Full wwPDB EM Validation Report ⓘ

Mar 11, 2024 – 02:32 AM EDT

PDB ID	:	6UGM
EMDB ID	:	EMD-20765
Title	:	Structural basis of COMPASS eCM recognition of an unmodified nucleosome
Authors	:	Hsu, P.L.; Shi, H.; Zheng, N.
Deposited on	:	2019-09-26
Resolution	:	3.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

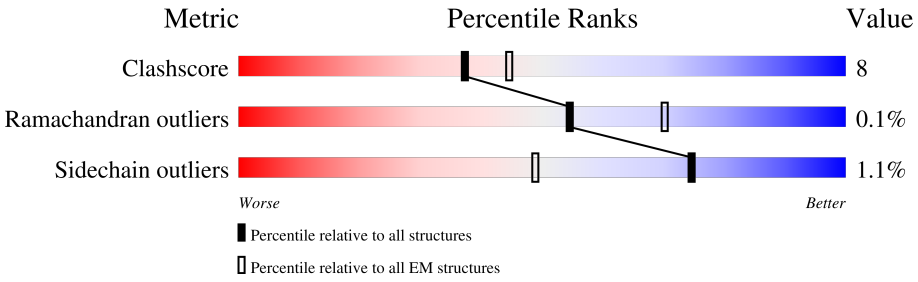
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	64% 8% 28%
1	E	135	59% 11% • 29%
2	B	102	71% 10% 20%
2	F	102	72% 13% 16%
3	C	107	• 84% 14% •
3	G	107	• 84% 16%
4	D	125	64% 10% • 26%
5	H	125	60% 14% 26%

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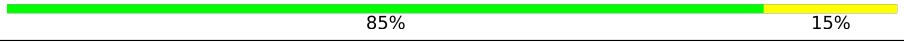
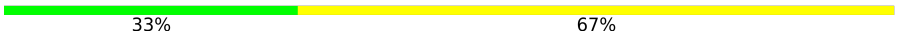
Mol	Chain	Length	Quality of chain
6	I	147	
7	J	146	
8	K	327	
9	M	275	
10	N	439	
11	R	3	
12	X	342	
13	L	405	
14	O	134	
14	P	134	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 23609 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			799	504	155	138	2		
1	E	96	Total	C	N	O	S	0	0
			793	499	154	137	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	82	Total	C	N	O	S	0	0
			657	416	128	112	1		
2	F	86	Total	C	N	O	S	0	0
			694	436	140	117	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			823	519	161	143		
3	G	107	Total	C	N	O	0	0
			823	519	161	143		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	7	PRO	ALA	conflict	UNP A0A1L8FQ56

- Molecule 5 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 6 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 7 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

- Molecule 8 is a protein called Swd3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	305	Total	C	N	O	S	0	0
			2365	1498	395	453	19		

- Molecule 9 is a protein called Histone-lysine N-methyltransferase, H3 lysine-4 specific.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	188	Total	C	N	O	S	0	0
			1490	944	261	277	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	761	GLU	ASP	conflict	UNP Q6CIT4

- Molecule 10 is a protein called Swd1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	408	Total	C	N	O	S	0	0
			3273	2095	539	622	17		

- Molecule 11 is a protein called H3 N-terminus.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	3	Total	C	N	O	S	0	0
			24	14	4	5	1		

- Molecule 12 is a protein called Spp1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	73	Total	C	N	O	0	0
			604	379	108	117		

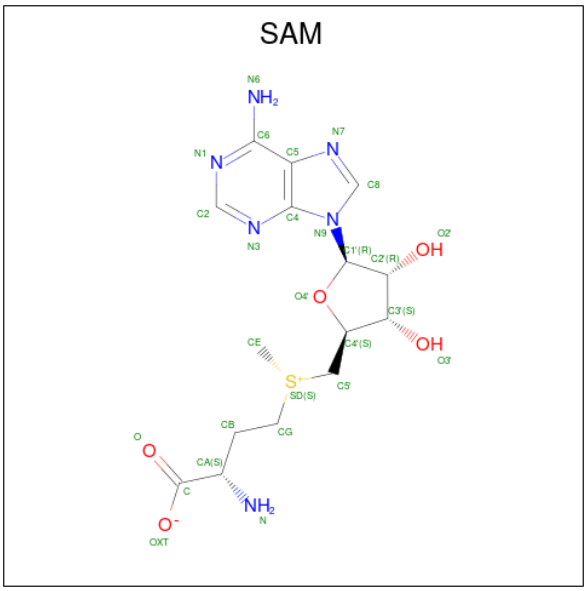
- Molecule 13 is a protein called Bre2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	382	Total	C	N	O	S	0	0
			3128	1985	519	609	15		

- Molecule 14 is a protein called Sdc1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	42	Total	C	N	O	S	0	0
			342	216	63	62	1		
14	P	43	Total	C	N	O	S	0	0
			329	211	57	59	2		

- Molecule 15 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



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

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

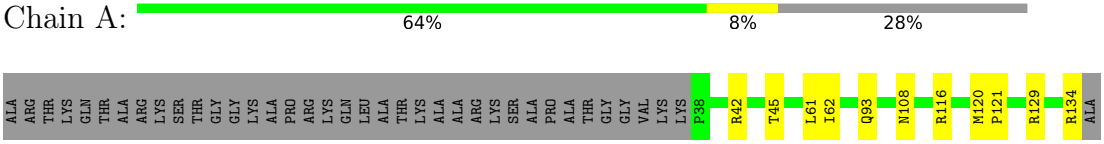
Mol	Chain	Residues	Atoms		AltConf
16	M	1	Total	Zn	0
			1	1	

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.

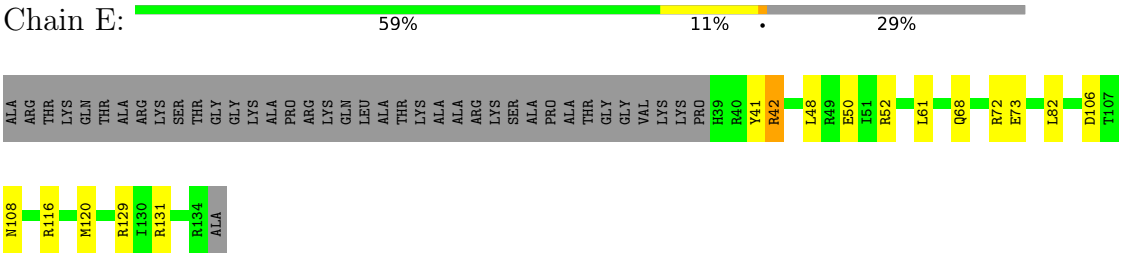
• Molecule 1: Histone H3

Chain A:



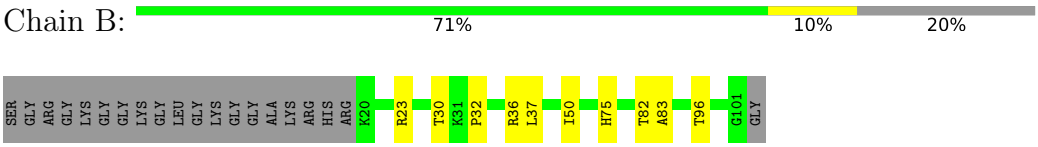
• Molecule 1: Histone H3

Chain E:



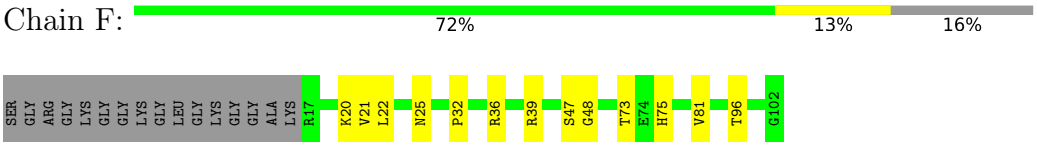
• Molecule 2: Histone H4

Chain B:



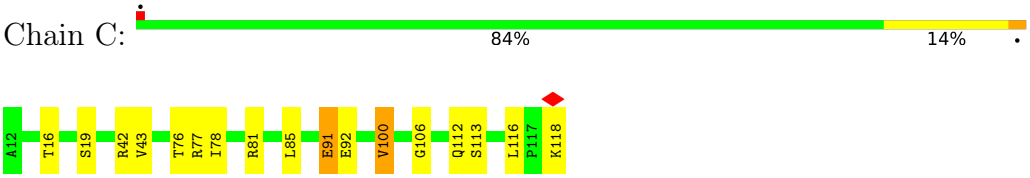
• Molecule 2: Histone H4

Chain F:



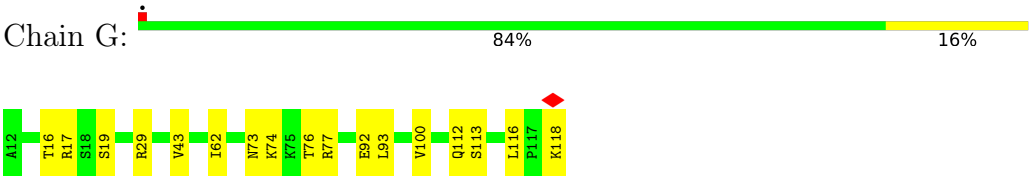
• Molecule 3: Histone H2A

Chain C:



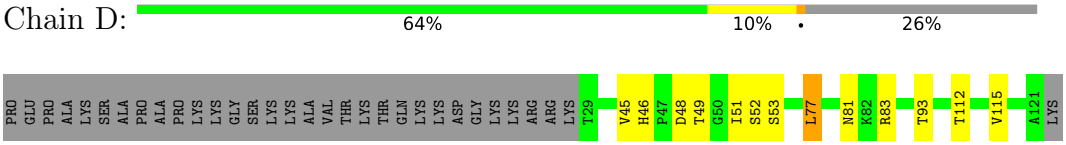
• Molecule 3: Histone H2A

Chain G:



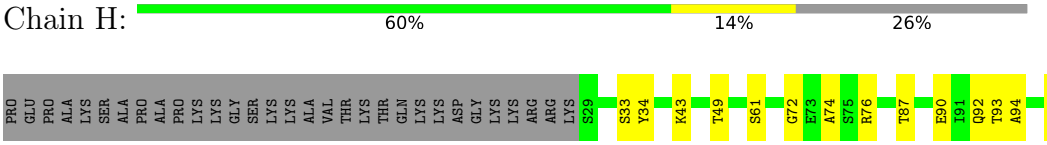
• Molecule 4: Histone H2B

Chain D:



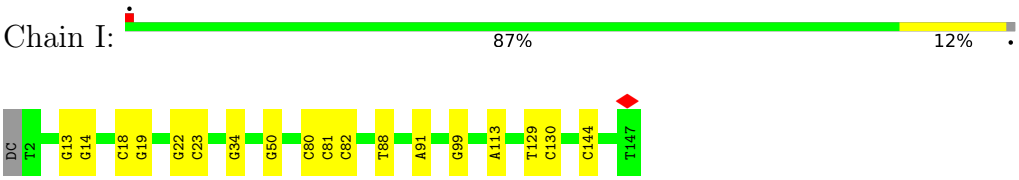
• Molecule 5: Histone H2B 1.1

Chain H:



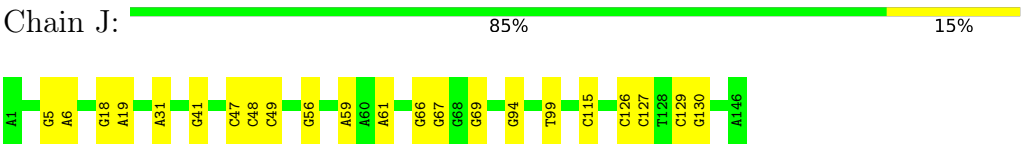
• Molecule 6: DNA (146-MER)

Chain I:



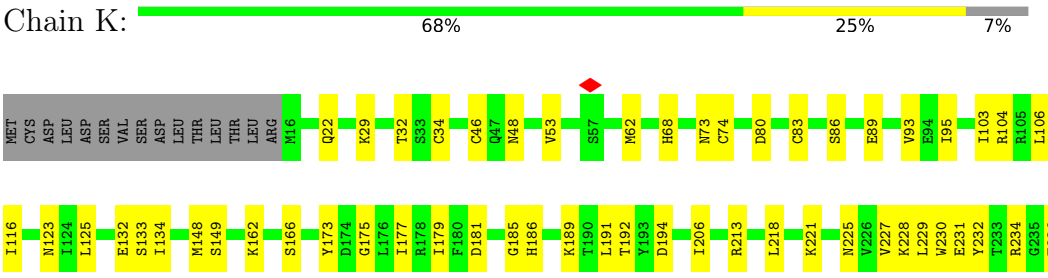
• Molecule 7: DNA (146-MER)

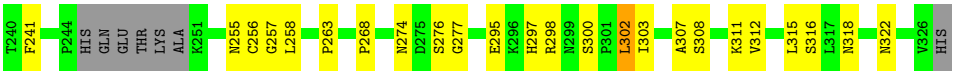
Chain J:



• Molecule 8: Swd3

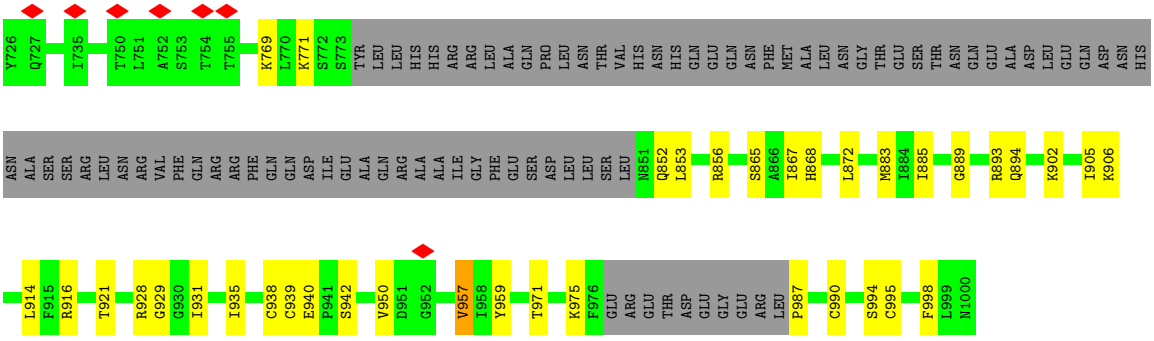
Chain K:





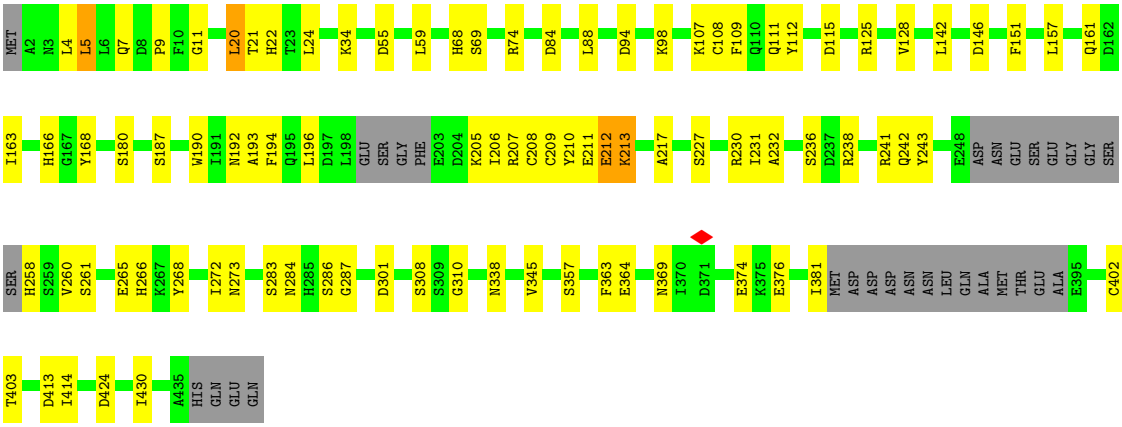
• Molecule 9: Histone-lysine N-methyltransferase, H3 lysine-4 specific

Chain M:



• Molecule 10: Swd1

Chain N:

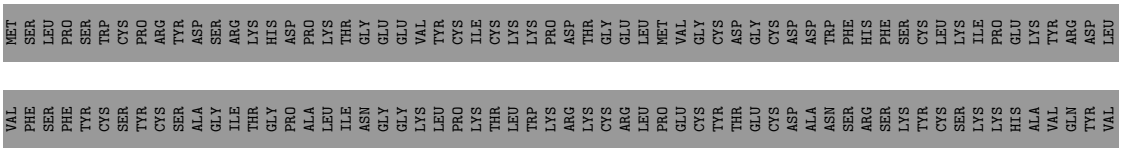


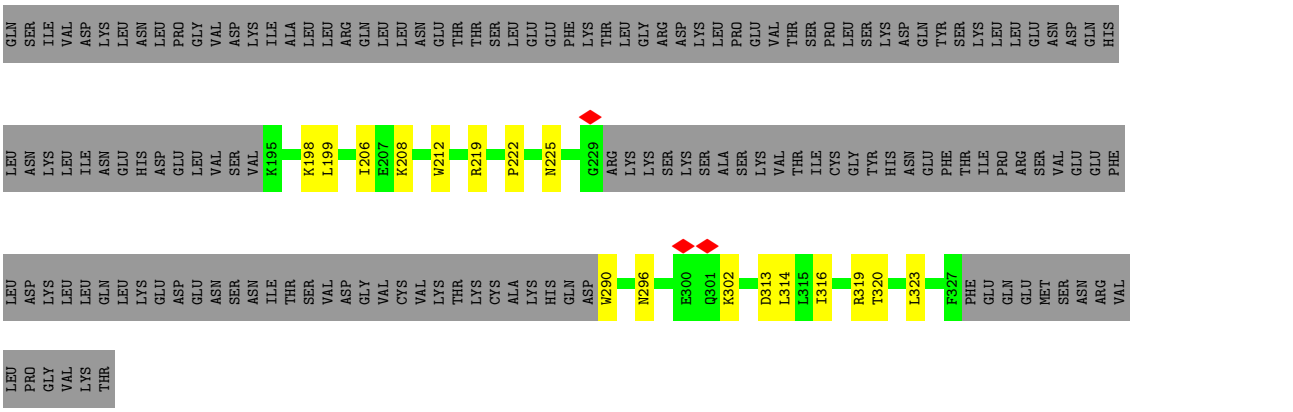
• Molecule 11: H3 N-terminus

Chain R:

• Molecule 12: Spp1

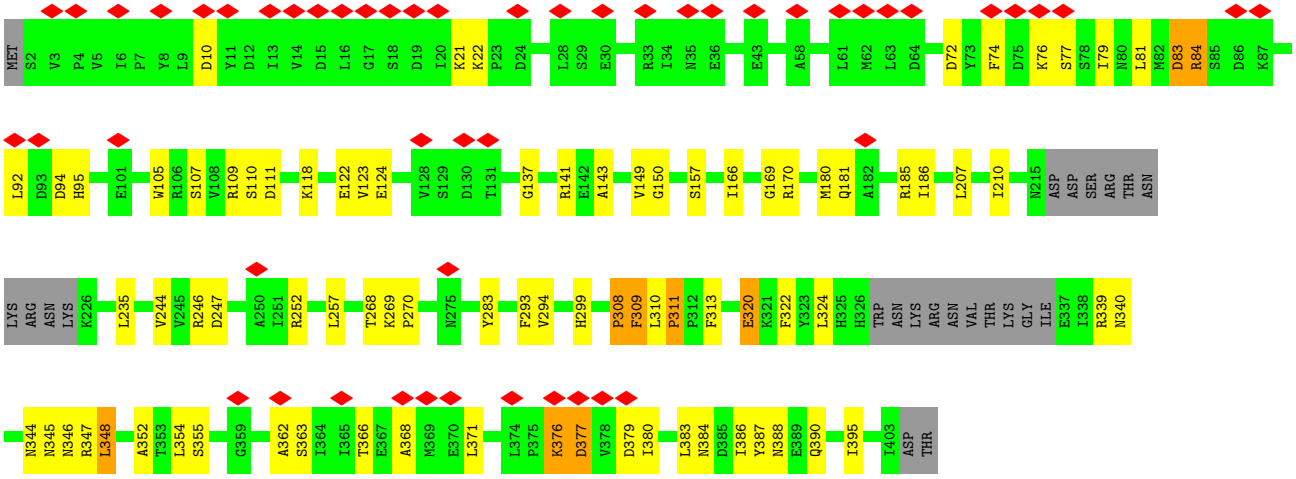
Chain X:





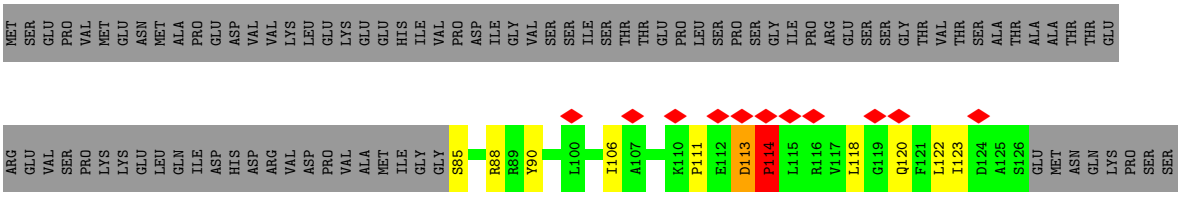
• Molecule 13: Bre2

Chain L:



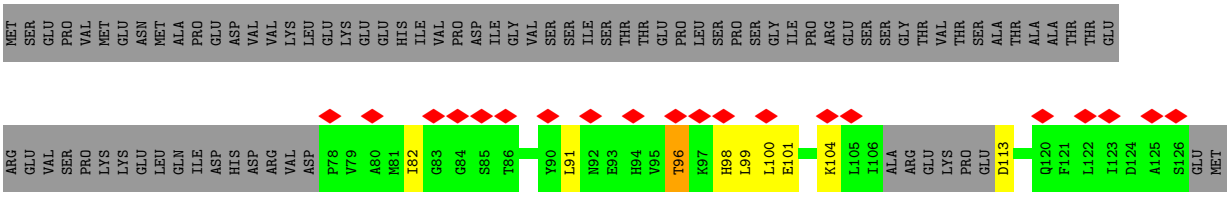
• Molecule 14: Sdc1

Chain O:



• Molecule 14: Sdc1

Chain P:




ASN
GLN
LYS
PRO
SER
SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	100905	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 ($e^-/Å^2$)	74	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	0.119	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	342.144, 342.144, 342.144	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	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, 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	A	0.59	0/811	0.64	0/1087
1	E	0.61	0/804	0.82	2/1077 (0.2%)
2	B	0.74	0/664	0.79	0/889
2	F	0.67	0/702	0.68	0/937
3	C	0.57	0/833	0.66	0/1124
3	G	0.56	0/833	0.67	0/1124
4	D	0.64	0/737	0.65	0/993
5	H	0.68	0/736	0.69	1/991 (0.1%)
6	I	0.99	0/3333	1.04	0/5137
7	J	1.00	0/3381	1.02	2/5221 (0.0%)
8	K	0.35	0/2410	0.73	5/3262 (0.2%)
9	M	0.39	0/1514	0.74	1/2031 (0.0%)
10	N	0.38	0/3360	0.72	11/4577 (0.2%)
11	R	0.44	0/23	0.84	0/29
12	X	0.36	0/612	0.79	1/825 (0.1%)
13	L	0.35	0/3198	0.80	12/4323 (0.3%)
14	O	0.42	1/347 (0.3%)	0.77	2/466 (0.4%)
14	P	0.32	0/333	0.73	1/447 (0.2%)
All	All	0.66	1/24631 (0.0%)	0.83	38/34540 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
8	K	0	1
13	L	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	O	114	PRO	N-CD	6.12	1.56	1.47

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	41	TYR	CB-CA-C	-13.56	83.29	110.40
13	L	376	LYS	N-CA-C	-11.44	80.11	111.00
10	N	20	LEU	CB-CA-C	-10.90	89.50	110.20
13	L	376	LYS	CB-CA-C	10.68	131.76	110.40
10	N	212	GLU	CB-CA-C	9.28	128.96	110.40
8	K	302	LEU	CB-CA-C	-8.91	93.27	110.20
13	L	309	PHE	N-CA-CB	-8.79	94.77	110.60
10	N	88	LEU	CB-CA-C	8.42	126.19	110.20
10	N	21	THR	CB-CA-C	-7.62	91.02	111.60
10	N	413	ASP	N-CA-C	-7.25	91.43	111.00
8	K	302	LEU	N-CA-C	6.89	129.60	111.00
10	N	20	LEU	N-CA-C	6.76	129.26	111.00
13	L	322	PHE	CB-CA-C	6.75	123.89	110.40
13	L	83	ASP	N-CA-C	-6.71	92.88	111.00
13	L	309	PHE	N-CA-C	6.70	129.09	111.00
10	N	414	ILE	N-CA-C	-6.70	92.92	111.00
10	N	213	LYS	N-CA-CB	6.50	122.30	110.60
13	L	310	LEU	CA-CB-CG	6.24	129.66	115.30
10	N	21	THR	N-CA-C	6.18	127.70	111.00
10	N	213	LYS	N-CA-C	-5.75	95.48	111.00
7	J	94	DG	P-O3'-C3'	5.71	126.55	119.70
5	H	98	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	E	42	ARG	N-CA-C	5.63	126.19	111.00
9	M	885	ILE	CG1-CB-CG2	-5.57	99.15	111.40
13	L	377	ASP	N-CA-CB	5.56	120.60	110.60
13	L	348	LEU	CA-CB-CG	5.52	127.99	115.30
8	K	125	LEU	CA-CB-CG	5.47	127.87	115.30
7	J	126	DC	P-O3'-C3'	5.41	126.19	119.70
12	X	314	LEU	CA-CB-CG	5.37	127.66	115.30
8	K	114	ILE	N-CA-C	5.34	125.41	111.00
14	O	122	LEU	CA-CB-CG	5.31	127.52	115.30
13	L	320	GLU	CB-CA-C	5.31	121.02	110.40
13	L	84	ARG	N-CA-CB	5.27	120.08	110.60
14	O	113	ASP	N-CA-C	-5.21	96.93	111.00
8	K	302	LEU	O-C-N	-5.15	114.46	122.70
10	N	88	LEU	N-CA-C	-5.11	97.19	111.00
13	L	257	LEU	CA-CB-CG	5.02	126.85	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	P	100	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	THR	Peptide
8	K	113	VAL	Mainchain
13	L	308	PRO	Mainchain
13	L	309	PHE	Peptide

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	799	0	834	8	0
1	E	793	0	829	13	0
2	B	657	0	706	6	0
2	F	694	0	742	10	0
3	C	823	0	882	10	0
3	G	823	0	882	15	0
4	D	726	0	747	10	0
5	H	725	0	745	15	0
6	I	2975	0	1639	18	0
7	J	3011	0	1639	18	0
8	K	2365	0	2376	52	0
9	M	1490	0	1513	30	0
10	N	3273	0	3136	79	0
11	R	24	0	23	5	0
12	X	604	0	605	10	0
13	L	3128	0	3011	54	0
14	O	342	0	355	7	0
14	P	329	0	341	7	0
15	M	27	0	22	2	0
16	M	1	0	0	0	0
All	All	23609	0	21027	313	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 8.

All (313) 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)
8:K:256:CYS:SG	8:K:302:LEU:O	2.09	1.11
10:N:210:TYR:HB2	10:N:260:VAL:CG1	1.83	1.08
10:N:210:TYR:HE1	10:N:261:SER:HA	1.08	1.08
10:N:210:TYR:CE1	10:N:261:SER:HA	1.88	1.08
9:M:914:LEU:HB2	11:R:3:THR:HG21	1.30	1.07
10:N:210:TYR:HB2	10:N:260:VAL:HG13	1.35	1.04
10:N:20:LEU:O	10:N:20:LEU:HG	1.20	1.01
10:N:20:LEU:O	10:N:20:LEU:CG	1.98	0.98
3:G:62:ILE:CD1	3:G:93:LEU:HD13	1.96	0.95
9:M:914:LEU:HB2	11:R:3:THR:CG2	2.04	0.88
3:G:62:ILE:HD13	3:G:93:LEU:HD13	1.58	0.85
10:N:161:GLN:HE22	10:N:208:CYS:HB3	1.45	0.80
9:M:865:SER:HB3	9:M:868:HIS:O	1.82	0.80
3:G:62:ILE:HD13	3:G:93:LEU:CD1	2.11	0.79
1:E:42:ARG:NH2	6:I:144:DC:OP2	2.17	0.78
3:G:92:GLU:OE2	5:H:102:GLU:HB2	1.84	0.76
13:L:376:LYS:O	13:L:377:ASP:OD2	2.03	0.76
13:L:74:PHE:HD2	13:L:76:LYS:O	1.69	0.76
10:N:210:TYR:CB	10:N:260:VAL:HG13	2.15	0.75
10:N:210:TYR:HD1	10:N:260:VAL:O	1.70	0.75
3:G:62:ILE:HD11	3:G:93:LEU:HD13	1.68	0.73
10:N:161:GLN:NE2	10:N:208:CYS:HB3	2.03	0.73
10:N:190:TRP:CE3	10:N:212:GLU:O	2.41	0.73
9:M:914:LEU:CB	11:R:3:THR:HG21	2.15	0.73
10:N:211:GLU:O	10:N:212:GLU:HB2	1.89	0.72
6:I:82:DC:H42	7:J:66:DG:H1	1.39	0.69
13:L:320:GLU:O	13:L:324:LEU:HG	1.92	0.69
8:K:134:ILE:N	8:K:148:MET:O	2.24	0.69
10:N:210:TYR:CD1	10:N:260:VAL:HG13	2.29	0.68
1:E:42:ARG:HD3	6:I:144:DC:OP2	1.94	0.67
3:C:42:ARG:HG2	6:I:113:DA:H5”	1.77	0.67
10:N:210:TYR:CD1	10:N:260:VAL:O	2.47	0.66
6:I:99:DG:H1	7:J:49:DC:H42	1.43	0.65
8:K:181:ASP:HB3	8:K:186:HIS:H	1.61	0.65
12:X:222:PRO:HA	12:X:225:ASN:HD22	1.61	0.65
9:M:940:GLU:OE2	9:M:994:SER:O	2.15	0.64
3:C:78:ILE:HB	4:D:51:ILE:HG13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:769:LYS:HD2	9:M:771:LYS:HG2	1.81	0.63
10:N:157:LEU:C	10:N:206:ILE:HD11	2.20	0.61
10:N:193:ALA:HB3	10:N:209:CYS:SG	2.40	0.61
12:X:320:THR:HA	12:X:323:LEU:HB2	1.83	0.61
3:G:62:ILE:CD1	3:G:93:LEU:CD1	2.71	0.60
10:N:22:HIS:HB3	10:N:59:LEU:HD21	1.83	0.60
3:G:73:ASN:O	3:G:74:LYS:HB2	2.01	0.60
13:L:124:GLU:HA	13:L:185:ARG:HG3	1.83	0.60
15:M:1101:SAM:HE1	11:R:4:MET:SD	2.42	0.60
10:N:68:HIS:HB3	10:N:107:LYS:HE3	1.82	0.59
8:K:134:ILE:HB	8:K:148:MET:HB2	1.83	0.59
13:L:157:SER:HB3	13:L:166:ILE:HD12	1.86	0.58
6:I:81:DC:H42	7:J:67:DG:H1	1.50	0.58
10:N:207:ARG:HH22	10:N:258:HIS:N	2.00	0.58
10:N:381:ILE:HB	13:L:170:ARG:HH11	1.69	0.58
3:C:100:VAL:HG23	2:F:96:THR:HB	1.86	0.57
13:L:395:ILE:HD13	14:P:91:LEU:HD13	1.86	0.57
1:E:68:GLN:HE21	1:E:72:ARG:HH21	1.53	0.57
14:P:98:HIS:HA	14:P:101:GLU:HB2	1.86	0.57
10:N:161:GLN:HE22	10:N:208:CYS:CB	2.15	0.57
10:N:207:ARG:NH2	10:N:258:HIS:N	2.53	0.57
1:E:48:LEU:HD23	1:E:52:ARG:HH12	1.70	0.57
10:N:142:LEU:HD22	10:N:151:PHE:HB3	1.87	0.56
6:I:34:DG:N2	7:J:115:DC:O2	2.38	0.56
8:K:74:CYS:HB3	8:K:116:ILE:HG12	1.86	0.56
13:L:110:SER:HB3	13:L:352:ALA:HB3	1.86	0.56
1:E:61:LEU:O	2:F:36:ARG:NH2	2.38	0.56
5:H:115:VAL:HG11	10:N:272:ILE:HD11	1.87	0.56
10:N:108:CYS:SG	10:N:109:PHE:N	2.79	0.56
2:B:75:HIS:HB2	4:D:93:THR:HG21	1.86	0.56
2:F:75:HIS:HB2	5:H:93:THR:HG21	1.88	0.56
1:E:116:ARG:NH1	1:E:120:MET:SD	2.79	0.55
5:H:43:LYS:NZ	5:H:49:THR:O	2.38	0.55
8:K:53:VAL:HB	8:K:62:MET:HB3	1.87	0.55
9:M:853:LEU:HD11	9:M:950:VAL:HG21	1.89	0.55
8:K:295:GLU:O	8:K:298:ARG:NH2	2.39	0.55
1:A:42:ARG:NH2	7:J:69:DG:OP1	2.38	0.55
9:M:872:LEU:HB2	9:M:935:ILE:HD13	1.89	0.55
1:E:42:ARG:HD3	6:I:144:DC:P	2.47	0.54
10:N:212:GLU:HG2	10:N:213:LYS:H	1.73	0.54
1:E:73:GLU:HB2	2:F:25:ASN:HD22	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:345:ASN:O	13:L:348:LEU:HD22	2.07	0.54
13:L:77:SER:H	13:L:384:ASN:HD21	1.53	0.54
9:M:883:MET:HG3	9:M:957:VAL:HG23	1.90	0.54
15:M:1101:SAM:CE	11:R:4:MET:SD	2.96	0.54
10:N:24:LEU:HB2	10:N:345:VAL:HB	1.89	0.54
10:N:161:GLN:OE1	10:N:208:CYS:SG	2.66	0.54
9:M:867:ILE:HG23	9:M:990:CYS:HA	1.90	0.54
10:N:210:TYR:HD1	10:N:260:VAL:HG13	1.72	0.54
10:N:230:ARG:NH1	10:N:287:GLY:O	2.41	0.54
10:N:301:ASP:OD1	10:N:301:ASP:N	2.41	0.53
4:D:83:ARG:NH1	7:J:41:DG:OP2	2.42	0.53
1:E:106:ASP:OD2	1:E:131:ARG:NH2	2.42	0.53
8:K:93:VAL:HB	8:K:106:LEU:HB2	1.90	0.53
9:M:893:ARG:NH1	10:N:374:GLU:OE1	2.41	0.53
8:K:80:ASP:OD1	8:K:80:ASP:N	2.42	0.53
8:K:225:ASN:ND2	8:K:274:ASN:OD1	2.41	0.53
12:X:206:ILE:HG23	12:X:313:ASP:HB3	1.91	0.53
13:L:109:ARG:NH1	13:L:143:ALA:O	2.42	0.53
8:K:228:LYS:HB3	8:K:237:VAL:HG21	1.90	0.53
8:K:103:ILE:HG22	8:K:104:ARG:HG2	1.90	0.52
8:K:132:GLU:OE1	9:M:769:LYS:NZ	2.40	0.52
14:O:85:SER:HB2	14:O:88:ARG:HB3	1.90	0.52
8:K:316:SER:OG	8:K:318:ASN:O	2.24	0.52
10:N:266:HIS:NE2	10:N:308:SER:O	2.43	0.52
13:L:137:GLY:HA3	13:L:157:SER:HA	1.92	0.52
4:D:52:SER:OG	4:D:53:SER:N	2.41	0.52
1:A:116:ARG:NH1	1:A:120:MET:SD	2.82	0.52
9:M:928:ARG:HG3	10:N:364:GLU:HB3	1.91	0.52
8:K:148:MET:CE	8:K:181:ASP:O	2.58	0.51
13:L:207:LEU:HD13	13:L:210:ILE:HD11	1.92	0.51
3:C:91:GLU:HG3	3:C:92:GLU:HG3	1.92	0.51
9:M:938:CYS:HB3	9:M:971:THR:HB	1.92	0.51
8:K:34:CYS:HB3	8:K:315:LEU:HB2	1.93	0.51
3:G:29:ARG:NH1	5:H:33:SER:O	2.43	0.51
10:N:357:SER:HA	10:N:363:PHE:HB2	1.92	0.51
6:I:130:DC:H42	7:J:18:DG:H1	1.58	0.51
14:O:111:PRO:HD2	14:O:114:PRO:HB3	1.93	0.51
3:G:92:GLU:OE1	5:H:103:LEU:HG	2.10	0.51
6:I:91:DA:N6	7:J:56:DG:O6	2.42	0.51
8:K:22:GLN:NE2	8:K:322:ASN:OD1	2.43	0.51
9:M:889:GLY:HA2	9:M:929:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:199:LEU:HB2	12:X:320:THR:HG21	1.93	0.51
8:K:175:GLY:HA2	8:K:206:ILE:HG12	1.93	0.51
10:N:217:ALA:HB1	10:N:236:SER:H	1.76	0.51
9:M:856:ARG:NH2	9:M:959:TYR:HE1	2.09	0.50
13:L:268:THR:OG1	13:L:269:LYS:N	2.44	0.50
8:K:179:ILE:HB	8:K:189:LYS:HB3	1.93	0.50
8:K:307:ALA:HA	8:K:312:VAL:HA	1.94	0.50
1:A:108:ASN:ND2	3:G:112:GLN:OE1	2.44	0.50
8:K:257:GLY:N	8:K:303:ILE:O	2.45	0.50
12:X:198:LYS:O	12:X:319:ARG:NH2	2.41	0.50
3:C:112:GLN:OE1	1:E:108:ASN:ND2	2.45	0.50
13:L:22:LYS:NZ	14:P:82:ILE:O	2.45	0.50
13:L:79:ILE:HD12	13:L:84:ARG:HH12	1.76	0.50
10:N:74:ARG:H	10:N:94:ASP:HB3	1.77	0.50
13:L:92:LEU:HD12	13:L:95:HIS:HE1	1.76	0.49
13:L:111:ASP:OD1	13:L:111:ASP:N	2.45	0.49
8:K:308:SER:HB2	8:K:311:LYS:H	1.76	0.49
13:L:74:PHE:CD2	13:L:76:LYS:O	2.56	0.49
14:O:111:PRO:HG2	14:O:113:ASP:O	2.10	0.49
8:K:218:LEU:O	8:K:230:TRP:N	2.45	0.49
10:N:283:SER:OG	10:N:284:ASN:N	2.45	0.49
13:L:150:GLY:O	13:L:169:GLY:N	2.44	0.49
9:M:987:PRO:HA	9:M:998:PHE:HA	1.94	0.49
10:N:161:GLN:NE2	10:N:208:CYS:CB	2.74	0.49
10:N:430:ILE:HD11	12:X:316:ILE:HG12	1.94	0.49
13:L:366:THR:HG22	13:L:383:LEU:HD13	1.95	0.49
1:A:129:ARG:O	1:A:129:ARG:NH1	2.40	0.49
10:N:192:ASN:HA	10:N:210:TYR:O	2.13	0.48
5:H:74:ALA:HB2	5:H:94:ALA:HB2	1.95	0.48
3:G:16:THR:O	3:G:19:SER:OG	2.32	0.48
2:B:30:THR:HG21	7:J:61:DA:H5"	1.96	0.48
10:N:210:TYR:HB2	10:N:260:VAL:HG11	1.85	0.48
4:D:112:THR:HA	4:D:115:VAL:HG12	1.96	0.48
13:L:94:ASP:OD1	13:L:94:ASP:N	2.45	0.48
14:O:120:GLN:HA	14:O:123:ILE:HD12	1.96	0.48
13:L:81:LEU:HA	13:L:84:ARG:HH21	1.78	0.48
13:L:235:LEU:HD22	13:L:340:ASN:HA	1.95	0.48
3:G:17:ARG:HB3	5:H:118:TYR:HE1	1.79	0.48
10:N:210:TYR:CB	10:N:260:VAL:CG1	2.75	0.48
5:H:90:GLU:O	5:H:94:ALA:N	2.44	0.47
2:F:20:LYS:NZ	2:F:21:VAL:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:83:CYS:HB2	8:K:95:ILE:HD11	1.95	0.47
13:L:247:ASP:OD2	13:L:339:ARG:NH2	2.46	0.47
4:D:45:VAL:O	4:D:46:HIS:ND1	2.47	0.47
8:K:238:VAL:O	8:K:239:ARG:NH1	2.45	0.47
10:N:210:TYR:CG	10:N:260:VAL:HG13	2.50	0.47
10:N:242:GLN:NE2	10:N:265:GLU:OE1	2.47	0.47
4:D:77:LEU:O	4:D:81:ASN:ND2	2.47	0.47
8:K:263:PRO:HD2	8:K:268:PRO:HA	1.96	0.47
1:A:62:ILE:O	1:A:93:GLN:NE2	2.47	0.47
8:K:166:SER:HB3	10:N:4:LEU:HG	1.96	0.47
6:I:88:DT:O4	7:J:59:DA:N6	2.48	0.47
8:K:148:MET:HE1	8:K:181:ASP:O	2.14	0.47
14:O:90:TYR:HH	14:P:113:ASP:N	2.12	0.47
8:K:123:ASN:ND2	10:N:55:ASP:OD1	2.45	0.47
12:X:208:LYS:HG3	12:X:212:TRP:HB2	1.97	0.47
4:D:48:ASP:OD1	4:D:48:ASP:N	2.39	0.47
6:I:129:DT:H3	7:J:19:DA:H61	1.63	0.47
8:K:179:ILE:HG21	10:N:7:GLN:HE22	1.80	0.47
9:M:889:GLY:N	10:N:369:ASN:OD1	2.46	0.47
10:N:207:ARG:HH22	10:N:258:HIS:CA	2.28	0.47
13:L:83:ASP:HB3	13:L:109:ARG:HH21	1.80	0.47
2:B:82:THR:OG1	2:B:83:ALA:N	2.48	0.47
8:K:162:LYS:HD3	8:K:213:ARG:HG3	1.97	0.47
9:M:902:LYS:O	9:M:906:LYS:N	2.48	0.47
9:M:856:ARG:HG2	9:M:856:ARG:O	2.15	0.46
10:N:115:ASP:OD1	10:N:115:ASP:N	2.47	0.46
13:L:180:MET:O	13:L:181:GLN:NE2	2.48	0.46
8:K:32:THR:OG1	8:K:46:CYS:SG	2.66	0.46
13:L:354:LEU:HD11	13:L:362:ALA:HB3	1.97	0.46
13:L:10:ASP:OD1	13:L:10:ASP:N	2.46	0.46
2:F:73:THR:HG21	2:F:81:VAL:HA	1.97	0.46
8:K:276:SER:OG	8:K:277:GLY:N	2.49	0.46
8:K:29:LYS:HD3	8:K:48:ASN:HB3	1.98	0.46
10:N:163:ILE:HB	10:N:166:HIS:HB2	1.97	0.46
3:G:17:ARG:NE	5:H:118:TYR:OH	2.44	0.46
8:K:73:ASN:ND2	8:K:89:GLU:OE1	2.46	0.46
8:K:227:VAL:HB	8:K:241:PHE:HB2	1.97	0.45
13:L:107:SER:HA	13:L:355:SER:HA	1.98	0.45
2:F:22:LEU:HD22	2:F:25:ASN:HD21	1.80	0.45
3:G:77:ARG:HE	3:G:77:ARG:HB3	1.59	0.45
8:K:148:MET:HE2	8:K:185:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:124:GLU:HB3	13:L:363:SER:HB2	1.99	0.45
13:L:244:VAL:HB	14:O:88:ARG:HH21	1.81	0.45
1:E:129:ARG:O	1:E:129:ARG:NH1	2.46	0.45
8:K:229:LEU:HB3	8:K:239:ARG:HB2	1.97	0.45
10:N:168:TYR:O	10:N:187:SER:N	2.48	0.45
10:N:5:LEU:H	10:N:5:LEU:HG	1.53	0.45
13:L:118:LYS:HB3	13:L:379:ASP:HB3	1.98	0.45
13:L:384:ASN:HA	13:L:387:TYR:HB3	1.98	0.45
7:J:5:DG:H2"	7:J:6:DA:H2'	1.98	0.45
3:C:16:THR:H	7:J:31:DA:H5"	1.81	0.45
8:K:221:LYS:HB2	8:K:258:LEU:HD12	1.98	0.45
13:L:149:VAL:HG23	13:L:157:SER:HB2	1.98	0.45
5:H:72:GLY:O	5:H:76:ARG:NH1	2.50	0.44
6:I:22:DG:N2	7:J:127:DC:O2	2.50	0.44
8:K:68:HIS:NE2	8:K:86:SER:OG	2.45	0.44
9:M:893:ARG:HA	9:M:921:THR:HA	1.97	0.44
9:M:939:CYS:HB3	9:M:995:CYS:HB2	1.99	0.44
5:H:61:SER:O	5:H:61:SER:OG	2.35	0.44
6:I:22:DG:H2"	6:I:23:DC:H5"	1.99	0.44
13:L:270:PRO:HB2	13:L:283:TYR:HD2	1.83	0.44
8:K:236:THR:OG1	8:K:237:VAL:N	2.49	0.44
9:M:894:GLN:OE1	9:M:916:ARG:NH1	2.50	0.44
6:I:50:DG:N2	7:J:99:DT:O2	2.51	0.44
8:K:175:GLY:O	8:K:192:THR:OG1	2.33	0.44
9:M:975:LYS:HB2	9:M:975:LYS:HE3	1.85	0.44
9:M:942:SER:N	9:M:971:THR:OG1	2.51	0.43
10:N:231:ILE:HG23	10:N:243:TYR:HB2	1.99	0.43
8:K:177:ILE:HB	8:K:191:LEU:HB2	2.00	0.43
10:N:84:ASP:OD1	10:N:84:ASP:N	2.47	0.43
10:N:210:TYR:HD1	10:N:260:VAL:C	2.21	0.43
9:M:935:ILE:HD12	9:M:935:ILE:HA	1.80	0.43
10:N:338:ASN:OD1	10:N:338:ASN:N	2.52	0.43
1:A:61:LEU:HD12	2:B:37:LEU:HD23	2.01	0.43
10:N:98:LYS:HD3	10:N:111:GLN:HB3	2.00	0.43
10:N:180:SER:OG	10:N:196:LEU:O	2.36	0.43
13:L:122:GLU:HG2	13:L:185:ARG:HG2	2.00	0.43
13:L:377:ASP:HB2	13:L:380:ILE:HG23	2.00	0.43
10:N:190:TRP:CD2	10:N:212:GLU:O	2.71	0.43
13:L:311:PRO:HD3	13:L:344:ASN:HD21	1.84	0.43
10:N:112:TYR:HB2	10:N:151:PHE:HD2	1.84	0.43
10:N:190:TRP:CE2	10:N:213:LYS:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:219:ARG:HA	12:X:222:PRO:HD2	2.01	0.43
3:C:76:THR:OG1	3:C:77:ARG:N	2.52	0.42
4:D:46:HIS:HB3	4:D:49:THR:HB	2.00	0.42
10:N:193:ALA:CB	10:N:209:CYS:SG	3.07	0.42
4:D:83:ARG:HA	4:D:83:ARG:HD3	1.88	0.42
1:E:50:GLU:OE1	2:F:39:ARG:NE	2.46	0.42
6:I:80:DC:O2	7:J:69:DG:N2	2.52	0.42
8:K:189:LYS:NZ	8:K:232:TYR:O	2.43	0.42
10:N:268:TYR:HE1	10:N:310:GLY:HA2	1.83	0.42
5:H:33:SER:OG	5:H:34:TYR:N	2.51	0.42
13:L:246:ARG:HH22	13:L:346:ASN:HB2	1.83	0.42
3:G:76:THR:OG1	3:G:77:ARG:N	2.52	0.42
10:N:24:LEU:HD23	10:N:24:LEU:HA	1.90	0.42
13:L:124:GLU:N	13:L:363:SER:O	2.52	0.42
5:H:92:GLN:HE22	10:N:273:ASN:HD21	1.68	0.42
10:N:205:LYS:HE3	10:N:205:LYS:HB2	1.83	0.42
14:P:96:THR:HA	14:P:99:LEU:HB2	2.00	0.42
8:K:133:SER:HA	8:K:149:SER:HA	2.01	0.42
10:N:34:LYS:HD2	10:N:34:LYS:HA	1.83	0.42
10:N:424:ASP:OD1	10:N:424:ASP:N	2.53	0.42
9:M:872:LEU:HD21	9:M:931:ILE:HG22	2.01	0.42
10:N:9:PRO:HB2	10:N:11:GLY:H	1.85	0.42
13:L:123:VAL:N	13:L:186:ILE:O	2.45	0.42
3:C:16:THR:O	3:C:19:SER:OG	2.32	0.41
6:I:18:DC:H2"	6:I:19:DG:C8	2.54	0.41
10:N:227:SER:HB3	10:N:286:SER:HA	2.01	0.41
13:L:21:LYS:HE3	13:L:21:LYS:HB2	1.85	0.41
14:P:101:GLU:HA	14:P:104:LYS:HG2	2.02	0.41
3:C:85:LEU:HD23	3:C:85:LEU:HA	1.92	0.41
14:P:91:LEU:H	14:P:91:LEU:HG	1.73	0.41
6:I:13:DG:H2'	6:I:14:DG:C8	2.55	0.41
8:K:239:ARG:HD3	8:K:239:ARG:HA	1.94	0.41
12:X:290:TRP:HE1	12:X:296:ASN:HD22	1.67	0.41
13:L:244:VAL:HG11	13:L:246:ARG:HE	1.85	0.41
13:L:294:VAL:HB	13:L:299:HIS:HE2	1.86	0.41
5:H:87:THR:N	5:H:90:GLU:OE1	2.46	0.41
10:N:146:ASP:N	10:N:146:ASP:OD1	2.53	0.41
13:L:141:ARG:HA	13:L:141:ARG:HD3	1.95	0.41
13:L:384:ASN:O	13:L:388:ASN:ND2	2.44	0.41
13:L:386:ILE:O	13:L:390:GLN:N	2.54	0.41
1:A:121:PRO:HG3	2:B:50:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:47:DC:H4'	7:J:48:DC:H5'	2.02	0.41
9:M:852:GLN:HG2	9:M:950:VAL:HG11	2.03	0.41
13:L:368:ALA:HA	13:L:371:LEU:HB2	2.03	0.41
1:A:134:ARG:HD3	1:A:134:ARG:HA	1.88	0.41
1:E:82:LEU:HD23	1:E:82:LEU:HA	1.96	0.41
8:K:173:TYR:OH	8:K:255:ASN:ND2	2.54	0.41
13:L:72:ASP:N	13:L:72:ASP:OD1	2.53	0.41
2:B:32:PRO:O	2:B:36:ARG:N	2.49	0.41
2:F:32:PRO:O	2:F:36:ARG:NH1	2.47	0.41
8:K:231:GLU:OE1	8:K:234:ARG:NE	2.54	0.41
9:M:902:LYS:HA	9:M:902:LYS:HD3	1.84	0.41
9:M:902:LYS:HA	9:M:905:ILE:HG22	2.02	0.41
10:N:376:GLU:HA	13:L:105:TRP:HE1	1.86	0.41
10:N:402:CYS:SG	10:N:403:THR:N	2.94	0.41
12:X:302:LYS:HA	12:X:302:LYS:HD2	1.90	0.41
8:K:134:ILE:O	8:K:148:MET:N	2.49	0.40
8:K:148:MET:HE2	8:K:181:ASP:O	2.21	0.40
10:N:125:ARG:HB2	10:N:128:VAL:HG12	2.02	0.40
13:L:308:PRO:O	13:L:313:PHE:CD2	2.74	0.40
13:L:346:ASN:HB3	13:L:347:ARG:HH21	1.87	0.40
14:O:106:ILE:HD13	14:O:118:LEU:HD22	2.04	0.40
2:F:47:SER:OG	2:F:48:GLY:N	2.55	0.40
7:J:129:DC:H2"	7:J:130:DG:N7	2.37	0.40
8:K:297:HIS:ND1	8:K:300:SER:OG	2.44	0.40
10:N:194:PHE:CE1	10:N:206:ILE:HD12	2.57	0.40
10:N:232:ALA:HA	10:N:242:GLN:HA	2.04	0.40
13:L:293:PHE:HD1	13:L:293:PHE:HA	1.77	0.40
3:C:81:ARG:HH11	3:C:106:GLY:HA3	1.85	0.40
8:K:133:SER:HA	8:K:148:MET:O	2.21	0.40
10:N:69:SER:HB3	10:N:107:LYS:HE2	2.03	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	95/135 (70%)	92 (97%)	3 (3%)	0	100	100
1	E	94/135 (70%)	90 (96%)	4 (4%)	0	100	100
2	B	80/102 (78%)	78 (98%)	2 (2%)	0	100	100
2	F	84/102 (82%)	80 (95%)	4 (5%)	0	100	100
3	C	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
3	G	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
4	D	91/125 (73%)	89 (98%)	2 (2%)	0	100	100
5	H	91/125 (73%)	87 (96%)	4 (4%)	0	100	100
8	K	301/327 (92%)	278 (92%)	23 (8%)	0	100	100
9	M	182/275 (66%)	162 (89%)	20 (11%)	0	100	100
10	N	400/439 (91%)	369 (92%)	31 (8%)	0	100	100
11	R	1/3 (33%)	1 (100%)	0	0	100	100
12	X	69/342 (20%)	64 (93%)	5 (7%)	0	100	100
13	L	376/405 (93%)	347 (92%)	28 (7%)	1 (0%)	41	74
14	O	40/134 (30%)	38 (95%)	1 (2%)	1 (2%)	5	35
14	P	39/134 (29%)	37 (95%)	2 (5%)	0	100	100
All	All	2153/2997 (72%)	2010 (93%)	141 (6%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	L	311	PRO
14	O	114	PRO

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	84/110 (76%)	84 (100%)	0	100	100
1	E	84/110 (76%)	84 (100%)	0	100	100
2	B	68/78 (87%)	66 (97%)	2 (3%)	42	66
2	F	71/78 (91%)	71 (100%)	0	100	100
3	C	84/84 (100%)	78 (93%)	6 (7%)	14	45
3	G	84/84 (100%)	79 (94%)	5 (6%)	19	50
4	D	79/105 (75%)	78 (99%)	1 (1%)	69	83
5	H	79/105 (75%)	79 (100%)	0	100	100
8	K	275/298 (92%)	274 (100%)	1 (0%)	91	95
9	M	161/238 (68%)	160 (99%)	1 (1%)	86	93
10	N	360/387 (93%)	357 (99%)	3 (1%)	81	89
11	R	3/3 (100%)	3 (100%)	0	100	100
12	X	70/319 (22%)	70 (100%)	0	100	100
13	L	352/375 (94%)	351 (100%)	1 (0%)	92	96
14	O	38/120 (32%)	38 (100%)	0	100	100
14	P	36/120 (30%)	35 (97%)	1 (3%)	43	67
All	All	1928/2614 (74%)	1907 (99%)	21 (1%)	74	85

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	23	ARG
2	B	96	THR
3	C	43	VAL
3	C	91	GLU
3	C	100	VAL
3	C	113	SER
3	C	116	LEU
3	C	118	LYS
4	D	77	LEU
3	G	43	VAL
3	G	100	VAL
3	G	113	SER
3	G	116	LEU
3	G	118	LYS
8	K	194	ASP
9	M	957	VAL

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Mol	Chain	Res	Type
10	N	5	LEU
10	N	238	ARG
10	N	241	ARG
13	L	252	ARG
14	P	96	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	81	ASN
1	E	68	GLN
2	F	25	ASN
2	F	75	HIS
3	G	73	ASN
5	H	81	ASN
9	M	937	HIS
10	N	3	ASN
10	N	7	GLN
10	N	110	GLN
10	N	161	GLN
10	N	166	HIS
10	N	273	ASN
10	N	276	GLN
12	X	211	ASN
12	X	225	ASN
12	X	296	ASN
12	X	307	ASN
13	L	181	GLN
13	L	295	ASN
13	L	344	ASN
13	L	384	ASN
14	O	98	HIS
14	P	120	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	SAM	M	1101	-	24,29,29	1.18	3 (12%)	23,42,42	1.53	4 (17%)

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
15	SAM	M	1101	-	-	6/12/33/33	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	M	1101	SAM	C2-N3	3.48	1.37	1.32
15	M	1101	SAM	C2-N1	2.28	1.38	1.33
15	M	1101	SAM	OXT-C	-2.27	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	M	1101	SAM	N3-C2-N1	-5.12	120.67	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	M	1101	SAM	C3'-C2'-C1'	2.91	105.36	100.98
15	M	1101	SAM	OXT-C-O	-2.31	118.84	124.09
15	M	1101	SAM	OXT-C-CA	2.01	120.25	113.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

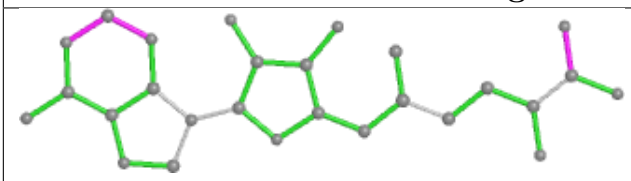
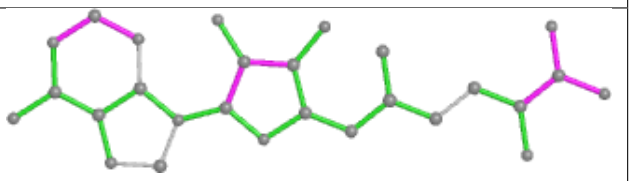
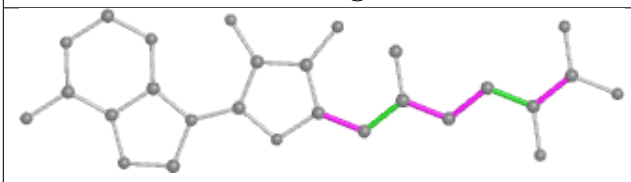
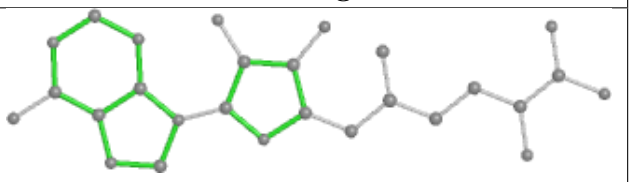
Mol	Chain	Res	Type	Atoms
15	M	1101	SAM	CB-CG-SD-CE
15	M	1101	SAM	CB-CG-SD-C5'
15	M	1101	SAM	O4'-C4'-C5'-SD
15	M	1101	SAM	C3'-C4'-C5'-SD
15	M	1101	SAM	CA-CB-CG-SD
15	M	1101	SAM	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	M	1101	SAM	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 SAM M 1101	
 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.

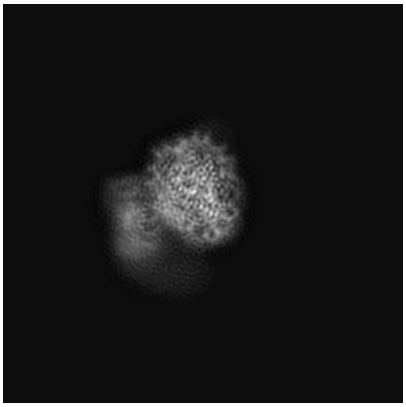
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20765. These allow visual inspection of the internal detail of the map and identification of artifacts.

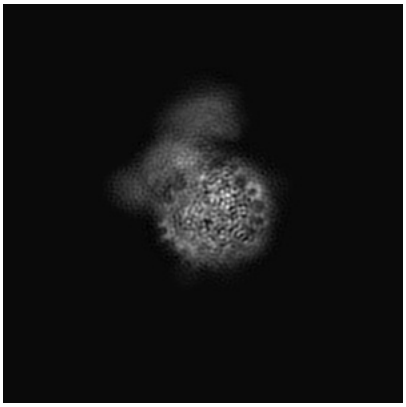
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

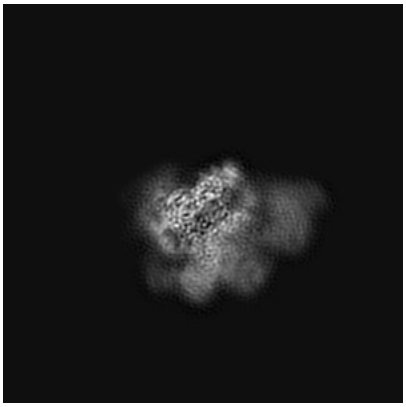
6.1.1 Primary map



X



Y

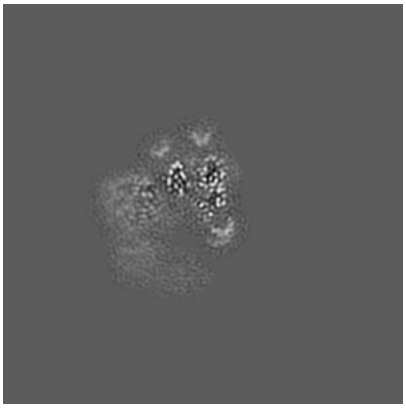


Z

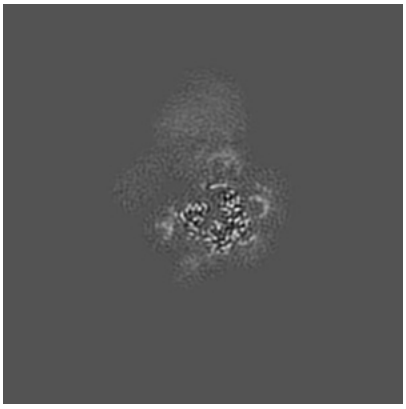
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 162



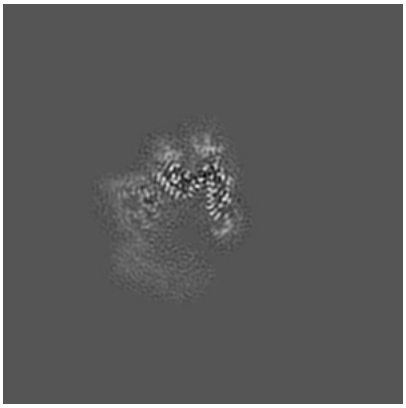
Y Index: 162

Z Index: 162

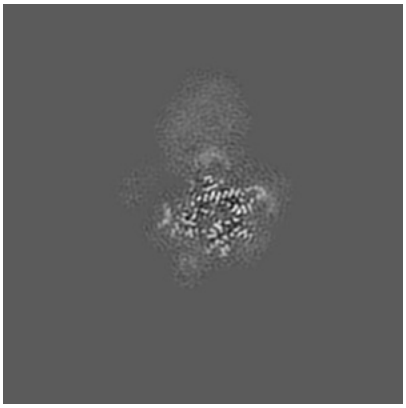
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

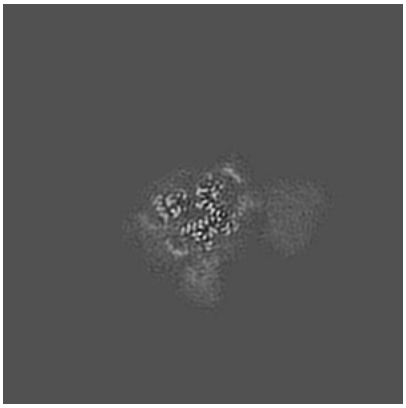
6.3.1 Primary map



X Index: 167



Y Index: 167

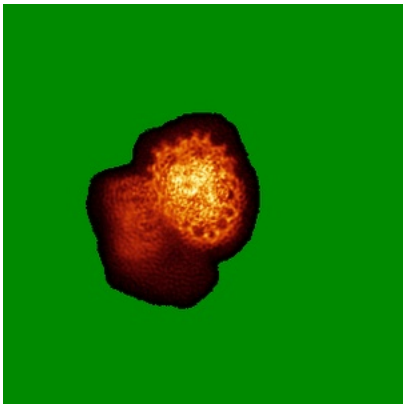


Z Index: 181

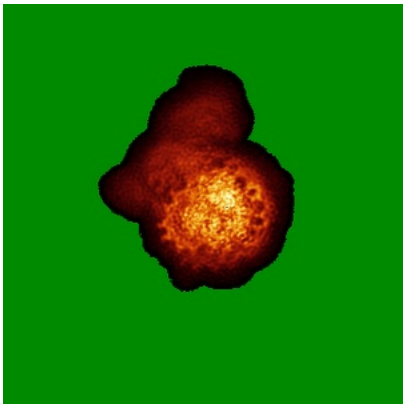
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

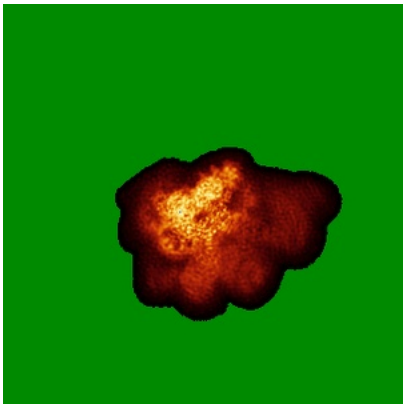
6.4.1 Primary map



X



Y

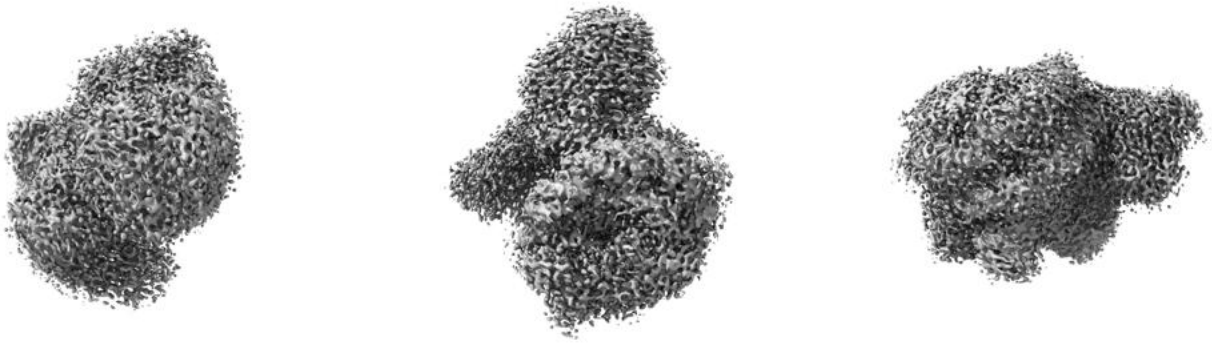


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

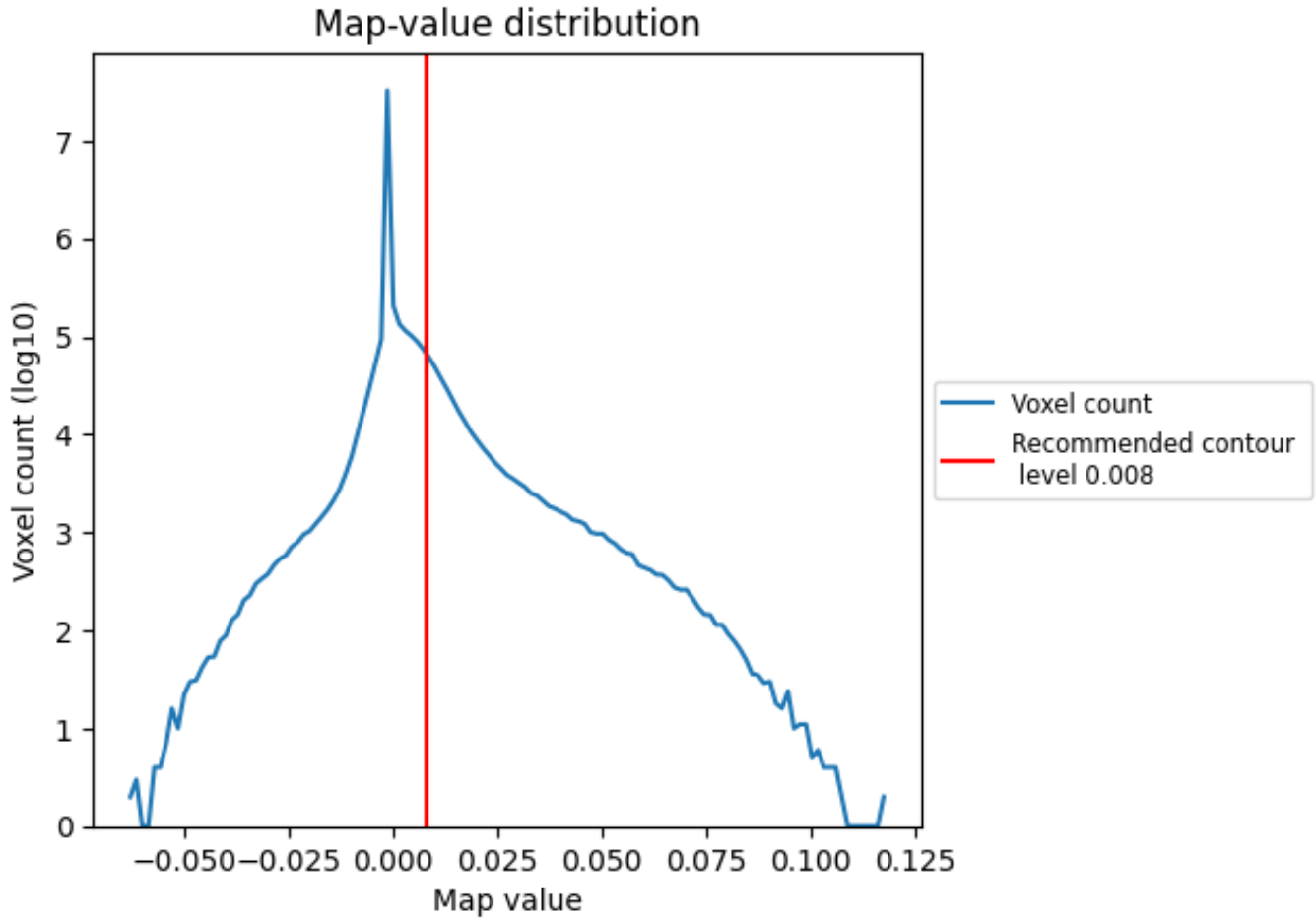
6.6 Mask visualisation (i)

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

7 Map analysis

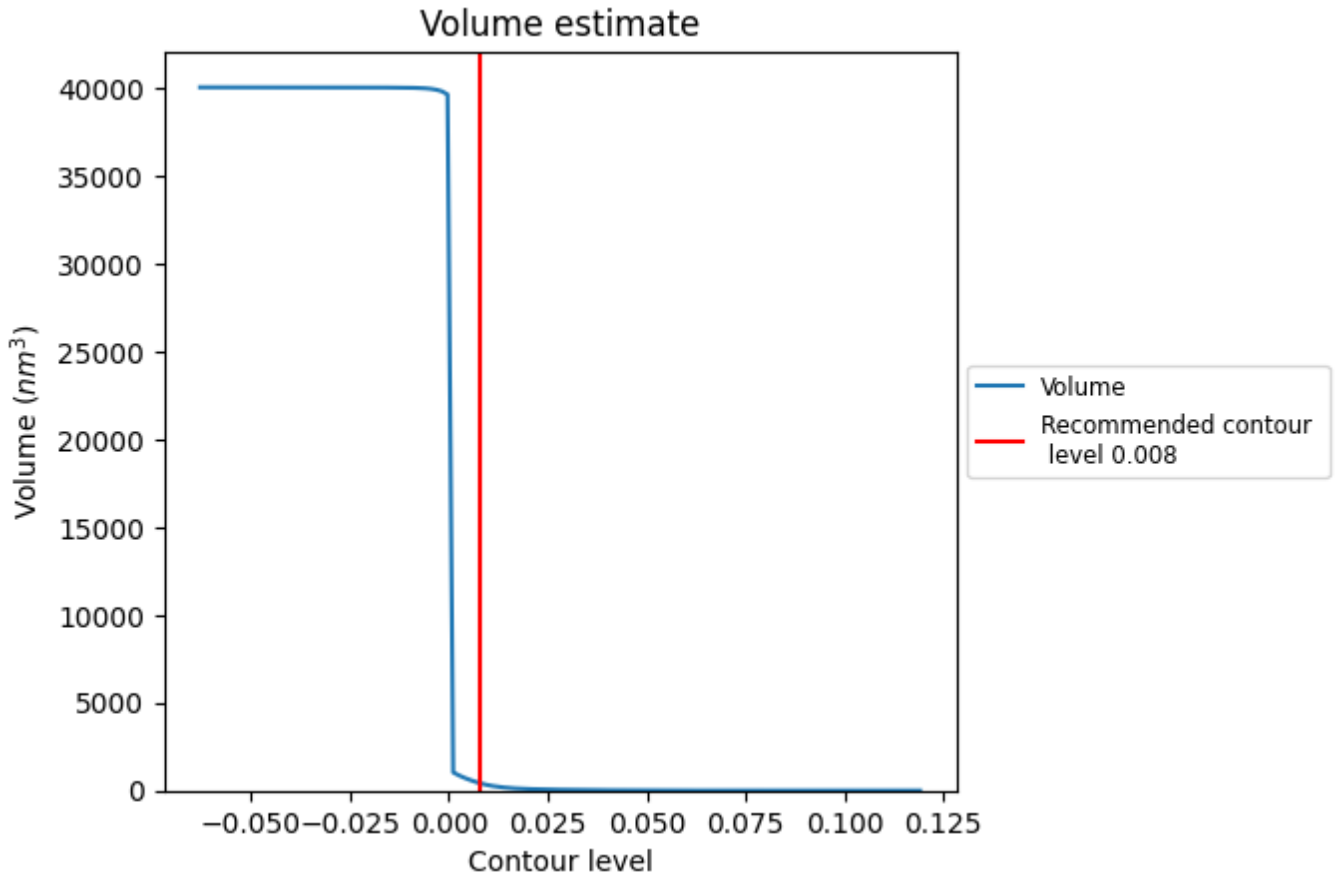
This section contains the results of statistical analysis of the map.

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.

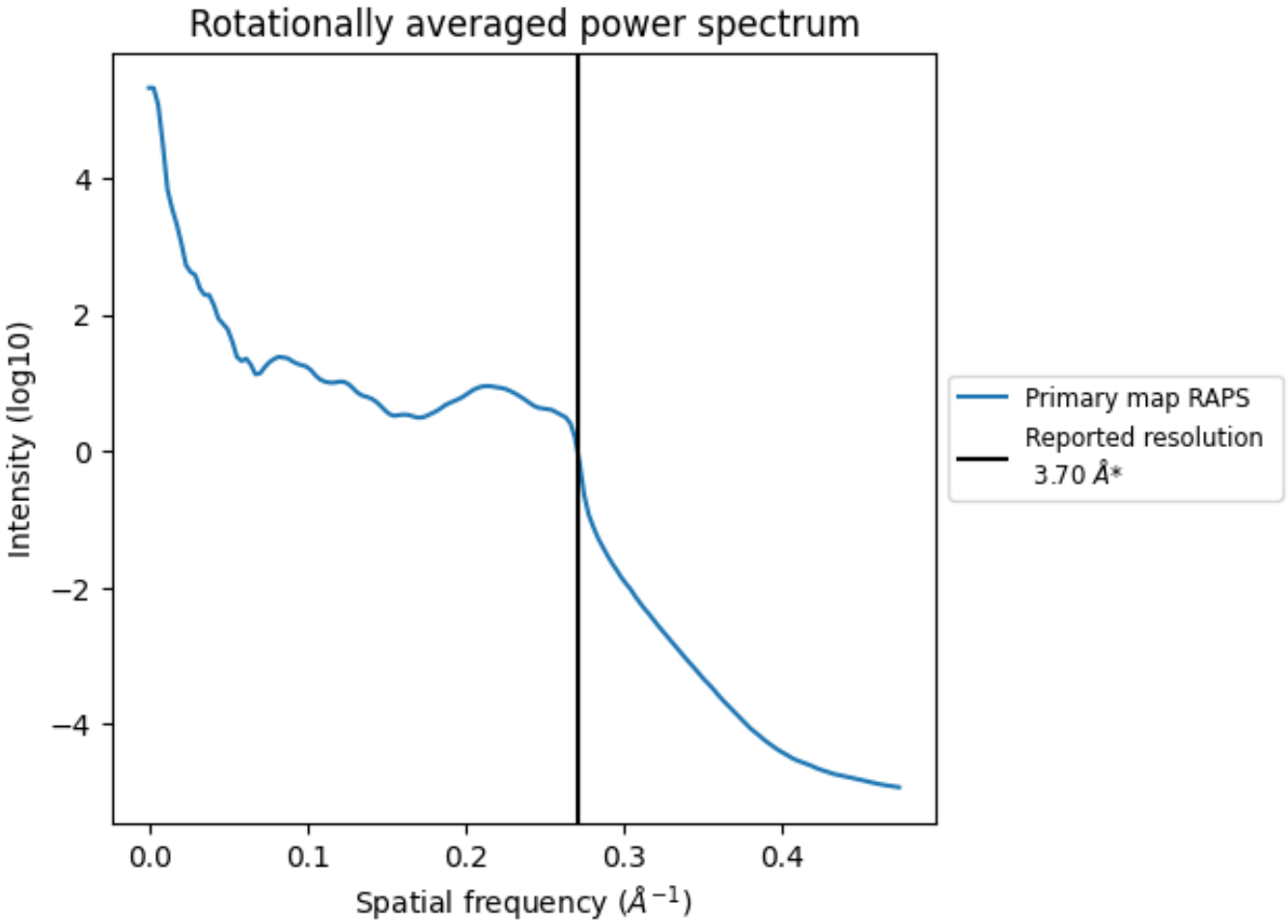
7.2 Volume estimate



The volume at the recommended contour level is 411 nm^3; this corresponds to an approximate mass of 371 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 0.270 $Å^{-1}$

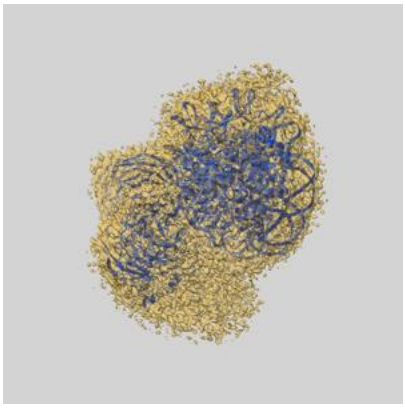
8 Fourier-Shell correlation (i)

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

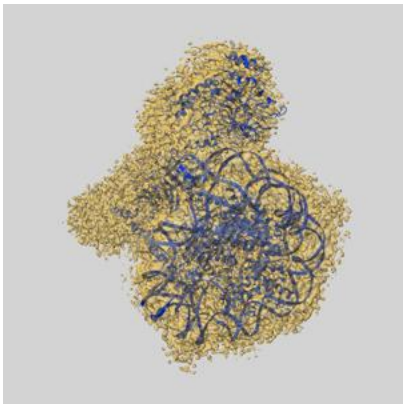
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20765 and PDB model 6UGM. Per-residue inclusion information can be found in section 3 on page 8.

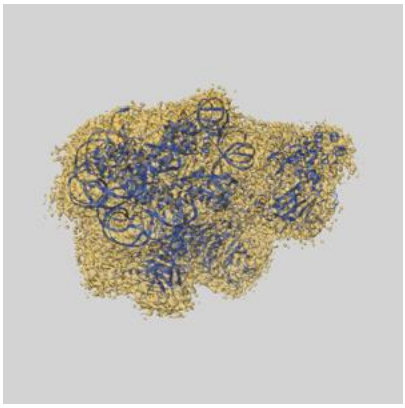
9.1 Map-model overlay



X



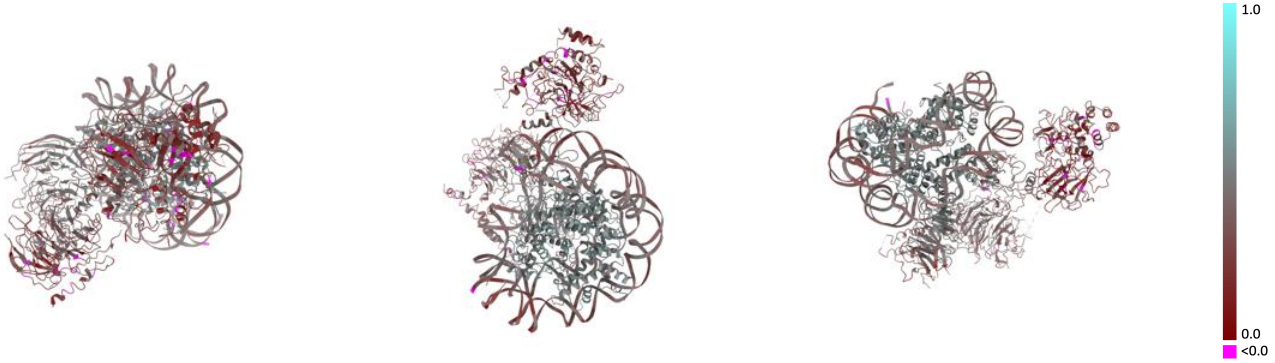
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

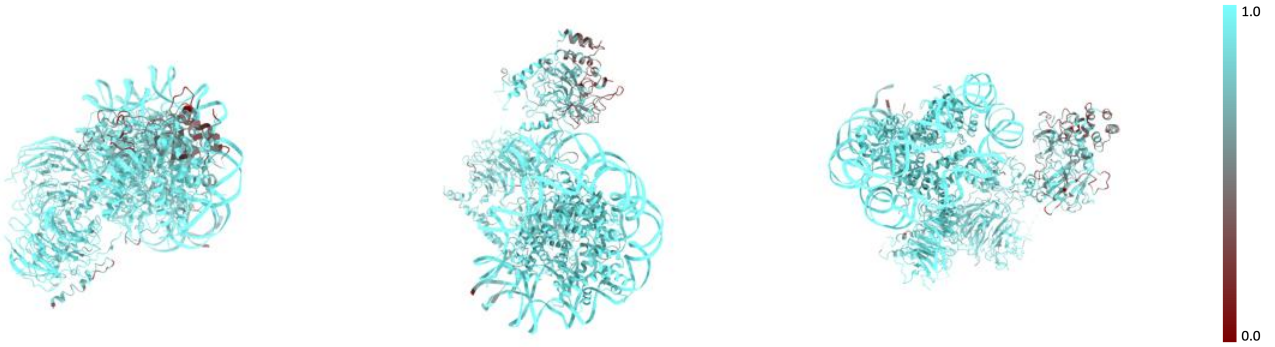
9.2 Q-score mapped to coordinate model



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.

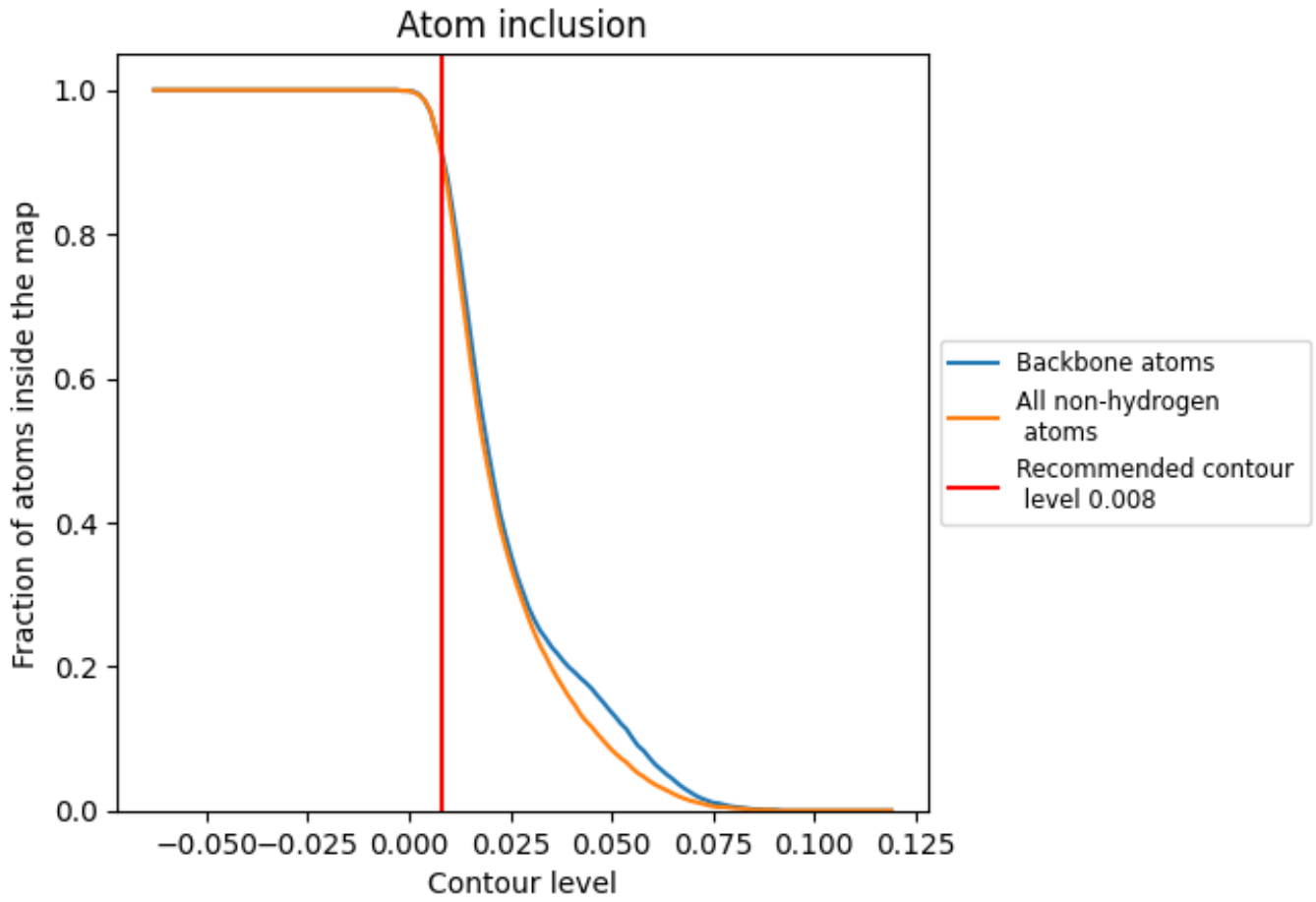
9.3 Atom inclusion mapped to coordinate model



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 (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9120	0.3850
A	0.9660	0.5170
B	0.9830	0.5190
C	0.9350	0.4790
D	0.9820	0.5090
E	0.9670	0.5260
F	0.9580	0.5190
G	0.9400	0.4950
H	0.9890	0.5160
I	0.9710	0.3770
J	0.9730	0.3780
K	0.9520	0.3300
L	0.7260	0.2460
M	0.8810	0.3680
N	0.9480	0.3980
O	0.6130	0.2420
P	0.4750	0.2670
R	0.9170	0.3180
X	0.8780	0.2810