Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 10:02 pm GMT

PDB ID	:	6R1U
EMDB ID	:	EMD-4705
Title	:	Structure of LSD2/NPAC-linker/nucleosome core particle complex: Class 2
Authors	:	Marabelli, C.; Pilotto, S.; Chittori, S.; Subramaniam, S.; Mattevi, A.
Deposited on	:	2019-03-15
Resolution	:	4.36 Å(reported)
Based on initial models	:	4HSU, 6ESF

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:

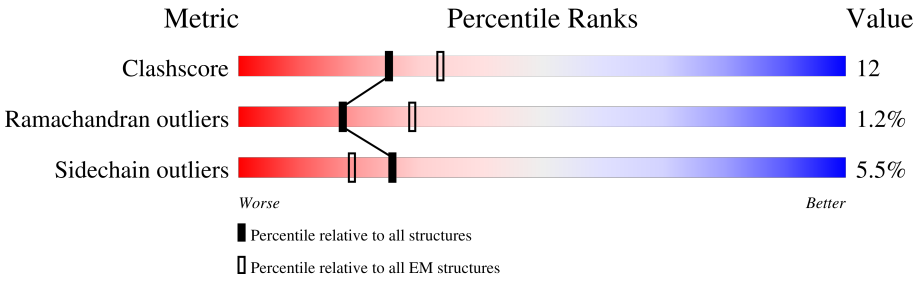
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.36 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 >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	135	51% 17% 27%
1	E	135	51% 19% 27%
2	B	102	58% 19% 5% 17%
2	F	102	60% 15% 22%
3	C	129	63% 16% 19%
3	G	129	67% 16% 12%
4	D	122	64% 11% 21%
4	H	122	61% 13% 20%

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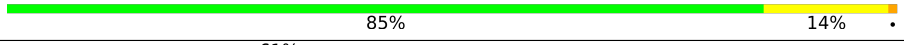
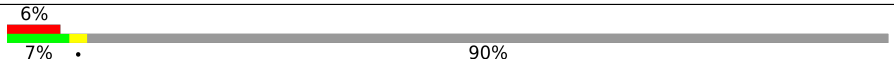
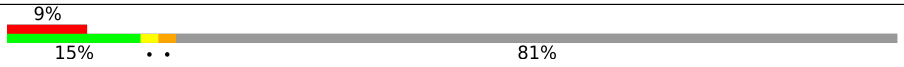
Mol	Chain	Length	Quality of chain
5	I	147	
6	J	147	
7	K	776	
8	L	124	
9	M	135	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 18394 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	99	Total	C	N	O	S	0	0
			816	515	158	140	3		
1	E	99	Total	C	N	O	S	0	0
			820	518	159	140	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	conflict	UNP P84233
E	102	ALA	GLY	conflict	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	85	Total	C	N	O	S	0	0
			689	434	139	115	1		
2	F	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	105	Total	C	N	O	0	0
			811	511	158	142		
3	G	113	Total	C	N	O	0	0
			870	547	172	151		

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			757	475	140	140	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	98	Total	C	N	O	S	0	0
			775	487	144	142	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	conflict	UNP P02281
H	29	THR	SER	conflict	UNP P02281

- Molecule 5 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	147	Total	C	N	O	P	0	0
			3031	1435	566	883	147		

- Molecule 6 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	147	Total	C	N	O	P	0	0
			2996	1423	545	881	147		

- Molecule 7 is a protein called Lysine-specific histone demethylase 1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	737	Total	C	N	O	S	0	0
			5837	3727	994	1075	41		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	47	PRO	-	expression tag	UNP Q8NB78
K	48	LEU	-	expression tag	UNP Q8NB78
K	49	GLY	-	expression tag	UNP Q8NB78
K	50	SER	-	expression tag	UNP Q8NB78

- Molecule 8 is a protein called Putative oxidoreductase GLYR1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	12	Total	C	N	O	0	0
			105	69	19	17		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	145	PRO	-	expression tag	UNP Q49A26
L	146	LEU	-	expression tag	UNP Q49A26
L	147	GLY	-	expression tag	UNP Q49A26
L	148	SER	-	expression tag	UNP Q49A26
L	149	PRO	-	expression tag	UNP Q49A26
L	150	GLU	-	expression tag	UNP Q49A26
L	151	PHE	-	expression tag	UNP Q49A26

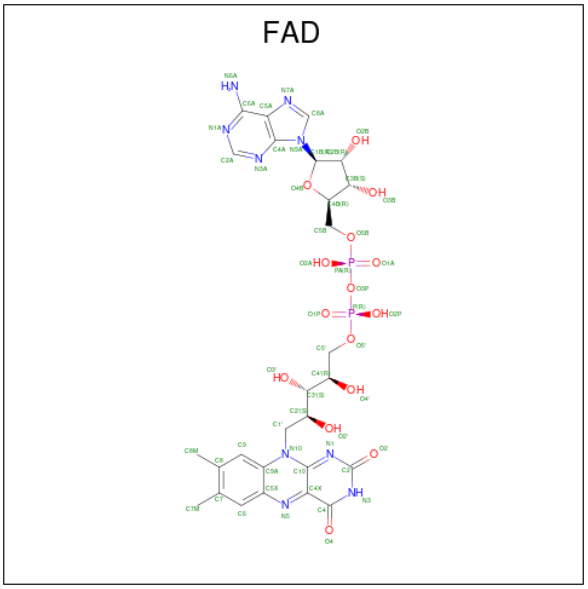
- Molecule 9 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	26	Total	C	N	O	S	0	0
			193	115	44	33	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	4	MET	LYS	conflict	UNP A0A310TTQ1

- Molecule 10 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					AltConf
10	K	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

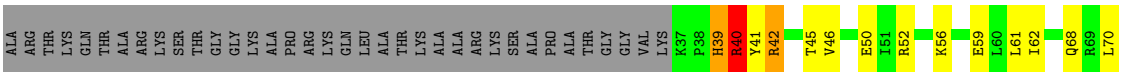
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
11	K	3	3	3	0

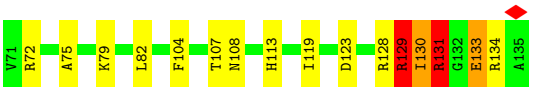
3 Residue-property plots (i)

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: Histone H3.2

Chain A:



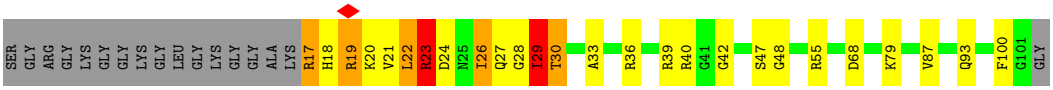


• Molecule 1: Histone H3.2

Chain E:

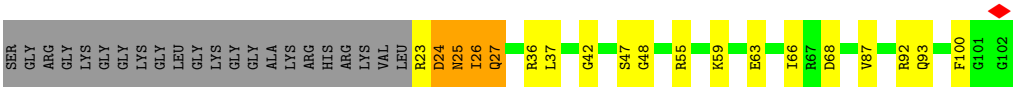
• Molecule 2: Histone H4

Chain B:



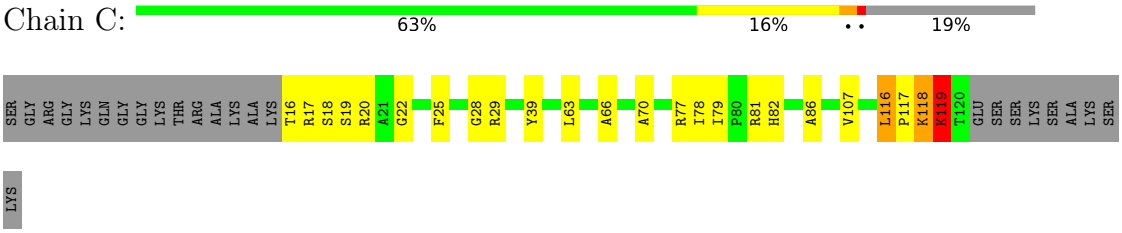
• Molecule 2: Histone H4

Chain F:



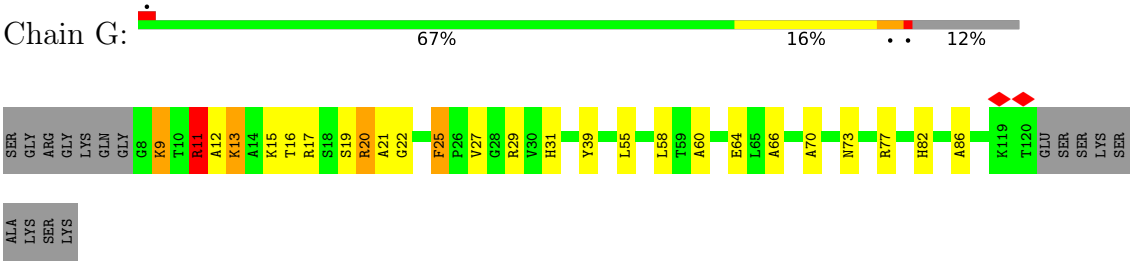
• Molecule 3: Histone H2A

Chain C:



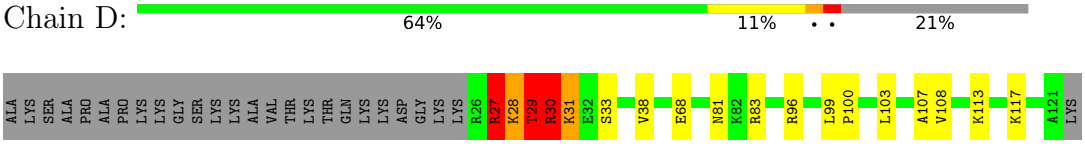
• Molecule 3: Histone H2A

Chain G:



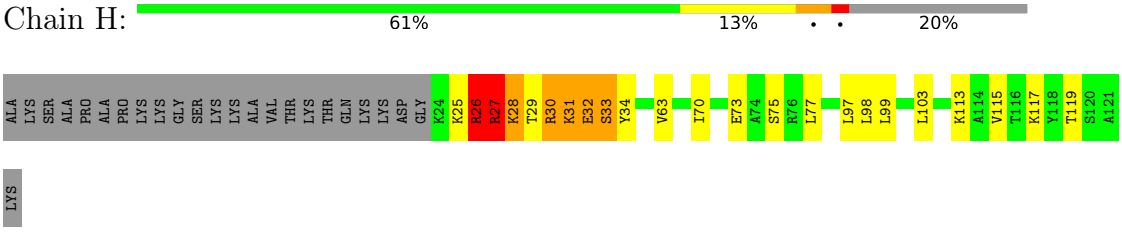
• Molecule 4: Histone H2B 1.1

Chain D:



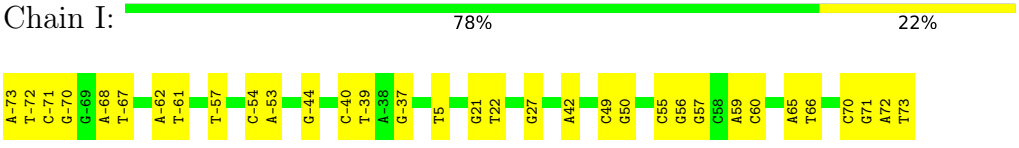
• Molecule 4: Histone H2B 1.1

Chain H:



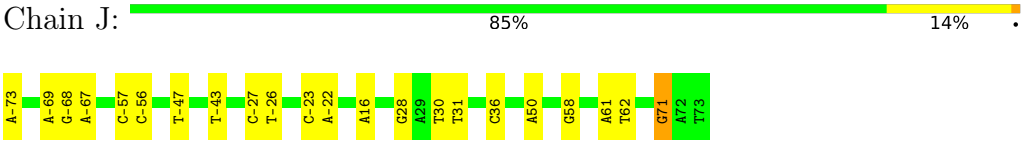
• Molecule 5: DNA (147-MER)

Chain I:



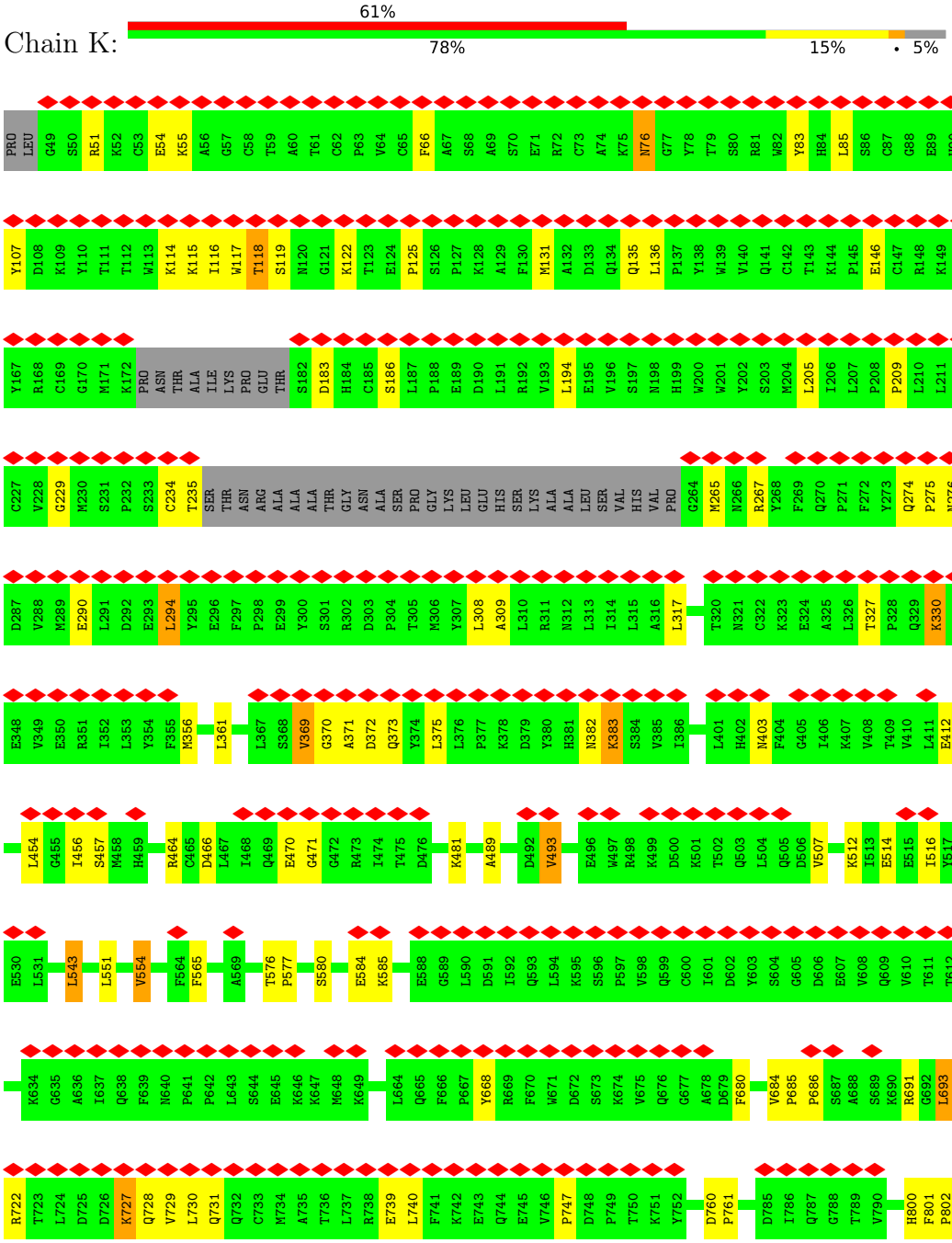
• Molecule 6: DNA (147-MER)

Chain J:



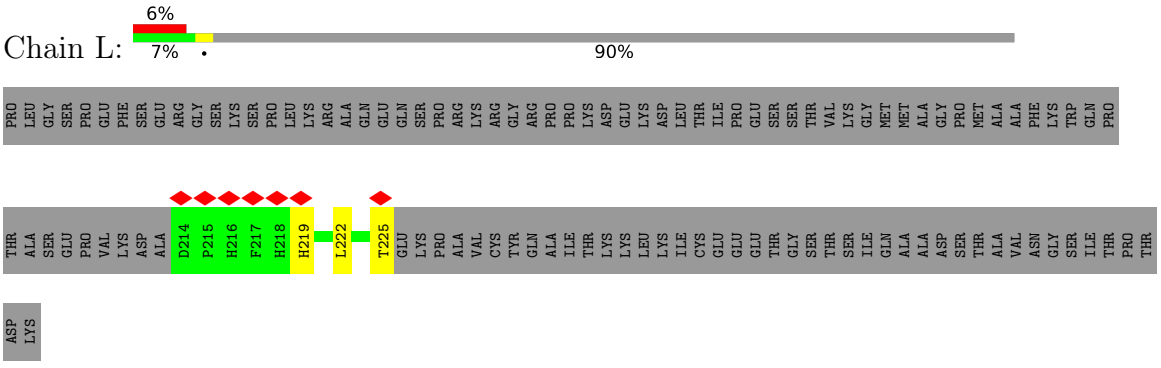
• Molecule 7: Lysine-specific histone demethylase 1B

Chain K:

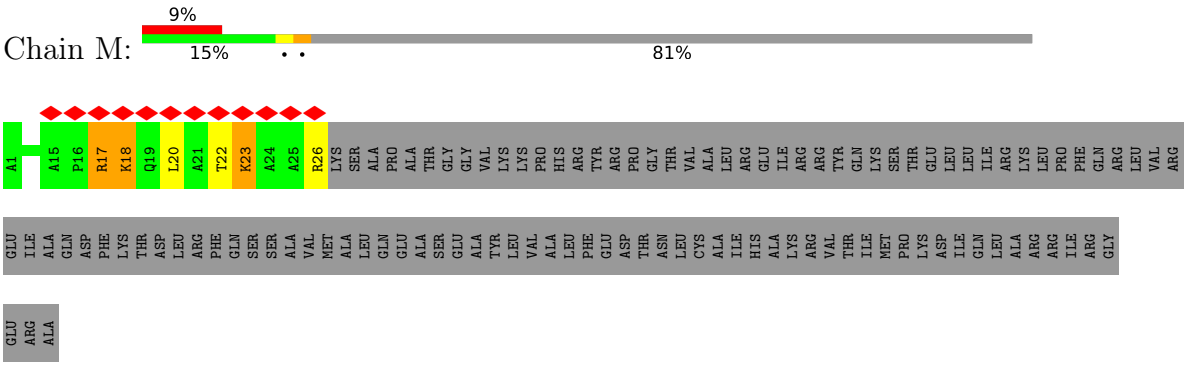


• Molecule 8: Putative oxidoreductase GLYR1

Chain L:



• Molecule 9: Histone H3



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	72315	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	0.7	Depositor
Maximum defocus (nm)	3.05	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0112	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ZN, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.43	0/828	0.60	0/1111
1	E	0.41	0/832	0.61	0/1115
2	B	0.40	0/697	0.58	0/932
2	F	0.44	0/645	0.55	0/862
3	C	0.42	0/821	0.62	0/1109
3	G	0.40	0/880	0.60	0/1185
4	D	0.44	0/768	0.56	0/1032
4	H	0.44	0/786	0.56	0/1054
5	I	0.88	1/3403 (0.0%)	1.05	2/5255 (0.0%)
6	J	0.87	1/3357 (0.0%)	1.03	0/5174
7	K	0.32	0/5981	0.46	1/8100 (0.0%)
8	L	0.27	0/110	0.42	0/149
9	M	0.34	0/193	0.45	0/254
All	All	0.60	2/19301 (0.0%)	0.76	3/27332 (0.0%)

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	A	0	3
3	G	0	1
4	D	0	1
4	H	0	3
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	71	DG	C1'-N9	-8.28	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	71	DG	C1'-N9	-7.44	1.36	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	151	ARG	NE-CZ-NH1	-5.27	117.67	120.30
5	I	42	DA	O4'-C1'-N9	5.17	111.62	108.00
5	I	-57	DT	O4'-C1'-N1	5.06	111.54	108.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ARG	Sidechain
1	A	131	ARG	Sidechain
1	A	40	ARG	Sidechain
4	D	27	ARG	Sidechain
3	G	11	ARG	Sidechain
4	H	26	ARG	Sidechain
4	H	27	ARG	Sidechain
4	H	30	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	816	0	858	52	0
1	E	820	0	866	59	0
2	B	689	0	739	38	0
2	F	638	0	676	33	0
3	C	811	0	866	35	0
3	G	870	0	938	28	0
4	D	757	0	783	36	0
4	H	775	0	809	43	0
5	I	3031	0	1651	51	0
6	J	2996	0	1650	28	0
7	K	5837	0	5749	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	105	0	91	2	0
9	M	193	0	218	11	0
10	K	53	0	30	2	0
11	K	3	0	0	0	0
All	All	18394	0	15924	393	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 12.

All (393) 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:E:70:LEU:HA	2:F:25:ASN:OD1	1.31	1.30
1:A:41:TYR:O	1:A:42:ARG:CG	1.82	1.28
1:E:70:LEU:CA	2:F:25:ASN:OD1	1.83	1.26
4:D:30:ARG:O	4:D:31:LYS:HG3	1.19	1.24
5:I:-70:DG:C2	6:J:71:DG:N2	2.08	1.22
4:H:32:GLU:OE1	4:H:33:SER:O	1.60	1.19
3:G:17:ARG:HD2	6:J:-43:DT:OP2	1.43	1.18
3:G:29:ARG:CZ	4:H:32:GLU:OE2	1.94	1.16
1:E:69:ARG:C	2:F:25:ASN:OD1	1.84	1.15
1:E:70:LEU:N	2:F:25:ASN:OD1	1.79	1.13
1:E:37:LYS:HD2	1:E:38:PRO:CD	1.81	1.11
5:I:-70:DG:N2	6:J:71:DG:C2	2.21	1.09
1:E:37:LYS:H	1:E:38:PRO:CD	1.66	1.08
4:D:30:ARG:CG	4:D:31:LYS:H	1.67	1.07
2:B:27:GLN:OE1	2:B:55:ARG:HD3	1.53	1.07
1:E:69:ARG:CB	2:F:25:ASN:HD21	1.68	1.07
1:A:41:TYR:O	1:A:42:ARG:HG3	0.89	1.06
1:A:129:ARG:HH21	1:A:129:ARG:HB2	1.19	1.06
2:F:23:ARG:HD2	7:K:101:ARG:HD2	1.30	1.05
4:D:30:ARG:HG2	4:D:31:LYS:H	0.92	1.05
4:D:30:ARG:HG2	4:D:31:LYS:N	1.73	1.04
1:E:37:LYS:CD	1:E:38:PRO:HD3	1.87	1.04
4:D:30:ARG:O	4:D:31:LYS:CG	2.05	1.04
5:I:-70:DG:C2	6:J:71:DG:C2	2.49	1.00
5:I:-73:DA:H2"	5:I:-72:DT:C7	1.91	1.00
4:H:31:LYS:HB2	5:I:50:DG:OP1	1.62	1.00
3:G:29:ARG:NH2	4:H:32:GLU:OE2	1.94	0.99
1:E:37:LYS:H	1:E:38:PRO:HD3	1.23	0.99
3:G:29:ARG:NH1	4:H:32:GLU:CD	2.16	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:HIS:NE2	5:I:-67:DT:OP1	1.96	0.98
5:I:72:DA:H3'	5:I:73:DT:H71	1.47	0.95
1:E:69:ARG:O	2:F:25:ASN:OD1	1.86	0.94
9:M:17:ARG:H	9:M:17:ARG:HD3	1.31	0.94
7:K:369:VAL:HG22	7:K:373:GLN:HB3	1.48	0.93
7:K:580:SER:O	7:K:584:GLU:HG2	1.69	0.92
5:I:-70:DG:N2	6:J:71:DG:N2	2.14	0.92
1:E:69:ARG:HB3	2:F:25:ASN:HD21	1.31	0.92
1:E:37:LYS:HD2	1:E:38:PRO:HD3	0.95	0.91
4:D:30:ARG:CG	4:D:31:LYS:N	2.28	0.91
7:K:727:LYS:HE3	7:K:731:GLN:HE22	1.36	0.89
2:B:17:ARG:HG2	2:B:17:ARG:HH21	1.37	0.89
4:H:26:ARG:HG2	4:H:26:ARG:HH11	1.38	0.89
1:E:36:LYS:HD2	1:E:37:LYS:HG3	1.54	0.89
3:G:17:ARG:CD	6:J:-43:DT:OP2	2.21	0.88
4:D:28:LYS:HD2	4:D:28:LYS:N	1.87	0.88
5:I:-73:DA:H2"	5:I:-72:DT:H71	1.55	0.87
7:K:727:LYS:HE3	7:K:731:GLN:NE2	1.89	0.87
3:G:29:ARG:CZ	4:H:32:GLU:CD	2.43	0.87
3:G:11:ARG:HB2	3:G:11:ARG:HH21	1.41	0.86
9:M:17:ARG:HD3	9:M:17:ARG:N	1.91	0.85
2:B:22:LEU:O	2:B:24:ASP:N	2.09	0.85
1:E:73:GLU:OE1	2:F:25:ASN:HB2	1.77	0.85
3:C:118:LYS:NZ	3:C:118:LYS:O	2.09	0.85
1:E:39:HIS:HE1	5:I:-67:DT:C5'	1.89	0.85
4:H:29:THR:OG1	6:J:30:DT:OP1	1.95	0.85
1:A:41:TYR:C	1:A:42:ARG:HG3	1.96	0.84
3:G:29:ARG:NH1	4:H:32:GLU:OE2	2.08	0.84
7:K:209:PRO:HG3	7:K:341:VAL:HG21	1.60	0.84
2:F:23:ARG:CD	7:K:101:ARG:HD2	2.07	0.83
3:C:119:LYS:O	3:C:119:LYS:NZ	2.11	0.83
4:H:32:GLU:OE2	5:I:49:DC:OP1	1.97	0.83
3:C:118:LYS:H	3:C:118:LYS:CE	1.92	0.82
1:E:69:ARG:HB2	2:F:25:ASN:HD21	1.44	0.82
3:G:19:SER:O	3:G:22:GLY:N	2.11	0.81
1:A:129:ARG:HH21	1:A:129:ARG:CB	1.93	0.81
1:E:39:HIS:HE1	5:I:-67:DT:H5"	1.46	0.81
1:E:37:LYS:N	1:E:38:PRO:CD	2.43	0.81
7:K:493:VAL:HG22	7:K:516:ILE:HD13	1.63	0.81
1:E:69:ARG:HB3	2:F:25:ASN:ND2	1.96	0.80
4:H:31:LYS:HE2	4:H:31:LYS:HA	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:5:DT:OP1	9:M:23:LYS:NZ	2.14	0.80
2:B:24:ASP:HB2	2:B:27:GLN:HB2	1.64	0.80
2:F:26:ILE:CD1	2:F:59:LYS:HD2	2.13	0.79
1:A:68:GLN:HE21	1:A:72:ARG:HH21	1.30	0.78
2:B:27:GLN:OE1	2:B:55:ARG:CD	2.30	0.78
1:E:38:PRO:O	1:E:40:ARG:N	2.18	0.77
2:F:26:ILE:HD11	2:F:59:LYS:HD2	1.66	0.76
5:I:-70:DG:N3	6:J:71:DG:N2	2.33	0.76
1:E:68:GLN:HE21	1:E:72:ARG:HH21	1.33	0.76
1:E:52:ARG:O	1:E:56:LYS:HB2	1.86	0.75
5:I:-70:DG:N1	6:J:71:DG:N1	2.35	0.75
3:C:119:LYS:HE3	3:C:119:LYS:N	2.02	0.74
4:H:26:ARG:HG2	4:H:26:ARG:NH1	1.96	0.74
3:C:118:LYS:H	3:C:118:LYS:CD	2.00	0.74
2:B:29:ILE:N	2:B:29:ILE:HD12	2.01	0.72
3:G:11:ARG:HB2	3:G:11:ARG:NH2	2.03	0.72
1:E:39:HIS:CE1	5:I:-67:DT:C5'	2.72	0.72
2:F:23:ARG:HD3	7:K:103:HIS:HE1	1.55	0.72
3:G:12:ALA:O	3:G:13:LYS:O	2.07	0.71
1:A:129:ARG:HB2	1:A:129:ARG:NH2	2.02	0.71
4:D:28:LYS:HD2	4:D:28:LYS:H	1.54	0.71
7:K:327:THR:OG1	7:K:330:LYS:HG2	1.89	0.71
4:D:30:ARG:HD2	4:D:31:LYS:N	2.05	0.70
2:F:27:GLN:HA	2:F:27:GLN:NE2	2.06	0.70
7:K:209:PRO:HG3	7:K:341:VAL:CG2	2.22	0.70
1:E:46:VAL:O	1:E:50:GLU:HB2	1.93	0.69
1:A:70:LEU:HD11	2:B:26:ILE:HG13	1.75	0.69
1:E:37:LYS:HD2	1:E:37:LYS:N	2.07	0.69
3:C:117:PRO:HD3	1:E:48:LEU:CD1	2.23	0.68
1:E:37:LYS:N	1:E:38:PRO:HD3	2.01	0.68
4:D:30:ARG:CZ	4:D:30:ARG:HB3	2.23	0.68
3:G:29:ARG:NH1	4:H:32:GLU:OE1	2.27	0.68
7:K:76:ASN:HD22	7:K:76:ASN:H	1.42	0.67
5:I:-73:DA:H2"	5:I:-72:DT:H73	1.77	0.67
7:K:276:ASN:HA	9:M:20:LEU:O	1.94	0.67
2:B:28:GLY:O	2:B:30:THR:N	2.26	0.67
4:D:30:ARG:CD	4:D:31:LYS:N	2.57	0.67
5:I:-73:DA:C2'	5:I:-72:DT:C7	2.70	0.67
1:E:37:LYS:HD2	1:E:37:LYS:H	1.60	0.66
7:K:382:ASN:O	7:K:383:LYS:HB3	1.96	0.66
1:A:41:TYR:HA	5:I:70:DC:H5"	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-73:DA:C2'	5:I:-72:DT:H71	2.24	0.65
1:A:130:ILE:HD13	1:E:106:ASP:HB3	1.79	0.65
1:A:70:LEU:HD13	2:B:26:ILE:HG12	1.79	0.64
7:K:668:TYR:CZ	7:K:747:PRO:HG3	2.32	0.64
7:K:727:LYS:HD3	7:K:728:GLN:N	2.13	0.64
9:M:17:ARG:H	9:M:17:ARG:CD	2.00	0.64
1:A:62:ILE:HG22	2:B:33:ALA:HB1	1.78	0.64
1:A:108:ASN:ND2	2:B:42:GLY:O	2.32	0.63
2:B:26:ILE:HD13	2:B:26:ILE:O	1.99	0.63
3:C:28:GLY:HA3	5:I:-44:DG:H3'	1.81	0.63
3:C:117:PRO:HD3	1:E:48:LEU:HD13	1.80	0.63
7:K:719:ALA:O	7:K:722:ARG:HG2	1.98	0.63
2:B:29:ILE:O	2:B:30:THR:O	2.17	0.63
3:G:82:HIS:O	3:G:86:ALA:HB2	1.99	0.62
3:C:66:ALA:O	3:C:70:ALA:HB2	2.00	0.62
7:K:99:TYR:CE2	7:K:131:MET:HE1	2.35	0.62
2:B:29:ILE:O	2:B:29:ILE:HD13	1.99	0.61
3:G:19:SER:O	3:G:21:ALA:N	2.34	0.61
4:H:28:LYS:HG3	4:H:29:THR:H	1.66	0.61
3:G:66:ALA:O	3:G:70:ALA:HB2	2.00	0.61
4:H:28:LYS:HG3	4:H:29:THR:N	2.16	0.60
1:E:108:ASN:ND2	2:F:42:GLY:O	2.34	0.60
2:B:17:ARG:HG2	2:B:17:ARG:NH2	2.07	0.60
1:A:40:ARG:H	1:A:40:ARG:NH1	2.00	0.59
4:H:31:LYS:NZ	4:H:31:LYS:HB3	2.17	0.59
2:F:24:ASP:OD1	2:F:27:GLN:HB2	2.03	0.59
6:J:61:DA:H2"	6:J:62:DT:H2'	1.84	0.59
1:A:131:ARG:CB	1:A:131:ARG:HH11	2.16	0.59
7:K:285:ARG:HD3	9:M:20:LEU:HD13	1.84	0.59
1:A:41:TYR:OH	6:J:-67:DA:H4'	2.04	0.58
4:D:30:ARG:HB2	6:J:50:DA:OP1	2.02	0.58
1:E:39:HIS:CE1	5:I:-67:DT:H5"	2.32	0.58
7:K:76:ASN:HD22	7:K:76:ASN:N	2.02	0.58
4:H:27:ARG:HD2	6:J:31:DT:OP1	2.04	0.58
3:G:29:ARG:NH1	4:H:33:SER:O	2.37	0.58
7:K:361:LEU:HD11	8:L:219:HIS:CE1	2.39	0.58
3:C:17:ARG:HG2	3:C:20:ARG:HD2	1.84	0.57
2:F:27:GLN:OE1	2:F:55:ARG:CZ	2.52	0.57
1:A:70:LEU:CD1	2:B:26:ILE:CG1	2.82	0.57
7:K:693:LEU:HD22	7:K:694:PHE:CE2	2.39	0.57
1:E:42:ARG:NH1	6:J:71:DG:OP2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:82:HIS:O	3:G:86:ALA:CB	2.53	0.57
4:D:30:ARG:HB3	4:D:30:ARG:NH1	2.19	0.57
4:H:99:LEU:HD12	4:H:103:LEU:HB3	1.87	0.57
1:A:130:ILE:CG2	1:E:130:ILE:HG21	2.34	0.57
4:H:31:LYS:HE2	4:H:31:LYS:CA	2.32	0.57
7:K:721:VAL:HG22	7:K:729:VAL:HG22	1.87	0.57
7:K:454:LEU:HD21	7:K:585:LYS:HG2	1.88	0.56
4:H:31:LYS:HA	4:H:31:LYS:CE	2.35	0.56
4:D:30:ARG:HG3	4:D:30:ARG:HH11	1.69	0.56
1:E:39:HIS:NE2	5:I:-68:DA:H4'	2.21	0.56
2:F:26:ILE:HD11	2:F:59:LYS:CD	2.35	0.56
5:I:-70:DG:C2	6:J:71:DG:N1	2.72	0.56
1:A:123:ASP:OD1	1:E:113:HIS:NE2	2.31	0.56
1:A:104:PHE:HA	1:A:107:THR:HG22	1.88	0.56
3:C:82:HIS:O	3:C:86:ALA:CB	2.55	0.55
2:B:29:ILE:HD11	2:B:55:ARG:HG2	1.88	0.55
7:K:514:GLU:OE1	7:K:518:LYS:HE3	2.07	0.55
1:A:129:ARG:O	1:A:129:ARG:HD3	2.06	0.55
5:I:73:DT:C2	6:J:-73:DA:N1	2.75	0.55
3:C:119:LYS:HZ2	3:C:119:LYS:C	2.05	0.54
3:C:82:HIS:O	3:C:86:ALA:HB2	2.06	0.54
4:D:30:ARG:CZ	4:D:30:ARG:CB	2.86	0.54
3:G:19:SER:O	3:G:20:ARG:C	2.44	0.54
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.32	0.54
4:D:30:ARG:O	4:D:31:LYS:CB	2.55	0.54
4:H:31:LYS:HB3	4:H:31:LYS:HZ3	1.73	0.54
3:C:118:LYS:H	3:C:118:LYS:HD3	1.72	0.53
5:I:-37:DG:O6	6:J:36:DC:N4	2.42	0.53
4:D:113:LYS:O	4:D:117:LYS:CB	2.57	0.53
2:F:92:ARG:HH12	4:H:97:LEU:HD22	1.73	0.53
7:K:122:LYS:O	7:K:122:LYS:HG2	2.09	0.53
1:A:41:TYR:CD2	5:I:70:DC:H5"	2.43	0.53
3:C:118:LYS:H	3:C:118:LYS:HE3	1.73	0.53
3:C:29:ARG:NH1	4:D:33:SER:O	2.42	0.53
1:E:97:GLU:O	1:E:101:VAL:HB	2.08	0.53
1:A:70:LEU:CD1	2:B:26:ILE:HG13	2.38	0.53
4:H:113:LYS:O	4:H:117:LYS:HB2	2.08	0.53
5:I:59:DA:H2"	5:I:60:DC:H2'	1.91	0.53
1:A:46:VAL:O	1:A:50:GLU:HB3	2.09	0.52
4:D:29:THR:HA	4:D:30:ARG:HH21	1.74	0.52
7:K:727:LYS:HD3	7:K:728:GLN:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:ILE:HG13	3:C:81:ARG:H	1.74	0.52
3:G:73:ASN:HB2	3:G:82:HIS:HE2	1.74	0.52
1:E:62:ILE:HD11	2:F:37:LEU:HD11	1.91	0.52
2:F:27:GLN:NE2	2:F:27:GLN:CA	2.73	0.52
3:C:119:LYS:N	3:C:119:LYS:CE	2.73	0.52
5:I:-73:DA:C2'	5:I:-72:DT:H73	2.38	0.52
1:A:70:LEU:CD1	2:B:26:ILE:HG12	2.39	0.52
7:K:223:TYR:CE1	7:K:275:PRO:HD3	2.44	0.52
7:K:456:ILE:HG23	7:K:577:PRO:HG2	1.92	0.52
1:A:79:LYS:HD3	1:A:82:LEU:HD21	1.90	0.52
3:C:39:TYR:OH	4:D:68:GLU:OE1	2.28	0.51
7:K:217:ALA:HB3	7:K:218:PRO:HD3	1.91	0.51
2:B:87:VAL:HG21	2:B:100:PHE:HB2	1.93	0.51
1:A:129:ARG:NH2	1:A:129:ARG:CG	2.73	0.51
4:D:113:LYS:O	4:D:117:LYS:HB2	2.09	0.51
5:I:73:DT:C7	5:I:73:DT:OP2	2.59	0.51
2:F:87:VAL:HG21	2:F:100:PHE:HB2	1.93	0.51
7:K:412:GLU:OE1	10:K:901:FAD:O3B	2.27	0.51
1:A:50:GLU:OE1	2:B:39:ARG:NH1	2.44	0.51
1:A:129:ARG:HH21	1:A:129:ARG:CG	2.24	0.51
1:E:39:HIS:HE2	5:I:-68:DA:H4'	1.76	0.51
1:A:131:ARG:NH1	1:A:131:ARG:CG	2.73	0.51
3:C:66:ALA:O	3:C:70:ALA:CB	2.59	0.51
3:G:27:VAL:O	3:G:31:HIS:HB2	2.11	0.51
7:K:114:LYS:HG3	7:K:125:PRO:HB2	1.92	0.50
3:C:118:LYS:CD	3:C:118:LYS:N	2.73	0.50
1:E:36:LYS:O	1:E:36:LYS:HD3	2.10	0.50
1:A:70:LEU:HD11	2:B:26:ILE:CG1	2.39	0.50
7:K:489:ALA:O	7:K:493:VAL:HG12	2.11	0.50
7:K:551:LEU:HA	7:K:554:VAL:HG13	1.92	0.50
7:K:668:TYR:CE2	7:K:747:PRO:HG3	2.47	0.50
3:C:18:SER:O	3:C:22:GLY:N	2.44	0.50
4:D:30:ARG:CG	4:D:30:ARG:HH11	2.25	0.50
1:A:52:ARG:O	1:A:56:LYS:HB2	2.11	0.49
5:I:73:DT:O2	6:J:-73:DA:C2	2.66	0.49
4:D:30:ARG:HD2	4:D:30:ARG:C	2.33	0.49
9:M:18:LYS:HB3	9:M:18:LYS:NZ	2.27	0.49
1:A:40:ARG:NH1	1:A:40:ARG:N	2.61	0.49
1:A:131:ARG:NH1	1:A:131:ARG:HG3	2.28	0.49
2:B:19:ARG:HB3	6:J:16:DA:OP2	2.12	0.49
3:C:77:ARG:HH11	5:I:-54:DC:H5'	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:65:DA:H1'	5:I:66:DT:H5'	1.94	0.49
1:E:39:HIS:CE1	5:I:-67:DT:O5'	2.66	0.49
6:J:-69:DA:H2"	6:J:-68:DG:H2'	1.95	0.49
2:B:47:SER:OG	2:B:48:GLY:N	2.46	0.49
4:D:30:ARG:CG	4:D:30:ARG:NH1	2.75	0.49
1:A:130:ILE:HG22	1:E:130:ILE:HG21	1.96	0.48
5:I:-72:DT:H2"	5:I:-71:DC:C5	2.48	0.48
1:E:69:ARG:CB	2:F:25:ASN:ND2	2.51	0.48
2:F:59:LYS:NZ	2:F:63:GLU:OE2	2.42	0.48
4:D:29:THR:OG1	4:D:30:ARG:N	2.45	0.48
7:K:576:THR:OG1	7:K:577:PRO:HD3	2.13	0.48
7:K:685:PRO:HB3	7:K:691:ARG:HA	1.96	0.48
4:D:29:THR:HA	4:D:30:ARG:NH2	2.29	0.48
7:K:99:TYR:HD1	7:K:106:GLY:O	1.96	0.48
1:A:46:VAL:O	1:A:50:GLU:CB	2.62	0.48
2:F:47:SER:OG	2:F:48:GLY:N	2.45	0.48
1:E:39:HIS:CE1	5:I:-68:DA:H4'	2.49	0.47
7:K:83:TYR:HE2	7:K:93:ASN:HD22	1.61	0.47
7:K:146:GLU:CD	7:K:146:GLU:H	2.17	0.47
9:M:20:LEU:HD23	9:M:20:LEU:HA	1.73	0.47
7:K:215:VAL:HG21	7:K:317:LEU:HD21	1.97	0.47
1:E:103:LEU:HD21	1:E:124:ILE:HG23	1.96	0.47
7:K:802:PRO:O	7:K:803:GLN:HB2	2.15	0.47
7:K:383:LYS:HA	7:K:621:GLN:OE1	2.15	0.47
1:A:130:ILE:HG21	1:E:130:ILE:HG21	1.97	0.47
4:D:27:ARG:HD2	4:D:27:ARG:N	2.29	0.47
3:C:77:ARG:HH21	6:J:58:DG:H5'	1.79	0.47
7:K:512:LYS:HD2	7:K:512:LYS:HA	1.69	0.47
4:H:30:ARG:NH2	6:J:-47:DT:C1'	2.69	0.46
4:H:113:LYS:O	4:H:117:LYS:CB	2.63	0.46
7:K:285:ARG:HD3	9:M:20:LEU:CD1	2.45	0.46
3:C:78:ILE:HG23	3:C:82:HIS:HB2	1.97	0.46
7:K:136:LEU:HD13	7:K:339:GLY:HA3	1.98	0.46
1:A:61:LEU:HD12	2:B:36:ARG:HE	1.80	0.46
1:E:69:ARG:C	2:F:25:ASN:CG	2.69	0.46
6:J:-57:DC:H4'	6:J:-56:DC:H5'	1.98	0.46
3:C:119:LYS:C	3:C:119:LYS:HD2	2.35	0.46
1:E:37:LYS:H	1:E:38:PRO:HD2	1.65	0.46
1:E:61:LEU:O	2:F:36:ARG:NH2	2.39	0.46
1:E:46:VAL:O	1:E:50:GLU:CB	2.62	0.46
1:A:45:THR:OG1	5:I:70:DC:OP1	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:GLN:HE22	2:F:55:ARG:CD	2.29	0.46
7:K:183:ASP:OD2	7:K:186:SER:HB3	2.16	0.46
4:D:99:LEU:HA	4:D:100:PRO:HD3	1.82	0.46
2:B:29:ILE:N	2:B:29:ILE:CD1	2.73	0.46
3:C:18:SER:OG	3:C:25:PHE:O	2.34	0.46
3:G:39:TYR:HD1	4:H:75:SER:HB2	1.81	0.46
4:H:70:ILE:HG23	4:H:98:LEU:HD12	1.97	0.46
7:K:131:MET:HE1	7:K:135:GLN:HG3	1.97	0.46
3:C:118:LYS:N	3:C:118:LYS:HZ2	2.13	0.45
7:K:285:ARG:HA	7:K:286:PRO:HD3	1.86	0.45
5:I:21:DG:H2'	5:I:22:DT:H71	1.98	0.45
4:H:29:THR:HG22	4:H:29:THR:O	2.16	0.45
4:H:30:ARG:NH2	6:J:-47:DT:H1'	2.32	0.45
7:K:76:ASN:H	7:K:76:ASN:ND2	2.11	0.45
1:A:59:GLU:O	2:B:40:ARG:NH2	2.42	0.45
1:A:130:ILE:HG22	1:E:130:ILE:CG2	2.47	0.45
7:K:470:GLU:HA	7:K:471:GLY:HA2	1.62	0.45
4:H:33:SER:OG	4:H:34:TYR:N	2.50	0.45
7:K:131:MET:CE	7:K:135:GLN:HG3	2.47	0.45
1:E:37:LYS:CD	1:E:37:LYS:N	2.73	0.45
4:D:30:ARG:N	4:D:30:ARG:NE	2.65	0.45
4:H:31:LYS:NZ	4:H:31:LYS:CB	2.80	0.45
3:G:55:LEU:HD23	4:H:63:VAL:HG13	1.98	0.45
5:I:-54:DC:H2"	5:I:-53:DA:C8	2.52	0.45
9:M:17:ARG:N	9:M:17:ARG:CD	2.61	0.45
1:A:39:HIS:CG	1:A:39:HIS:O	2.70	0.44
2:B:29:ILE:O	2:B:30:THR:C	2.55	0.44
2:B:22:LEU:C	2:B:24:ASP:N	2.71	0.44
7:K:102:SER:HA	7:K:107:TYR:CD1	2.53	0.44
7:K:225:PRO:HD3	9:M:26:ARG:NH2	2.32	0.44
7:K:507:VAL:HG21	7:K:512:LYS:HD3	1.98	0.44
7:K:371:ALA:O	7:K:372:ASP:HB2	2.18	0.44
2:B:68:ASP:OD2	2:B:93:GLN:NE2	2.50	0.44
3:G:16:THR:O	3:G:20:ARG:NE	2.41	0.44
4:H:73:GLU:O	4:H:77:LEU:CB	2.65	0.44
5:I:-62:DA:H2'	5:I:-61:DT:H71	1.98	0.44
3:G:77:ARG:HH22	5:I:57:DG:H4'	1.83	0.44
4:H:31:LYS:CA	4:H:31:LYS:CE	2.93	0.44
1:A:128:ARG:HA	1:A:133:GLU:HB3	2.00	0.44
2:B:23:ARG:CZ	2:B:23:ARG:HB3	2.48	0.43
1:A:75:ALA:HB1	1:A:82:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:O	1:A:133:GLU:N	2.52	0.43
2:F:68:ASP:OD2	2:F:93:GLN:NE2	2.51	0.43
7:K:684:VAL:HA	7:K:685:PRO:HD3	1.85	0.43
4:D:28:LYS:HD2	4:D:28:LYS:O	2.19	0.43
1:A:129:ARG:HD3	1:A:129:ARG:C	2.38	0.43
2:F:23:ARG:CD	7:K:103:HIS:HE1	2.29	0.43
1:A:129:ARG:C	1:A:129:ARG:CD	2.85	0.43
7:K:565:PHE:CD1	7:K:800:HIS:CE1	3.06	0.43
5:I:73:DT:O5'	7:K:481:LYS:HD2	2.18	0.43
6:J:-27:DC:H4'	6:J:-26:DT:H5'	2.00	0.43
7:K:801:PHE:O	7:K:807:GLY:HA3	2.18	0.43
7:K:370:GLY:O	7:K:373:GLN:HB2	2.19	0.43
3:C:116:LEU:HD23	3:C:116:LEU:HA	1.84	0.43
3:G:58:LEU:HD21	4:H:99:LEU:HD11	2.01	0.43
7:K:117:TRP:CD1	7:K:125:PRO:HG3	2.53	0.43
4:D:81:ASN:HB3	4:D:83:ARG:HH11	1.84	0.42
5:I:73:DT:OP2	5:I:73:DT:H72	2.19	0.42
2:B:29:ILE:CD1	2:B:29:ILE:C	2.87	0.42
3:C:118:LYS:CE	3:C:118:LYS:N	2.73	0.42
7:K:464:ARG:NH1	7:K:466:ASP:OD2	2.53	0.42
7:K:219:LEU:HD11	7:K:265:MET:HE1	2.01	0.42
7:K:290:GLU:O	7:K:294:LEU:HD22	2.19	0.42
2:B:22:LEU:HD13	2:B:22:LEU:HA	1.85	0.42
1:E:37:LYS:NZ	1:E:38:PRO:HD3	2.34	0.42
5:I:-72:DT:H71	5:I:-72:DT:OP2	2.19	0.42
7:K:685:PRO:HA	7:K:686:PRO:HD3	1.93	0.42
4:D:103:LEU:O	4:D:107:ALA:HB2	2.20	0.42
1:E:71:VAL:HG13	2:F:66:ILE:HD11	2.01	0.42
1:E:83:ARG:NH1	5:I:27:DG:OP1	2.52	0.42
7:K:115:LYS:HA	7:K:118:THR:OG1	2.20	0.42
7:K:471:GLY:HA2	7:K:739:GLU:O	2.20	0.42
7:K:760:ASP:HA	7:K:761:PRO:HD3	1.88	0.41
2:B:79:LYS:N	6:J:28:DG:OP1	2.49	0.41
1:E:36:LYS:HB3	1:E:37:LYS:HE3	2.02	0.41
7:K:229:GLY:HA3	7:K:309:ALA:HB2	2.02	0.41
1:A:107:THR:HG23	1:A:119:ILE:HD12	2.02	0.41
2:B:29:ILE:CD1	2:B:55:ARG:HG2	2.49	0.41
1:E:61:LEU:HA	1:E:63:ARG:HH21	1.85	0.41
4:H:26:ARG:NH1	4:H:26:ARG:CG	2.73	0.41
5:I:55:DC:H2"	5:I:56:DG:N7	2.36	0.41
2:B:28:GLY:O	2:B:30:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:THR:O	3:C:19:SER:OG	2.33	0.41
3:G:25:PHE:HD1	3:G:25:PHE:HA	1.70	0.41
7:K:803:GLN:O	10:K:901:FAD:O3'	2.37	0.41
1:A:41:TYR:HA	5:I:70:DC:C5'	2.47	0.41
1:A:131:ARG:HH11	1:A:131:ARG:HB3	1.85	0.41
4:D:96:ARG:HG3	4:D:108:VAL:HG21	2.03	0.41
2:B:17:ARG:NH2	2:B:17:ARG:CG	2.74	0.41
3:C:70:ALA:HA	3:C:82:HIS:CD2	2.55	0.41
4:D:30:ARG:CD	4:D:30:ARG:C	2.86	0.41
7:K:115:LYS:HD3	7:K:116:ILE:HG13	2.03	0.41
7:K:290:GLU:HG3	8:L:222:LEU:HD13	2.02	0.41
3:G:9:LYS:HG3	3:G:11:ARG:NH2	2.36	0.41
4:H:115:VAL:O	4:H:119:THR:OG1	2.30	0.41
5:I:-40:DC:H2'	5:I:-39:DT:C6	2.55	0.41
5:I:72:DA:H2'	5:I:73:DT:C6	2.56	0.41
7:K:274:GLN:O	7:K:277:GLU:HB2	2.21	0.41
5:I:-73:DA:H2"	5:I:-72:DT:C5	2.52	0.41
7:K:234:CYS:O	7:K:235:THR:HG22	2.20	0.41
7:K:456:ILE:CG2	7:K:577:PRO:HG2	2.50	0.41
3:C:63:LEU:HD11	4:D:38:VAL:HG13	2.02	0.40
4:H:27:ARG:HG3	6:J:31:DT:OP1	2.22	0.40
4:H:28:LYS:CG	4:H:29:THR:N	2.81	0.40
4:H:32:GLU:O	4:H:33:SER:HB2	2.21	0.40
2:B:27:GLN:C	2:B:29:ILE:HD12	2.40	0.40
3:G:60:ALA:O	3:G:64:GLU:HB2	2.21	0.40
4:H:73:GLU:O	4:H:77:LEU:HB2	2.21	0.40
6:J:-23:DC:H2"	6:J:-22:DA:H8	1.86	0.40
7:K:54:GLU:HG3	7:K:55:LYS:N	2.36	0.40
7:K:375:LEU:HD12	7:K:403:ASN:HB3	2.02	0.40
7:K:543:LEU:HD12	7:K:543:LEU:HA	1.93	0.40
4:H:29:THR:O	4:H:30:ARG:C	2.60	0.40
1:A:61:LEU:HD13	1:A:61:LEU:HA	1.91	0.40
3:C:81:ARG:NH2	3:C:107:VAL:O	2.54	0.40
3:C:118:LYS:NZ	3:C:118:LYS:N	2.70	0.40
4:D:28:LYS:O	4:D:29:THR:O	2.40	0.40
7:K:66:PHE:CD1	7:K:66:PHE:C	2.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	97/135 (72%)	90 (93%)	5 (5%)	2 (2%)	7 39
1	E	97/135 (72%)	90 (93%)	3 (3%)	4 (4%)	3 25
2	B	83/102 (81%)	73 (88%)	6 (7%)	4 (5%)	2 23
2	F	78/102 (76%)	74 (95%)	4 (5%)	0	100 100
3	C	103/129 (80%)	97 (94%)	5 (5%)	1 (1%)	15 54
3	G	111/129 (86%)	101 (91%)	7 (6%)	3 (3%)	5 34
4	D	94/122 (77%)	88 (94%)	3 (3%)	3 (3%)	4 30
4	H	96/122 (79%)	85 (88%)	9 (9%)	2 (2%)	7 39
7	K	731/776 (94%)	704 (96%)	27 (4%)	0	100 100
8	L	10/124 (8%)	10 (100%)	0	0	100 100
9	M	24/135 (18%)	22 (92%)	2 (8%)	0	100 100
All	All	1524/2011 (76%)	1434 (94%)	71 (5%)	19 (1%)	17 50

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	23	ARG
2	B	29	ILE
2	B	30	THR
4	D	29	THR
4	D	31	LYS
1	E	37	LYS
1	E	39	HIS
1	E	40	ARG
3	G	13	LYS
3	C	119	LYS
1	E	38	PRO
3	G	20	ARG
1	A	134	ARG

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Mol	Chain	Res	Type
4	H	33	SER
2	B	18	HIS
4	H	28	LYS
1	A	42	ARG
4	D	30	ARG
3	G	11	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	86/110 (78%)	80 (93%)	6 (7%)	15 41
1	E	87/110 (79%)	84 (97%)	3 (3%)	37 61
2	B	71/78 (91%)	63 (89%)	8 (11%)	6 24
2	F	65/78 (83%)	61 (94%)	4 (6%)	18 45
3	C	84/101 (83%)	81 (96%)	3 (4%)	35 60
3	G	89/101 (88%)	86 (97%)	3 (3%)	37 61
4	D	82/102 (80%)	78 (95%)	4 (5%)	25 51
4	H	84/102 (82%)	79 (94%)	5 (6%)	19 46
7	K	632/662 (96%)	601 (95%)	31 (5%)	25 51
8	L	12/106 (11%)	11 (92%)	1 (8%)	11 36
9	M	18/110 (16%)	14 (78%)	4 (22%)	1 6
All	All	1310/1660 (79%)	1238 (94%)	72 (6%)	25 49

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	40	ARG
1	A	129	ARG
1	A	130	ILE
1	A	131	ARG

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Mol	Chain	Res	Type
1	A	133	GLU
2	B	17	ARG
2	B	19	ARG
2	B	20	LYS
2	B	21	VAL
2	B	22	LEU
2	B	23	ARG
2	B	26	ILE
2	B	29	ILE
3	C	116	LEU
3	C	118	LYS
3	C	119	LYS
4	D	27	ARG
4	D	28	LYS
4	D	29	THR
4	D	30	ARG
1	E	36	LYS
1	E	37	LYS
1	E	39	HIS
2	F	24	ASP
2	F	25	ASN
2	F	26	ILE
2	F	27	GLN
3	G	9	LYS
3	G	15	LYS
3	G	25	PHE
4	H	25	LYS
4	H	26	ARG
4	H	27	ARG
4	H	31	LYS
4	H	32	GLU
7	K	51	ARG
7	K	76	ASN
7	K	85	LEU
7	K	118	THR
7	K	119	SER
7	K	165	LYS
7	K	194	LEU
7	K	205	LEU
7	K	267	ARG
7	K	283	CYS
7	K	294	LEU

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Mol	Chain	Res	Type
7	K	308	LEU
7	K	330	LYS
7	K	344	ARG
7	K	356	MET
7	K	369	VAL
7	K	383	LYS
7	K	430	VAL
7	K	457	SER
7	K	493	VAL
7	K	527	GLN
7	K	543	LEU
7	K	554	VAL
7	K	625	VAL
7	K	680	PHE
7	K	693	LEU
7	K	707	SER
7	K	721	VAL
7	K	727	LYS
7	K	730	LEU
7	K	740	LEU
8	L	225	THR
9	M	17	ARG
9	M	18	LYS
9	M	22	THR
9	M	23	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
4	D	46	HIS
4	D	81	ASN
1	E	68	GLN
4	H	46	HIS
4	H	81	ASN
7	K	76	ASN
7	K	93	ASN
7	K	98	HIS
7	K	103	HIS
7	K	134	GLN
7	K	276	ASN
7	K	400	GLN

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Mol	Chain	Res	Type
7	K	527	GLN
7	K	731	GLN
8	L	218	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are 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	$\#\|Z\| > 2$
10	FAD	K	901	-	53,58,58	2.31	29 (54%)	68,89,89	1.43	13 (19%)

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
10	FAD	K	901	-	-	2/30/50/50	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	901	FAD	PA-O5B	-5.00	1.39	1.59
10	K	901	FAD	PA-O1A	-3.95	1.36	1.50
10	K	901	FAD	P-O2P	-3.79	1.37	1.55
10	K	901	FAD	O4B-C1B	-3.66	1.36	1.41
10	K	901	FAD	PA-O2A	-3.60	1.38	1.55
10	K	901	FAD	P-O1P	-3.51	1.38	1.50
10	K	901	FAD	C5X-N5	-3.25	1.33	1.39
10	K	901	FAD	P-O5'	-3.07	1.46	1.59
10	K	901	FAD	C4A-N3A	-3.02	1.31	1.35
10	K	901	FAD	C5A-N7A	-2.86	1.29	1.39
10	K	901	FAD	O3'-C3'	-2.79	1.36	1.43
10	K	901	FAD	C2-N3	-2.64	1.32	1.39
10	K	901	FAD	C5A-C4A	-2.63	1.34	1.40
10	K	901	FAD	C4X-C10	-2.62	1.36	1.44
10	K	901	FAD	O2-C2	-2.57	1.19	1.24
10	K	901	FAD	O5B-C5B	-2.56	1.34	1.44
10	K	901	FAD	C2A-N1A	-2.54	1.29	1.33
10	K	901	FAD	C2B-C1B	-2.48	1.50	1.53
10	K	901	FAD	C9A-C5X	-2.48	1.37	1.41
10	K	901	FAD	C8A-N7A	-2.48	1.30	1.34
10	K	901	FAD	O4'-C4'	-2.43	1.38	1.43
10	K	901	FAD	C4-N3	-2.42	1.34	1.38
10	K	901	FAD	C9-C9A	-2.33	1.35	1.39
10	K	901	FAD	C9-C8	-2.31	1.36	1.39
10	K	901	FAD	C6-C5X	-2.30	1.36	1.40
10	K	901	FAD	C4X-C4	-2.24	1.36	1.44
10	K	901	FAD	C6-C7	-2.11	1.36	1.39
10	K	901	FAD	C4X-N5	2.10	1.34	1.30
10	K	901	FAD	C9A-N10	-2.02	1.37	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	901	FAD	N3A-C2A-N1A	-3.77	122.78	128.68
10	K	901	FAD	C4X-C10-N10	3.32	121.33	116.48
10	K	901	FAD	C4-N3-C2	-2.92	120.24	125.64
10	K	901	FAD	C9A-N10-C10	-2.79	116.42	120.77
10	K	901	FAD	C4X-C4-N3	2.70	120.05	113.19
10	K	901	FAD	C4A-C5A-N7A	-2.58	106.72	109.40
10	K	901	FAD	O4B-C1B-C2B	-2.55	103.20	106.93
10	K	901	FAD	C5X-C9A-N10	2.44	120.47	117.95
10	K	901	FAD	C4'-C3'-C2'	2.30	118.15	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	901	FAD	O4'-C4'-C5'	-2.27	104.82	109.92
10	K	901	FAD	C10-C4X-N5	-2.10	120.40	124.86
10	K	901	FAD	C4X-C10-N1	-2.01	120.06	124.73
10	K	901	FAD	C4-C4X-N5	2.01	121.09	118.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	K	901	FAD	C5'-O5'-P-O3P
10	K	901	FAD	O4B-C4B-C5B-O5B

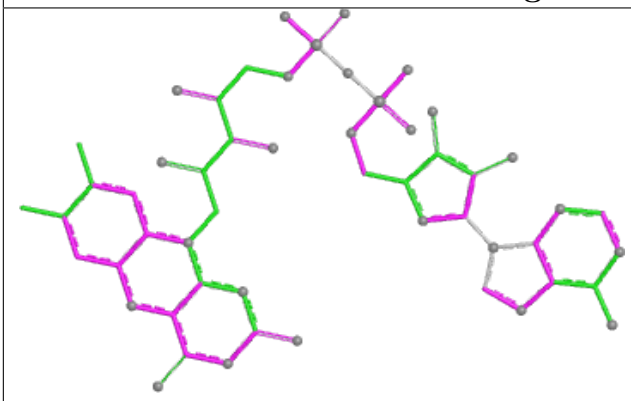
There are no ring outliers.

1 monomer is involved in 2 short contacts:

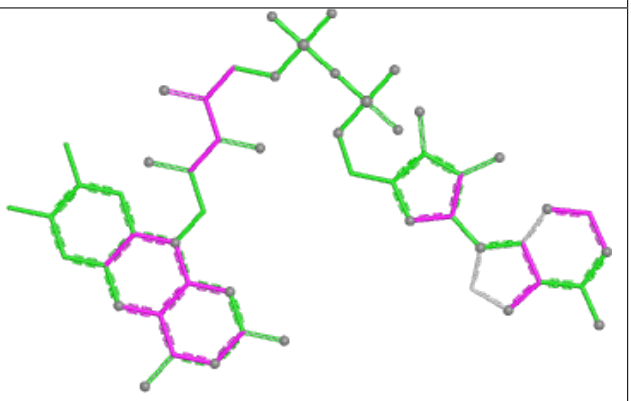
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	K	901	FAD	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

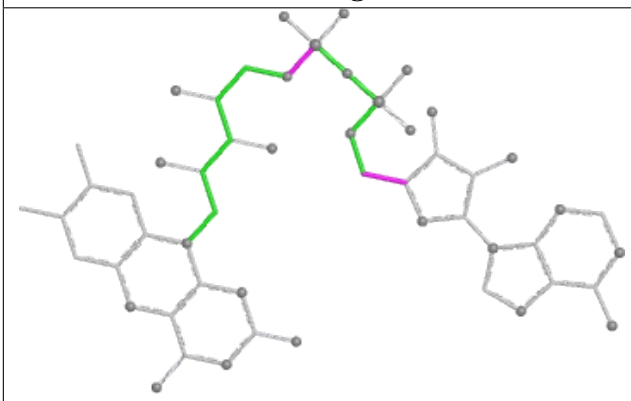
Ligand FAD K 901



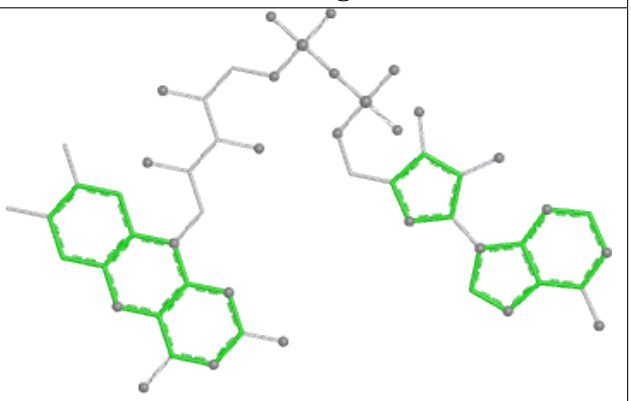
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

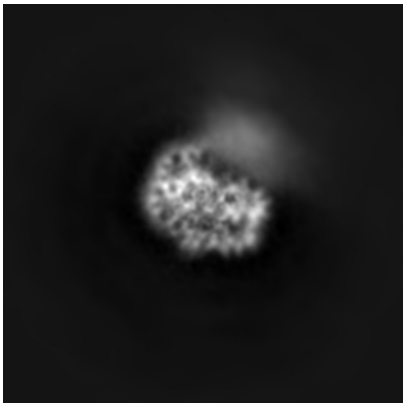
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4705. These allow visual inspection of the internal detail of the map and identification of artifacts.

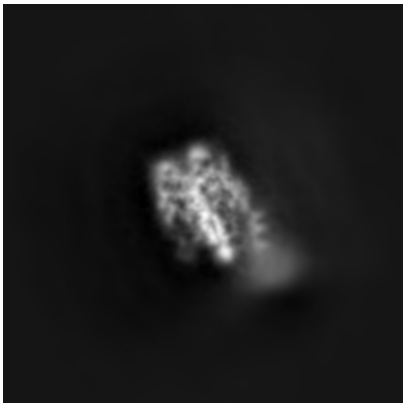
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

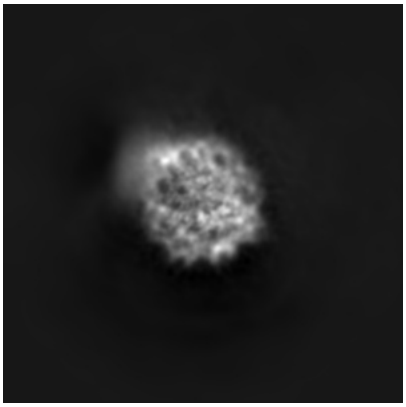
6.1.1 Primary map



X



Y

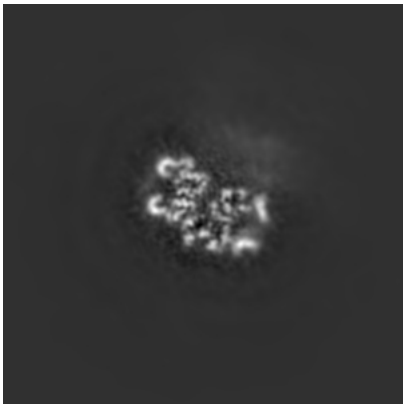


Z

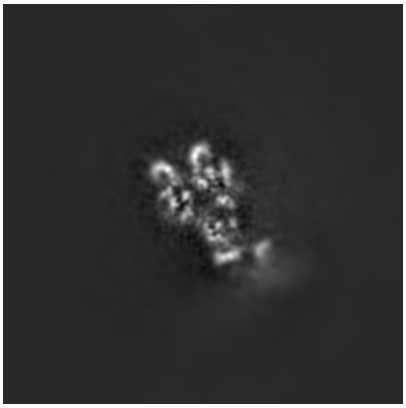
The images above show the map projected in three orthogonal directions.

6.2 Central slices

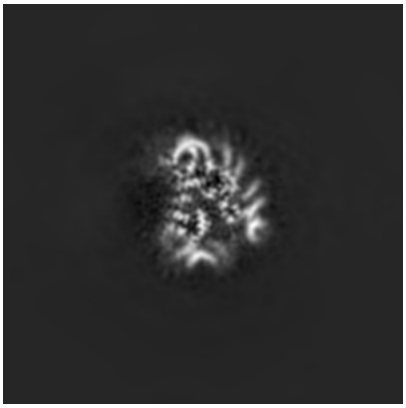
6.2.1 Primary map



X Index: 150



Y Index: 150

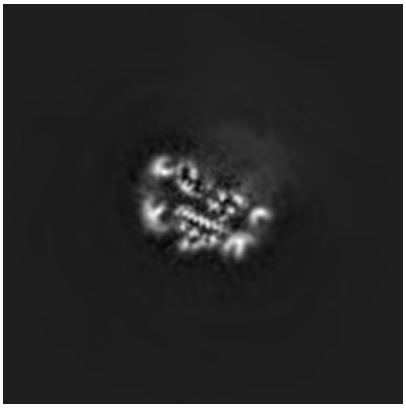


Z Index: 150

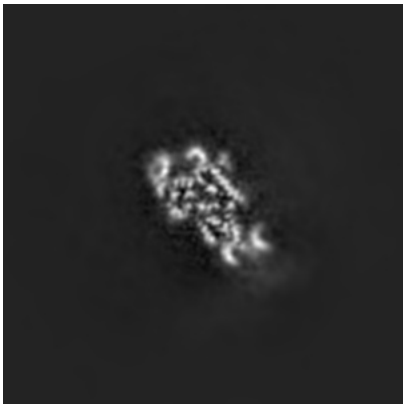
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

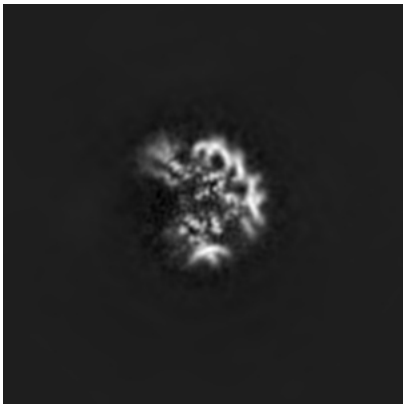
6.3.1 Primary map



X Index: 157



Y Index: 143

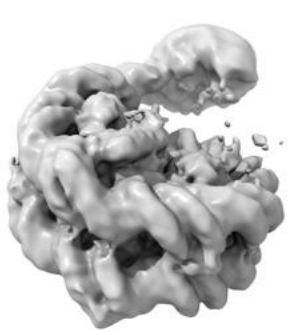


Z Index: 144

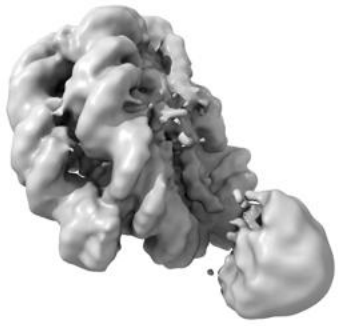
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

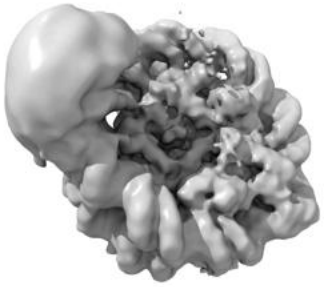
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

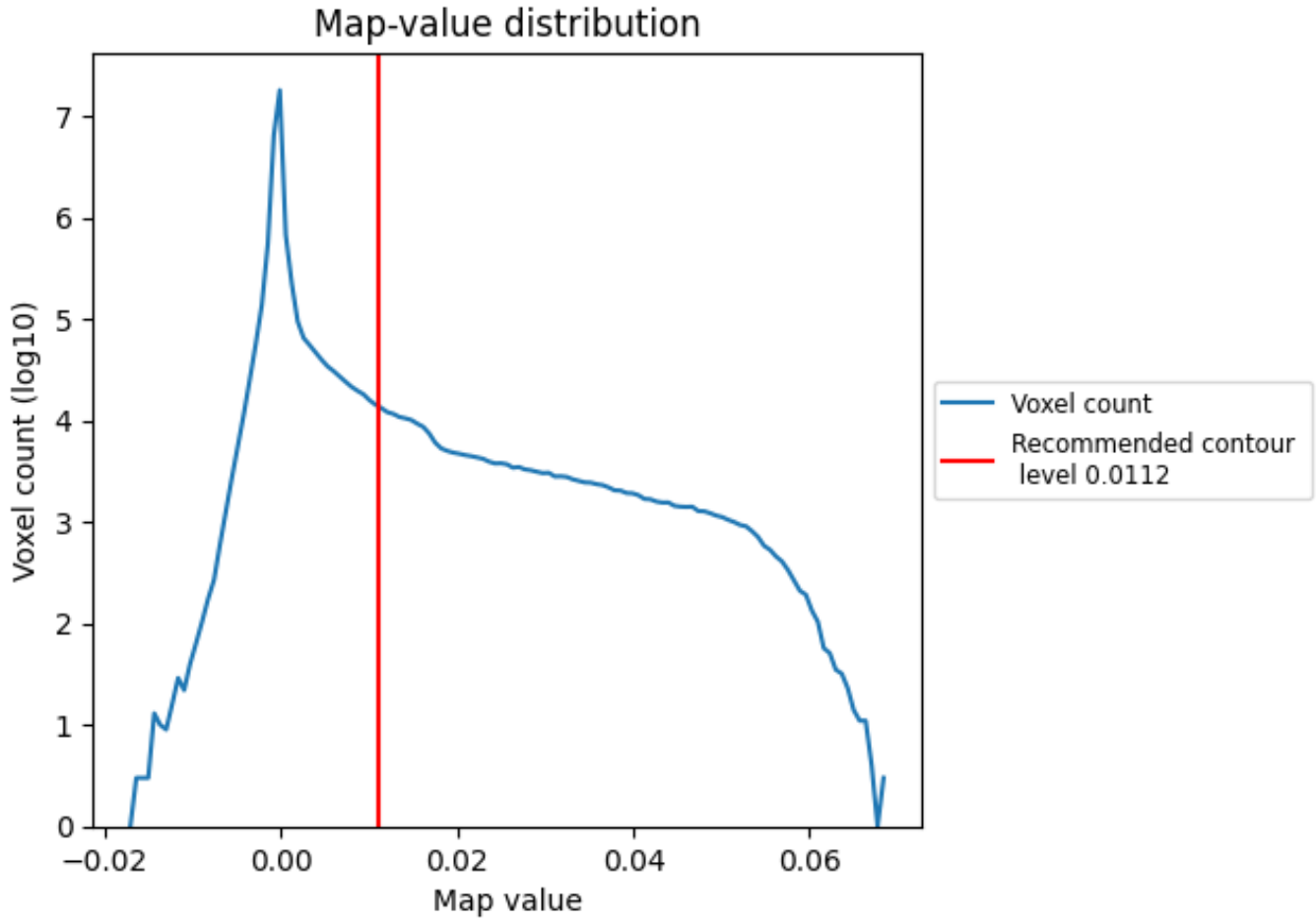
6.5 Mask visualisation (i)

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

7 Map analysis

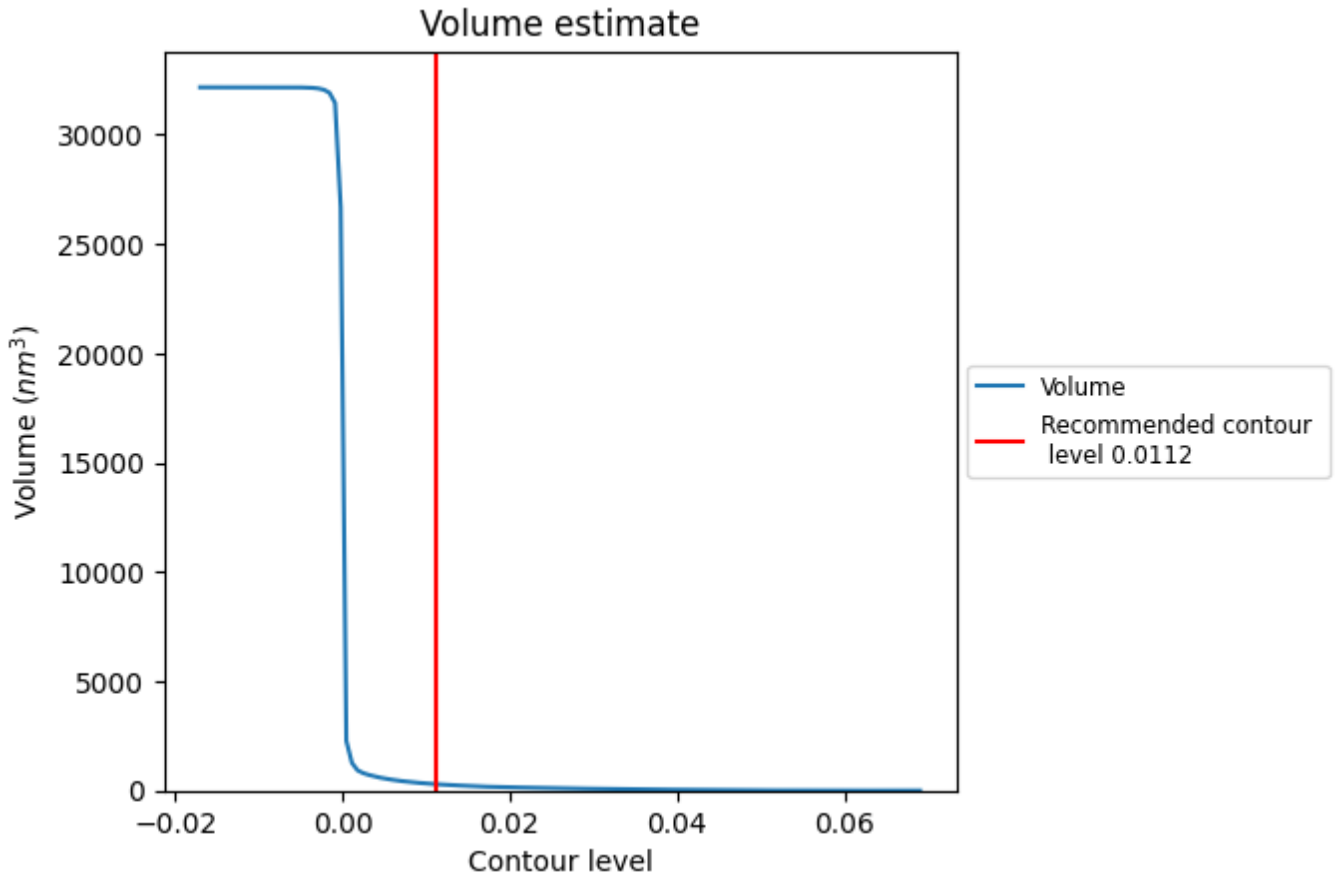
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

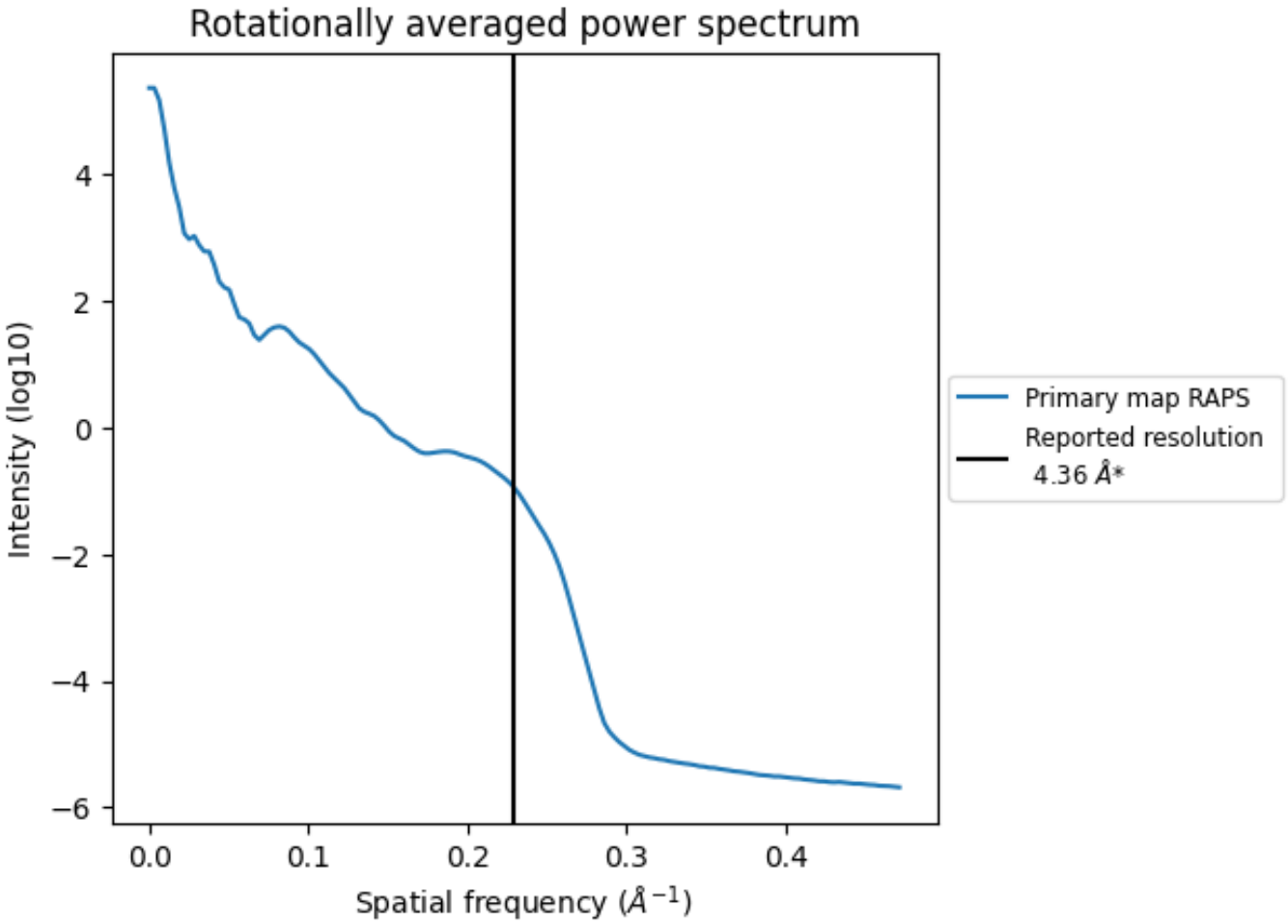
7.2 Volume estimate



The volume at the recommended contour level is 291 nm^3; this corresponds to an approximate mass of 263 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 (i)



*Reported resolution corresponds to spatial frequency of 0.229 Å^{-1}

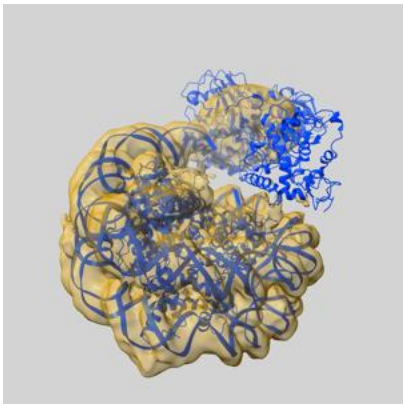
8 Fourier-Shell correlation

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

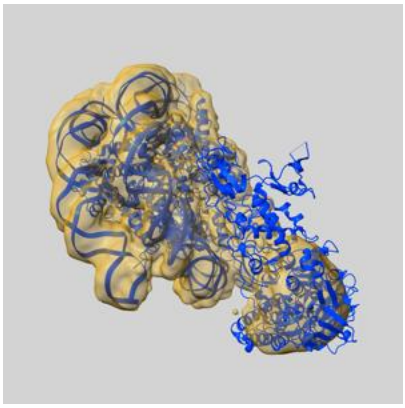
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4705 and PDB model 6R1U. Per-residue inclusion information can be found in section 3 on page 8.

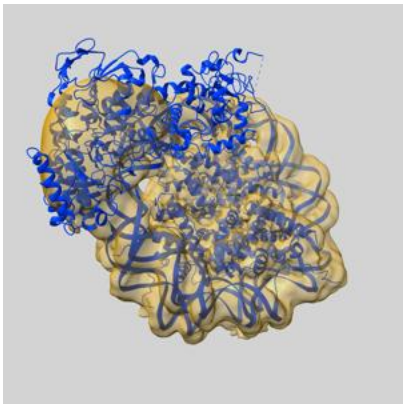
9.1 Map-model overlay



X



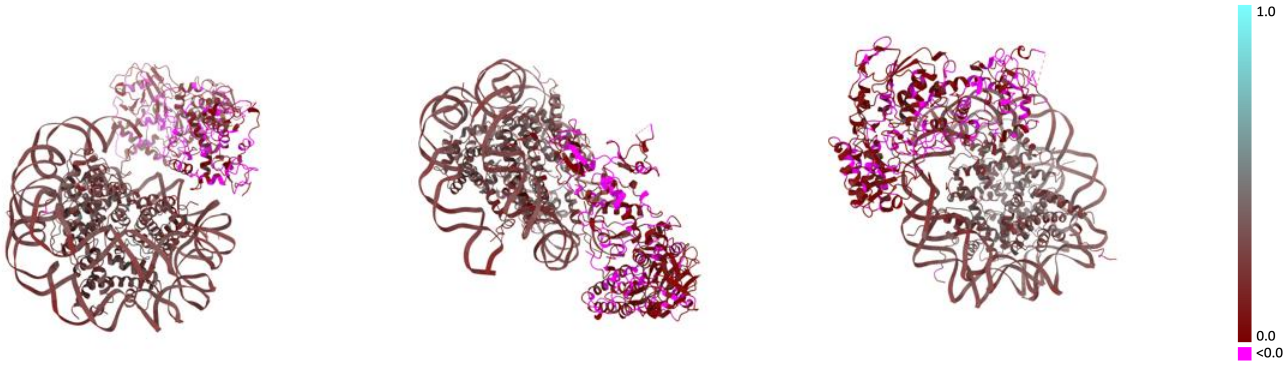
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0112 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.

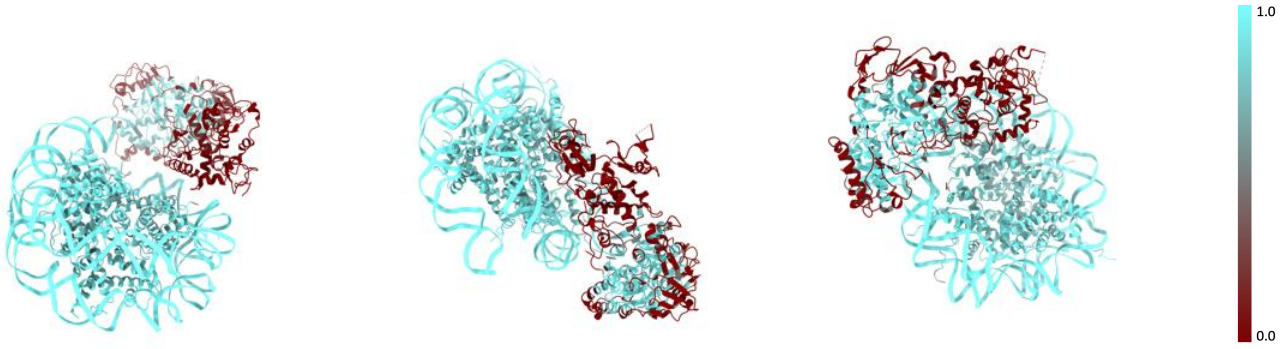
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

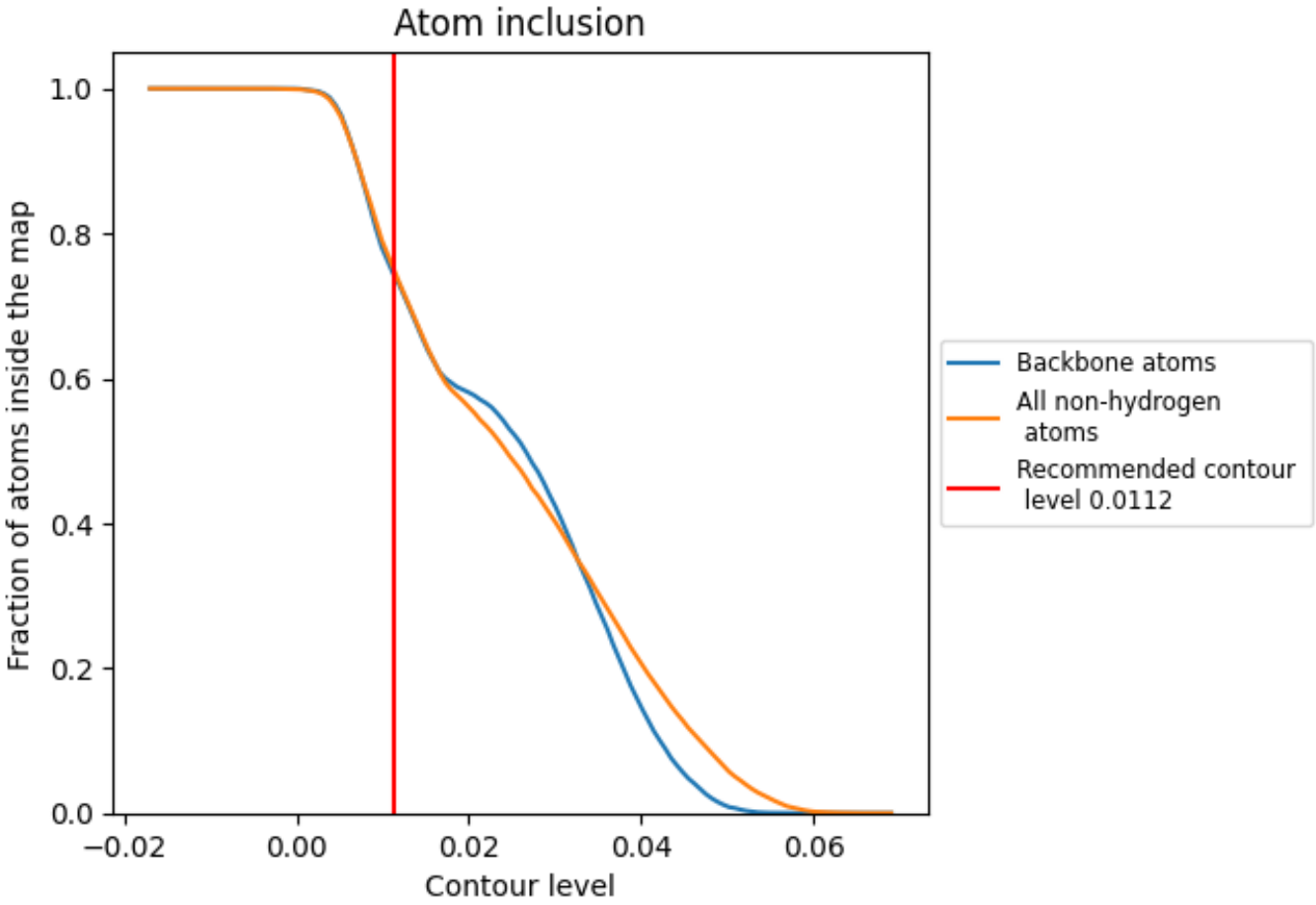
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0112).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 75% 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 (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7526	0.1980
A	0.9274	0.2920
B	0.9196	0.2950
C	0.9427	0.3110
D	0.9334	0.2910
E	0.9087	0.2540
F	0.9069	0.2910
G	0.9075	0.2850
H	0.9536	0.3150
I	0.9947	0.2610
J	0.9927	0.2680
K	0.3383	0.0390
L	0.3714	-0.0150
M	0.5027	0.0380