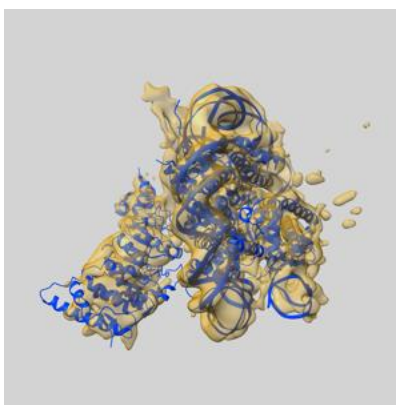
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9844 and PDB model 6JMA. Per-residue inclusion information can be found in section [3](#) on page [7](#).

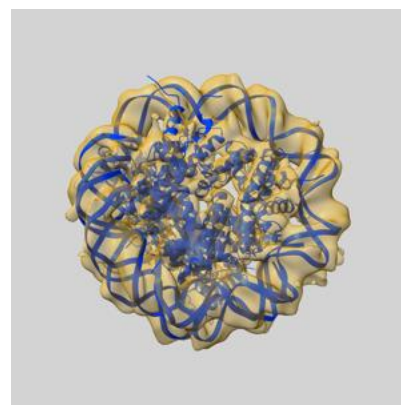
9.1 Map-model overlay [i](#)



X



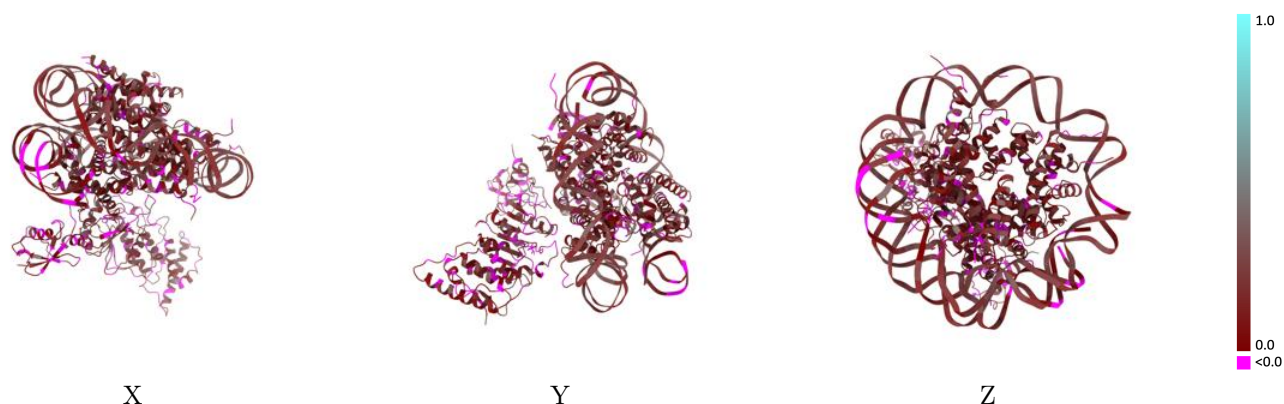
Y



Z

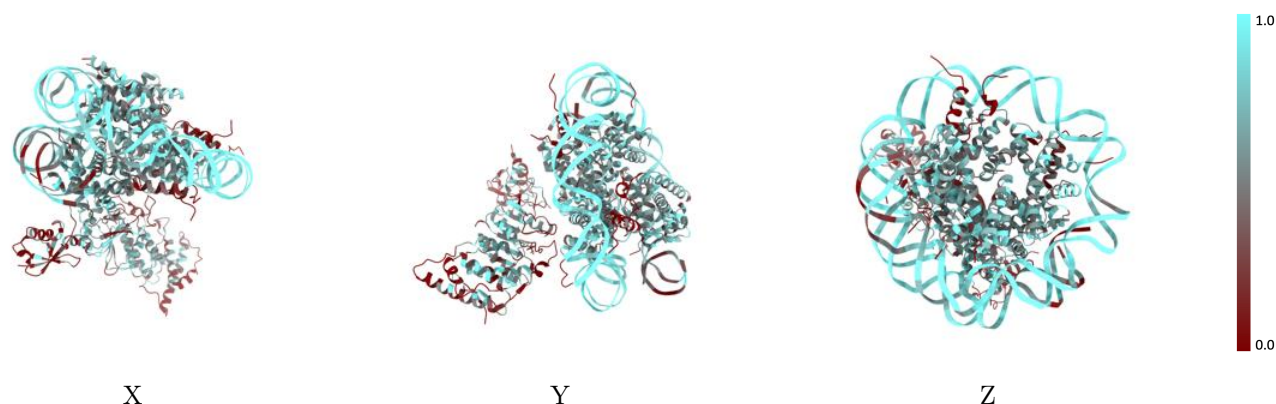
The images above show the 3D surface view of the map at the recommended contour level 0.0251 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



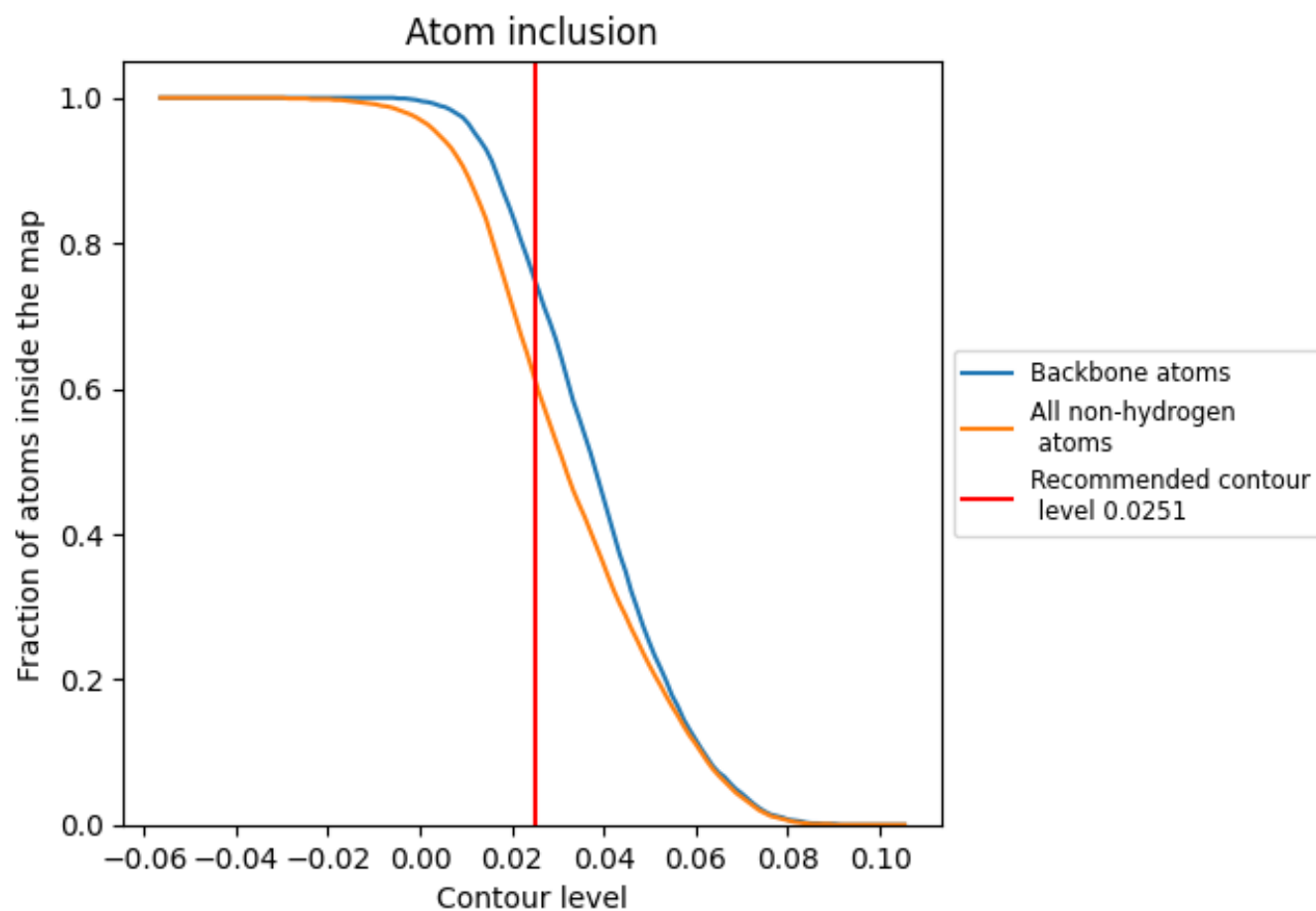
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0251).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 61% 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 (0.0251) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6100	0.1440
A	0.5410	0.1100
B	0.6170	0.1330
C	0.5470	0.1420
D	0.6120	0.1360
E	0.5120	0.1140
F	0.5740	0.1290
G	0.5590	0.1440
H	0.6160	0.1460
I	0.8150	0.1930
J	0.8030	0.1930
X	0.4420	0.1020
Y	0.1870	0.0650

