Full wwPDB EM Validation Report ⓘ

Jan 9, 2024 – 04:31 PM EST

PDB ID	:	8TOF
EMDB ID	:	EMD-41449
Title	:	Rpd3S bound to an H3K36Cme3 modified nucleosome
Authors	:	Markert, J.W.; Vos, S.M.; Farnung, L.
Deposited on	:	2023-08-03
Resolution	:	2.80 Å(reported)

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

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

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

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

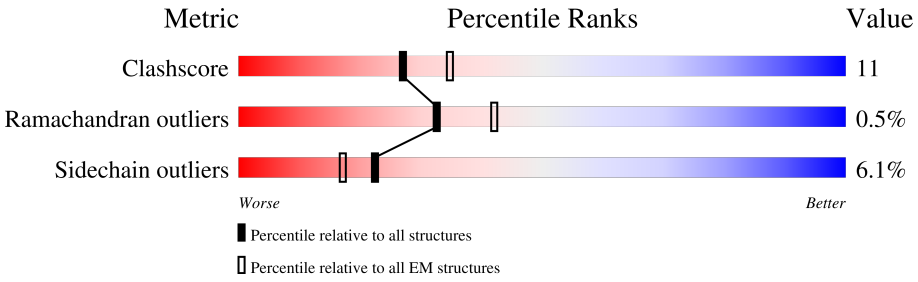
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1536	25% 9% 65%
2	B	433	65% 22% 11%
3	D	401	10% 54% 15% 28%
3	E	401	37% 46% 15% 37%
4	F	684	8% 10% 87%
4	G	684	7% 36% 15% 46%
5	H	5	20% 100%
6	N	206	8% 52% 33% 15%

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Mol	Chain	Length	Quality of chain
7	T	215	9% 55% 27% 18%
8	a	136	70% 26%
8	e	136	74% 26%
9	b	103	77% 21%
9	f	103	75% 24%
10	c	130	78% 21%
10	g	130	80% 19%
11	d	123	74% 23%
11	h	123	72% 24%
12	x	7	57% 100%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 29102 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 Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	545	Total	C	N	O	S	0	0
			4572	2936	774	848	14		

- Molecule 2 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	385	Total	C	N	O	S	0	0
			3057	1948	513	571	25		

- Molecule 3 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	289	Total	C	N	O	S	0	0
			2356	1513	387	443	13		
3	E	253	Total	C	N	O	S	0	0
			2080	1345	342	380	13		

- Molecule 4 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	89	Total	C	N	O	S	0	0
			724	463	121	131	9		
4	G	369	Total	C	N	O	S	0	0
			3010	1905	516	571	18		

- Molecule 5 is a protein called Rco1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	5	Total	C	N	O	0	0
			31	18	8	5		

- Molecule 6 is a DNA chain called DNA (176-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	176	Total	C	N	O	P	0	0
			3623	1719	651	1077	176		

- Molecule 7 is a DNA chain called DNA (176-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	176	Total	C	N	O	P	0	0
			3593	1702	680	1035	176		

- Molecule 8 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	101	Total	C	N	O	S	0	0
			836	528	161	143	4		
8	e	101	Total	C	N	O	S	0	0
			836	528	161	143	4		

- Molecule 9 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	81	Total	C	N	O	S	0	0
			646	407	126	112	1		
9	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 10 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	c	103	Total	C	N	O	0	0
			795	501	155	139		
10	g	105	Total	C	N	O	0	0
			809	510	158	141		

- Molecule 11 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	95	Total	C	N	O	S	0	0
			745	469	134	140	2		
11	h	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	0	MET	-	initiating methionine	UNP P02281
d	29	THR	SER	engineered mutation	UNP P02281
h	0	MET	-	initiating methionine	UNP P02281
h	29	THR	SER	engineered mutation	UNP P02281

- Molecule 12 is a protein called histone N-terminal tail.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	x	7	Total	C	N	O	0	0
			39	24	8	7		

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

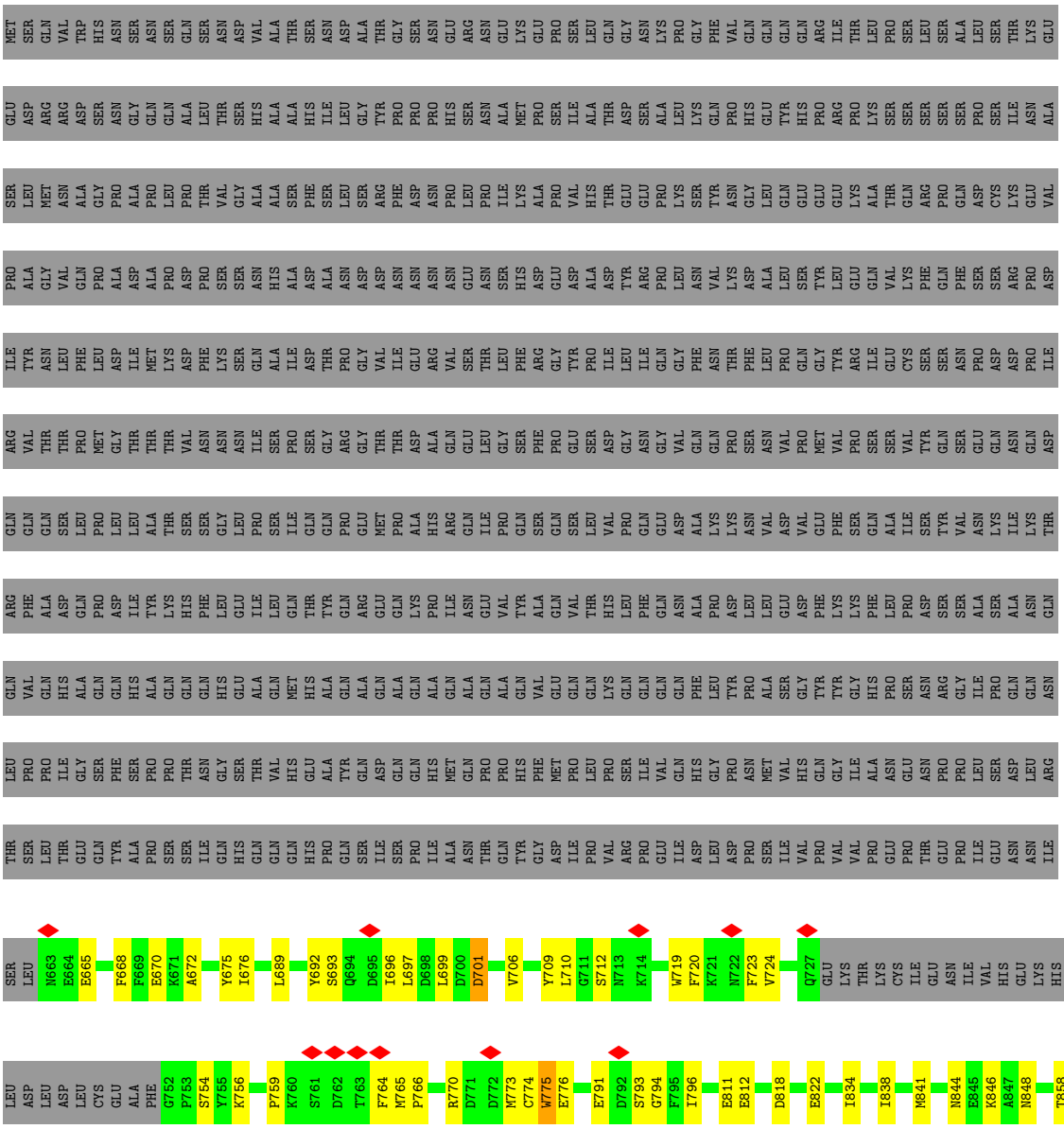
Mol	Chain	Residues	Atoms		AltConf
13	B	1	Total	Zn	0
			1	1	
13	G	4	Total	Zn	0
			4	4	

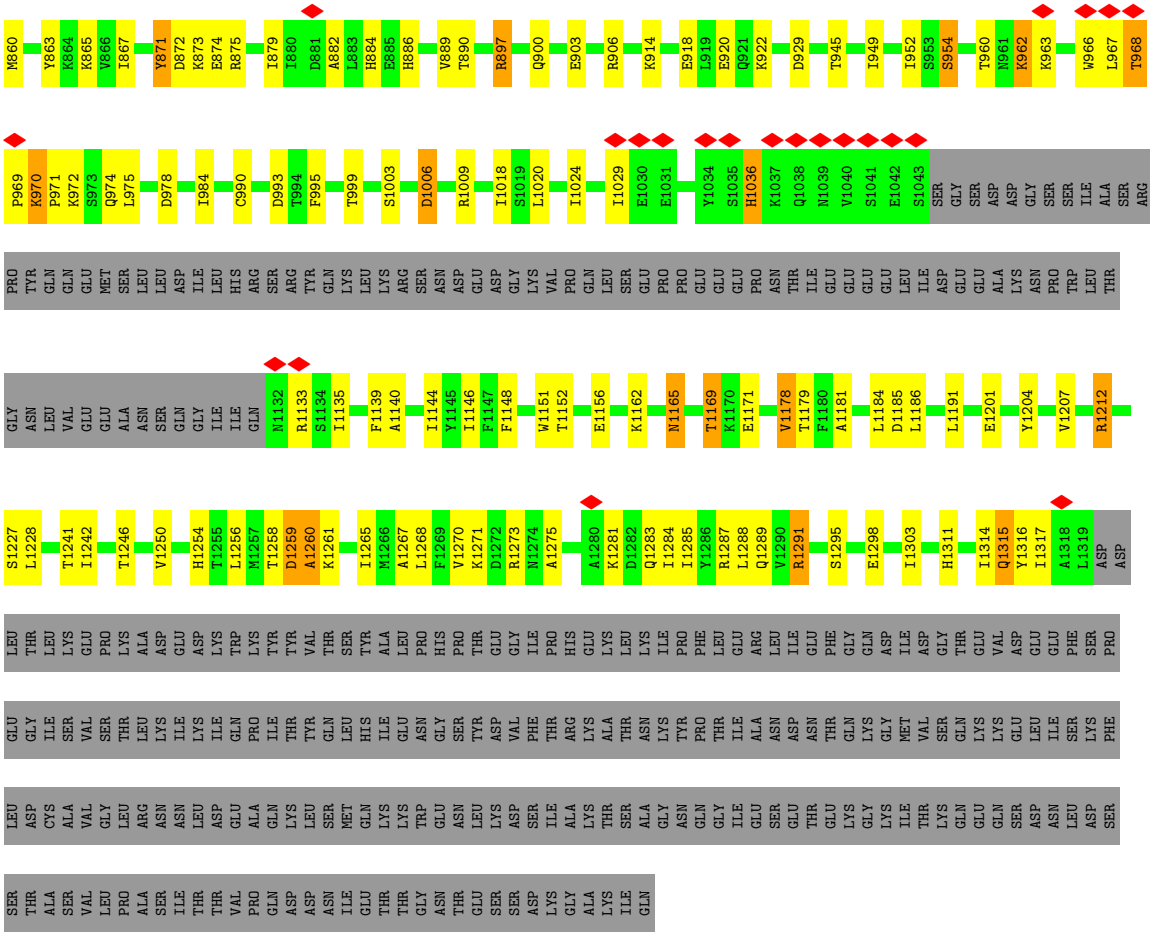
3 Residue-property plots (i)

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: Transcriptional regulatory protein SIN3

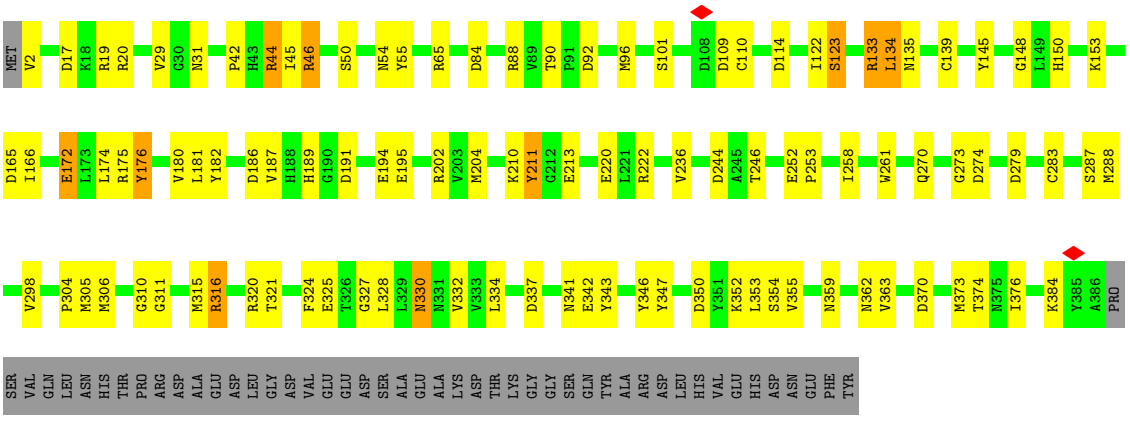
Chain A:





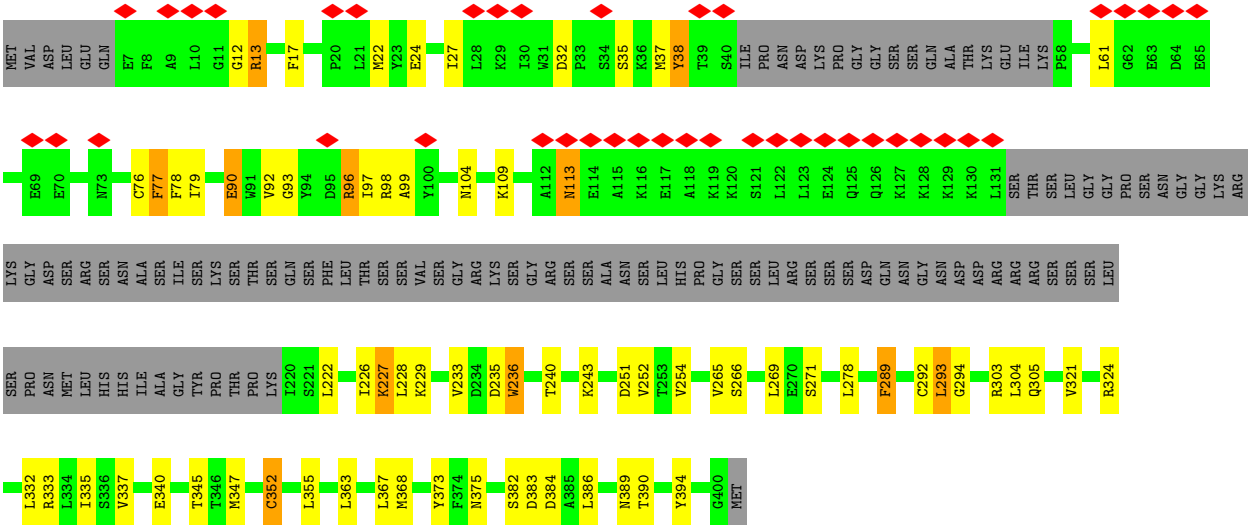
• Molecule 2: Histone deacetylase RPD3

Chain B:



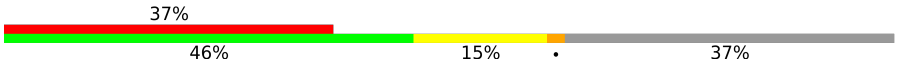
• Molecule 3: Chromatin modification-related protein EAF3

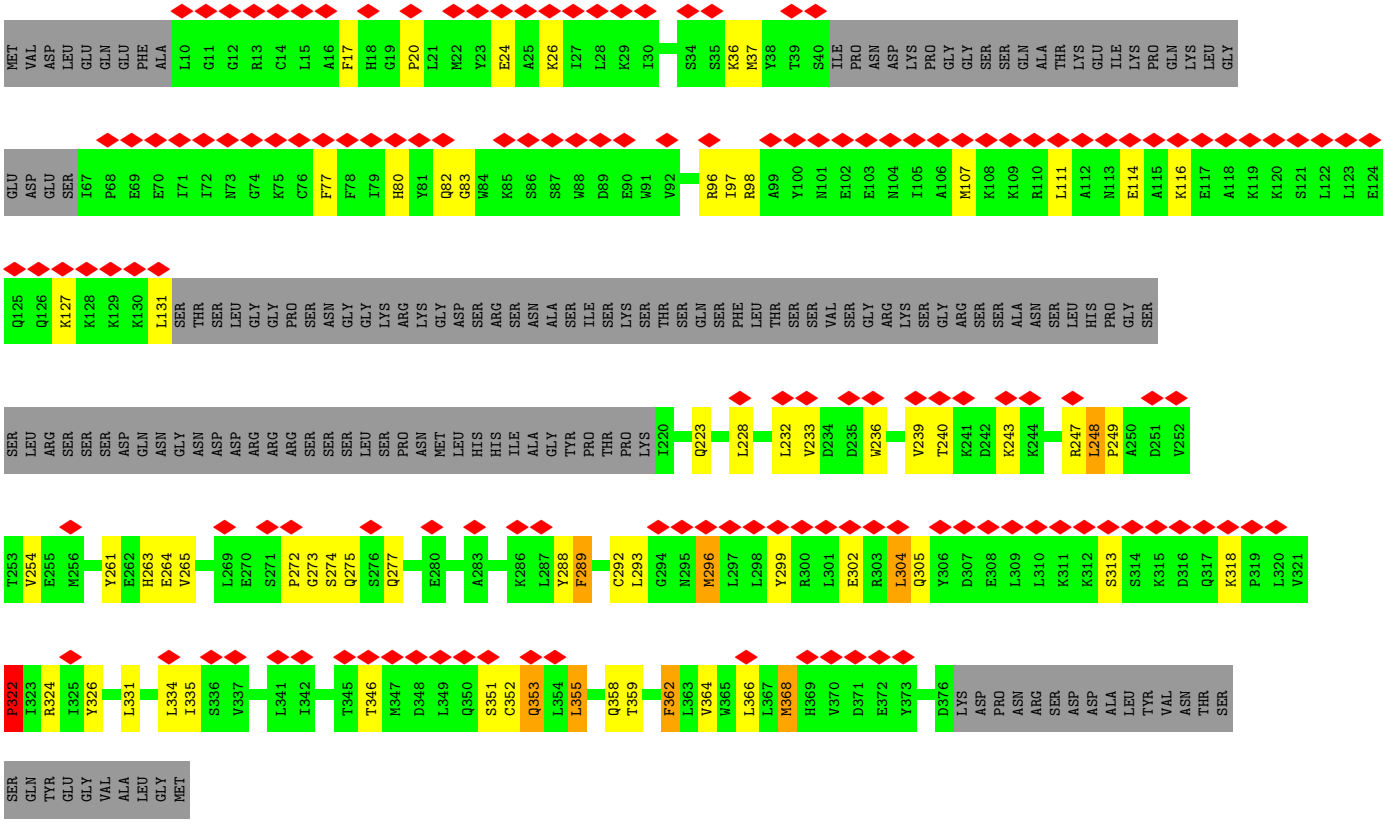
Chain D:



• Molecule 3: Chromatin modification-related protein EAF3

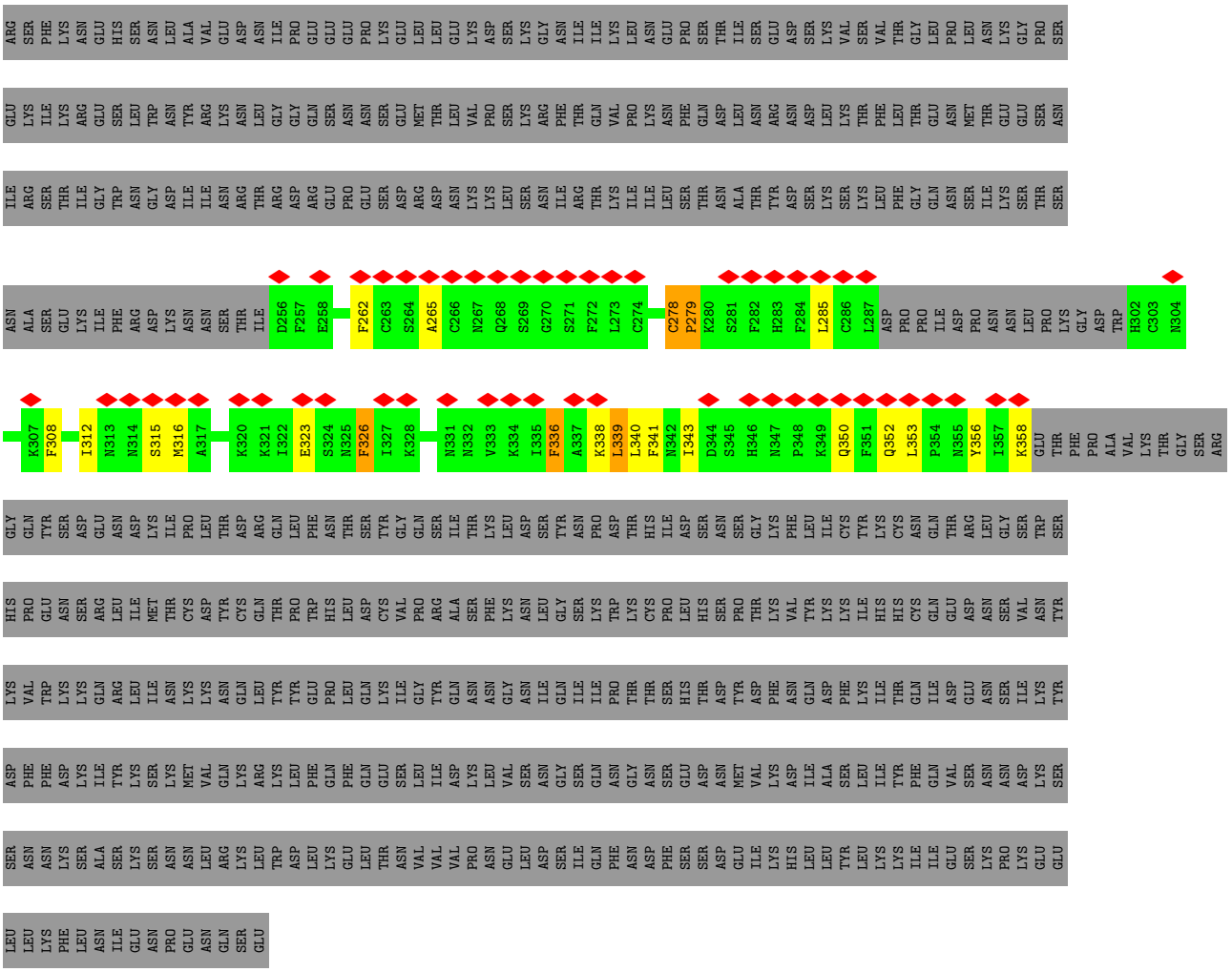
Chain E:





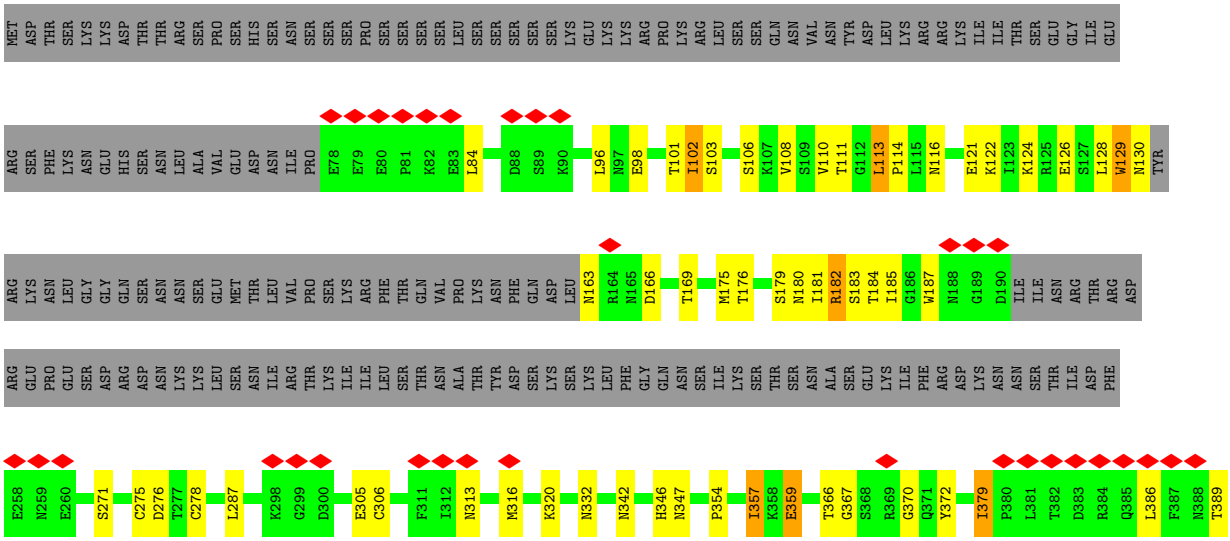
• Molecule 4: Transcriptional regulatory protein RCO1

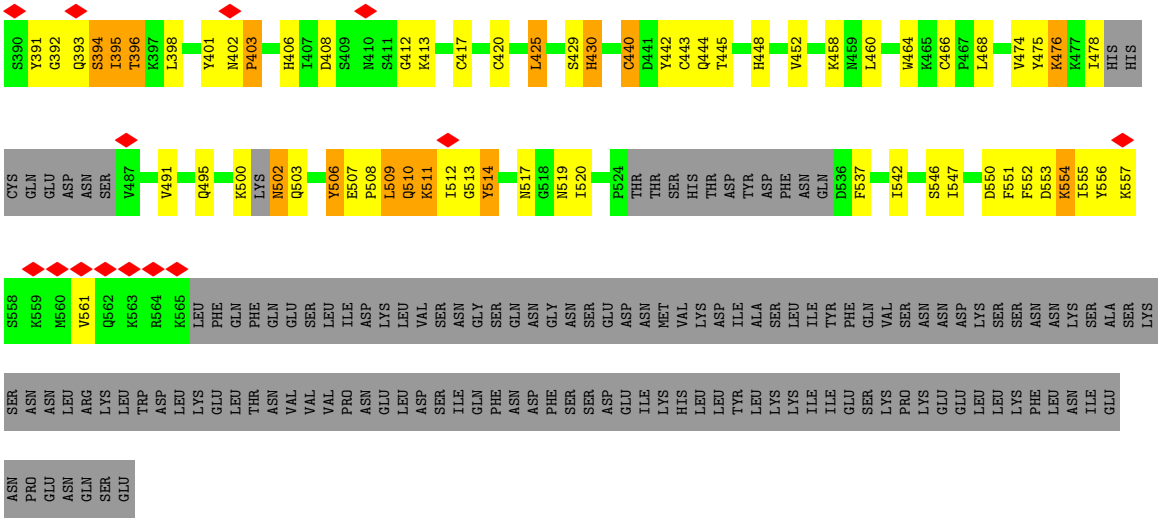
Chain F:



• Molecule 4: Transcriptional regulatory protein RCO1

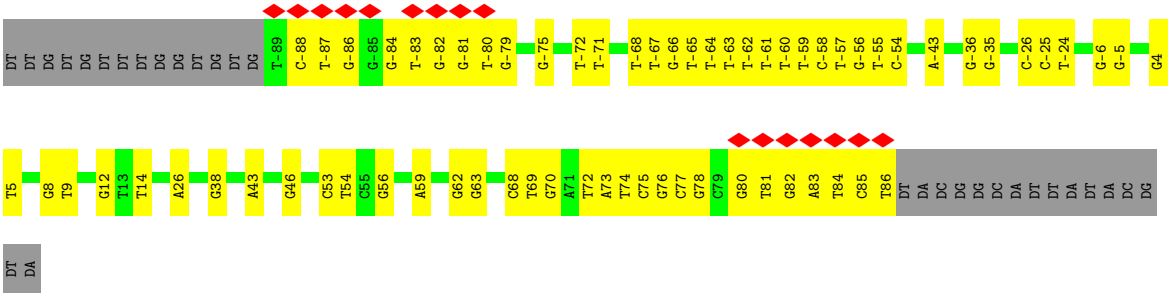
Chain G:



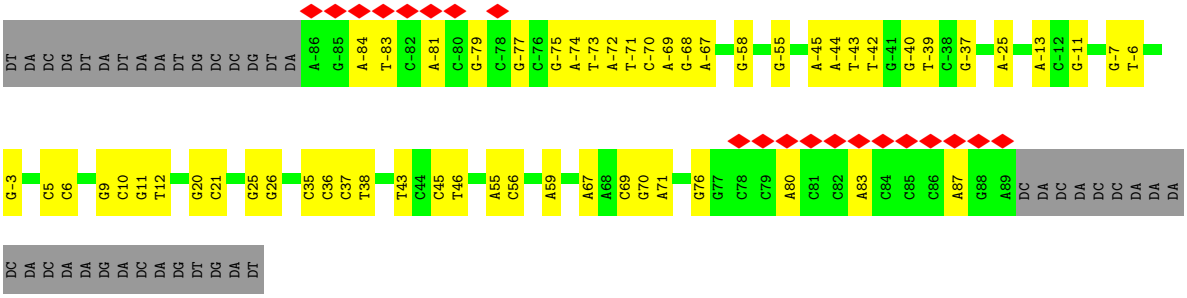


• Molecule 5: Rco1

• Molecule 6: DNA (176-MER)

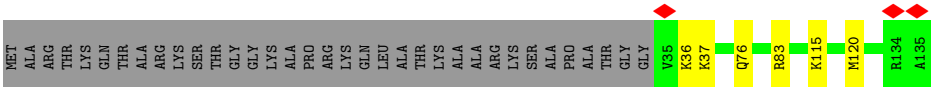


• Molecule 7: DNA (176-MER)



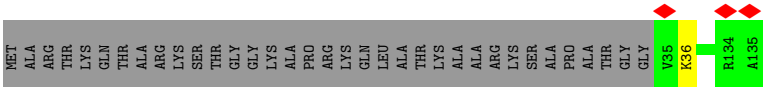
• Molecule 8: Histone H3

Chain a:



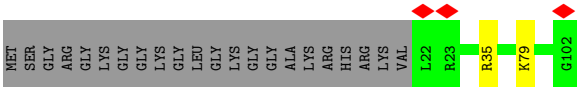
• Molecule 8: Histone H3

Chain e:



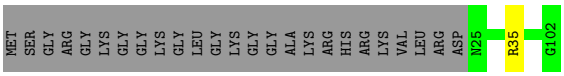
• Molecule 9: Histone H4

Chain b:



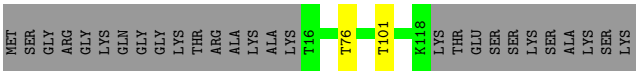
• Molecule 9: Histone H4

Chain f:



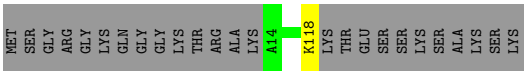
• Molecule 10: Histone H2A

Chain c:



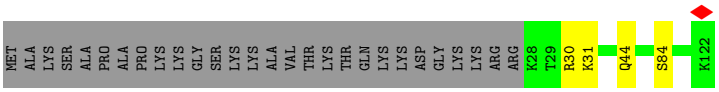
• Molecule 10: Histone H2A

Chain g:



• Molecule 11: Histone H2B 1.1

Chain d:

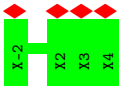


• Molecule 11: Histone H2B 1.1

Chain h:

• Molecule 12: histone N-terminal tail

Chain x:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	484141	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 ($e^-/Å^2$)	51.1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.614	Depositor
Minimum map value	-0.278	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07768	Depositor
Map size (Å)	369.90002, 369.90002, 369.90002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ML3, ZN

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	0.29	0/4675	0.51	0/6301
2	B	0.37	0/3137	0.52	0/4246
3	D	0.29	0/2403	0.50	0/3236
3	E	0.43	1/2122 (0.0%)	0.73	4/2856 (0.1%)
4	F	1.14	3/740 (0.4%)	1.08	6/991 (0.6%)
4	G	0.30	0/3077	0.53	1/4145 (0.0%)
5	H	0.21	0/10	1.06	0/11
6	N	0.81	0/4060	1.31	0/6272
7	T	0.88	0/4034	1.20	0/6216
8	a	0.32	0/835	0.56	0/1118
8	e	0.33	0/835	0.57	0/1118
9	b	0.33	0/653	0.56	0/873
9	f	0.34	0/626	0.56	0/837
10	c	0.32	0/805	0.55	0/1088
10	g	0.31	0/819	0.54	0/1106
11	d	0.34	0/756	0.48	0/1015
11	h	0.33	0/737	0.48	0/993
12	x	0.24	0/8	0.43	0/8
All	All	0.55	4/30332 (0.0%)	0.84	11/42430 (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
2	B	0	1
3	E	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	279	PRO	CB-CG	22.34	2.61	1.50
4	F	279	PRO	CG-CD	-18.41	0.89	1.50
3	E	322	PRO	CG-CD	-14.70	1.02	1.50
4	F	279	PRO	N-CD	5.40	1.55	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	279	PRO	CB-CG-CD	-25.12	8.51	106.50
3	E	322	PRO	N-CD-CG	-20.66	72.22	103.20
3	E	322	PRO	CA-CB-CG	-16.07	73.46	104.00
4	F	279	PRO	N-CA-CB	-10.45	90.77	103.30
4	G	403	PRO	CA-N-CD	-9.59	98.07	111.50
3	E	322	PRO	N-CA-CB	-9.06	92.43	103.30
4	F	279	PRO	CA-CB-CG	-8.71	87.46	104.00
4	F	279	PRO	CA-N-CD	-7.44	101.09	111.50
4	F	279	PRO	N-CD-CG	-7.34	92.19	103.20
4	F	278	CYS	C-N-CD	6.31	141.66	128.40
3	E	368	MET	CG-SD-CE	5.23	108.57	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	46	ARG	Sidechain
3	E	248	LEU	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	4572	0	4534	118	0
2	B	3057	0	2934	74	0
3	D	2356	0	2377	54	0
3	E	2080	0	2126	50	0
4	F	724	0	701	30	0
4	G	3010	0	2952	110	0
5	H	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	3623	0	1986	105	0
7	T	3593	0	1965	84	0
8	a	836	0	883	0	0
8	e	836	0	883	0	0
9	b	646	0	687	0	0
9	f	619	0	659	0	0
10	c	795	0	846	0	0
10	g	809	0	864	0	0
11	d	745	0	773	0	0
11	h	726	0	747	0	0
12	x	39	0	22	0	0
13	B	1	0	0	0	0
13	G	4	0	0	0	0
All	All	29102	0	25958	535	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 11.

All (535) 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)
4:F:279:PRO:N	4:F:279:PRO:CG	1.82	1.42
6:N:38:DG:C2	7:T:-37:DG:N2	1.90	1.38
6:N:59:DA:C2	7:T:-58:DG:N2	2.01	1.27
6:N:73:DA:C2	7:T:-72:DA:C2	2.24	1.25
4:F:279:PRO:CD	4:F:279:PRO:HG2	1.66	1.16
4:F:279:PRO:CD	4:F:279:PRO:HG3	1.66	1.13
6:N:-25:DC:H2"	6:N:-24:DT:C7	1.81	1.11
6:N:68:DC:H2"	6:N:69:DT:H71	1.15	1.08
4:F:279:PRO:CG	4:F:279:PRO:HD2	1.57	1.05
4:F:279:PRO:CG	4:F:279:PRO:HD3	1.57	1.03
6:N:-25:DC:C2'	6:N:-24:DT:H71	1.90	1.01
6:N:38:DG:N2	7:T:-37:DG:N2	2.07	1.01
7:T:25:DG:N2	7:T:26:DG:C2	2.30	0.99
6:N:-66:DG:N2	7:T:67:DA:C2	2.33	0.97
7:T:25:DG:N2	7:T:26:DG:N2	2.12	0.96
6:N:-25:DC:H2"	6:N:-24:DT:H71	0.97	0.96
6:N:68:DC:C2'	6:N:69:DT:H71	1.99	0.93
6:N:-66:DG:C2	7:T:67:DA:C2	2.57	0.92
4:G:101:THR:O	4:G:103:SER:N	2.05	0.89
4:F:279:PRO:CG	4:F:279:PRO:CD	0.89	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:-43:DT:C6	7:T:-42:DT:H72	2.09	0.87
6:N:73:DA:C2'	6:N:74:DT:H72	2.04	0.86
6:N:73:DA:N1	7:T:-72:DA:N1	2.23	0.86
4:G:305:GLU:N	4:G:305:GLU:OE1	2.09	0.85
7:T:-44:DA:C8	7:T:-43:DT:H72	2.11	0.84
1:A:1201:GLU:OE2	1:A:1201:GLU:N	2.10	0.84
3:E:313:SER:OG	3:E:318:LYS:O	1.96	0.83
1:A:945:THR:O	1:A:949:ILE:HD12	1.79	0.82
6:N:-66:DG:N2	7:T:67:DA:N3	2.26	0.82
2:B:153:LYS:NZ	2:B:195:GLU:OE1	2.13	0.82
6:N:38:DG:N2	7:T:-37:DG:C2	2.49	0.79
6:N:38:DG:C2	7:T:-37:DG:C2	2.71	0.79
3:D:294:GLY:O	3:D:303:ARG:NH2	2.17	0.78
3:E:331:LEU:O	3:E:335:ILE:HD12	1.83	0.78
6:N:68:DC:H2"	6:N:69:DT:C7	2.08	0.77
3:D:99:ALA:O	3:D:104:ASN:ND2	2.17	0.77
1:A:844:ASN:O	1:A:848:ASN:ND2	2.18	0.76
6:N:73:DA:C2	7:T:-72:DA:N1	2.53	0.76
1:A:838:ILE:O	1:A:846:LYS:NZ	2.19	0.76
3:D:17:PHE:N	3:D:96:ARG:O	2.19	0.75
1:A:858:THR:OG1	2:B:65:ARG:NH2	2.19	0.75
6:N:-36:DG:N2	6:N:-35:DG:N2	2.35	0.75
6:N:73:DA:C2	7:T:-72:DA:H2	2.03	0.74
1:A:1165:ASN:O	1:A:1169:THR:OG1	2.05	0.74
1:A:689:LEU:HD11	4:G:551:PHE:HB2	1.67	0.74
3:E:288:TYR:HB3	3:E:334:LEU:HD21	1.70	0.74
2:B:244:ASP:OD2	2:B:287:SER:OG	2.04	0.74
6:N:59:DA:C2	7:T:-58:DG:C2	2.76	0.73
2:B:342:GLU:OE2	4:G:169:THR:OG1	2.06	0.72
3:D:229:LYS:HG2	4:G:357:ILE:HG22	1.70	0.72
1:A:1258:THR:O	1:A:1258:THR:HG23	1.89	0.72
3:E:302:GLU:OE2	3:E:326:TYR:OH	2.05	0.72
6:N:-86:DG:C2	7:T:87:DA:C2	2.78	0.71
2:B:50:SER:OG	2:B:342:GLU:OE1	2.08	0.71
4:G:420:CYS:SG	4:G:448:HIS:CE1	2.83	0.71
6:N:73:DA:C2'	6:N:74:DT:C7	2.69	0.70
6:N:38:DG:N1	7:T:-37:DG:N2	2.39	0.70
6:N:73:DA:H2'	6:N:74:DT:H72	1.73	0.70
6:N:82:DG:C2	7:T:-81:DA:C2	2.80	0.70
1:A:1133:ARG:NH1	1:A:1275:ALA:O	2.22	0.69
4:G:181:ILE:O	4:G:184:THR:OG1	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:TYR:O	1:A:693:SER:OG	2.10	0.69
4:G:520:ILE:HG23	4:G:542:ILE:HG22	1.75	0.69
6:N:38:DG:N2	7:T:-37:DG:H21	1.82	0.69
7:T:5:DC:H2"	7:T:6:DC:C5	2.28	0.69
6:N:59:DA:N3	7:T:-58:DG:N2	2.40	0.68
6:N:73:DA:H2"	6:N:74:DT:C7	2.23	0.68
1:A:1261:LYS:O	1:A:1265:ILE:HD12	1.93	0.68
3:D:13:ARG:NH1	3:D:13:ARG:O	2.26	0.68
6:N:76:DG:C2	7:T:-75:DG:C2	2.82	0.68
1:A:1018:ILE:HG21	1:A:1151:TRP:CZ2	2.29	0.68
1:A:863:TYR:O	1:A:867:ILE:HD12	1.94	0.68
3:D:375:ASN:OD1	3:D:386:LEU:HD11	1.94	0.68
6:N:-36:DG:N2	6:N:-35:DG:C2	2.61	0.68
6:N:73:DA:C8	6:N:74:DT:H72	2.29	0.68
1:A:990:CYS:SG	1:A:1212:ARG:NH1	2.67	0.67
4:G:408:ASP:N	4:G:413:LYS:O	2.27	0.67
6:N:-82:DG:C2	7:T:83:DA:C2	2.83	0.67
3:E:26:LYS:NZ	3:E:82:GLN:OE1	2.19	0.67
4:G:444:GLN:OE1	4:G:444:GLN:N	2.28	0.67
4:G:474:VAL:HG12	4:G:474:VAL:O	1.94	0.67
3:E:351:SER:OG	4:G:509:LEU:HD21	1.96	0.66
1:A:995:PHE:O	1:A:999:THR:HG23	1.96	0.66
6:N:73:DA:N1	7:T:-72:DA:C2	2.64	0.66
4:G:84:LEU:HD21	4:G:96:LEU:HD11	1.77	0.66
2:B:273:GLY:N	2:B:311:GLY:O	2.29	0.66
6:N:80:DG:C2	7:T:-79:DG:C2	2.83	0.65
1:A:1135:ILE:HD12	1:A:1135:ILE:O	1.95	0.65
3:D:382:SER:OG	3:D:384:ASP:OD1	2.15	0.65
7:T:-7:DG:H2"	7:T:-6:DT:C7	2.27	0.65
1:A:1268:LEU:HD21	1:A:1289:GLN:HB3	1.79	0.65
6:N:80:DG:C2'	6:N:81:DT:H71	2.26	0.65
4:G:110:VAL:O	4:G:111:THR:OG1	2.09	0.65
7:T:-43:DT:N1	7:T:-42:DT:H72	2.12	0.64
6:N:80:DG:H2'	6:N:81:DT:H71	1.80	0.64
4:G:116:ASN:OD1	4:G:116:ASN:O	2.16	0.64
2:B:186:ASP:OD1	2:B:187:VAL:N	2.31	0.63
3:D:32:ASP:OD2	3:D:35:SER:OG	2.15	0.63
3:D:243:LYS:O	3:D:390:THR:OG1	2.16	0.63
6:N:-62:DT:C2'	6:N:-61:DT:H72	2.27	0.63
1:A:1281:LYS:O	1:A:1285:ILE:HD13	1.98	0.62
2:B:96:MET:SD	2:B:96:MET:N	2.73	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:289:PHE:CE1	3:E:293:LEU:HD13	2.34	0.62
3:E:346:THR:HG23	4:F:338:LYS:NZ	2.14	0.62
6:N:12:DG:N2	7:T:-11:DG:N3	2.48	0.62
6:N:78:DG:C2	7:T:-77:DG:C2	2.87	0.62
2:B:189:HIS:NE2	2:B:194:GLU:OE1	2.31	0.61
4:G:113:LEU:HB2	4:G:114:PRO:HD2	1.81	0.61
7:T:-7:DG:H2"	7:T:-6:DT:C5	2.35	0.61
3:D:226:ILE:HD13	4:G:537:PHE:CG	2.35	0.61
6:N:-84:DG:H2'	6:N:-83:DT:H71	1.81	0.61
1:A:696:ILE:HG22	4:G:474:VAL:HG11	1.81	0.61
7:T:-44:DA:N9	7:T:-43:DT:H72	2.15	0.61
4:F:278:CYS:C	4:F:279:PRO:CG	2.68	0.61
4:G:510:GLN:HA	4:G:510:GLN:OE1	1.99	0.61
1:A:791:GLU:N	1:A:791:GLU:OE1	2.33	0.60
3:D:92:VAL:HG13	3:D:96:ARG:HD2	1.83	0.60
6:N:53:DC:H2"	6:N:54:DT:H71	1.83	0.60
2:B:55:TYR:OH	2:B:337:ASP:O	2.18	0.60
6:N:-36:DG:C2	6:N:-35:DG:C2	2.89	0.60
3:D:233:VAL:HA	3:D:236:TRP:CD1	2.36	0.60
3:E:239:VAL:HG11	3:E:299:TYR:CD2	2.36	0.60
6:N:73:DA:H2	7:T:-72:DA:C2	2.12	0.60
4:G:429:SER:O	4:G:430:HIS:ND1	2.35	0.60
1:A:1003:SER:OG	1:A:1006:ASP:OD2	2.19	0.60
3:D:386:LEU:HD12	3:D:386:LEU:H	1.67	0.60
6:N:4:DG:N2	7:T:-3:DG:C2	2.70	0.60
7:T:-74:DA:H2"	7:T:-73:DT:H71	1.84	0.60
7:T:25:DG:C2	7:T:26:DG:C2	2.89	0.60
1:A:672:ALA:O	1:A:676:ILE:HD12	2.01	0.60
4:F:278:CYS:CA	4:F:279:PRO:HG3	2.32	0.60
4:G:474:VAL:O	4:G:474:VAL:CG1	2.50	0.60
7:T:25:DG:C2	7:T:26:DG:N1	2.70	0.59
3:D:303:ARG:NH1	4:G:287:LEU:O	2.34	0.59
7:T:11:DG:H2"	7:T:12:DT:H71	1.83	0.59
2:B:50:SER:O	2:B:54:ASN:ND2	2.34	0.59
3:D:304:LEU:HD23	3:D:394:TYR:CD1	2.37	0.59
2:B:134:LEU:HD23	2:B:304:PRO:CB	2.33	0.59
3:E:304:LEU:HD12	3:E:305:GLN:N	2.18	0.59
6:N:-84:DG:C2'	6:N:-83:DT:H71	2.33	0.59
4:G:555:ILE:HD12	4:G:556:TYR:N	2.18	0.58
1:A:1024:ILE:O	1:A:1024:ILE:HG22	2.03	0.58
4:G:512:ILE:HG22	4:G:513:GLY:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:181:ILE:O	4:G:182:ARG:CG	2.52	0.58
6:N:-26:DC:H2"	6:N:-25:DC:C6	2.39	0.58
3:E:293:LEU:HD11	3:E:326:TYR:CD2	2.39	0.58
4:F:278:CYS:HA	4:F:279:PRO:HG3	1.86	0.58
6:N:56:DG:N2	7:T:-55:DG:N2	2.51	0.58
6:N:-79:DG:C2	7:T:80:DA:C2	2.91	0.57
3:E:304:LEU:HD12	3:E:305:GLN:H	1.69	0.57
4:G:476:LYS:HD2	4:G:478:ILE:HG23	1.86	0.57
1:A:1020:LEU:CD1	1:A:1270:VAL:HG22	2.34	0.57
2:B:84:ASP:OD1	2:B:88:ARG:NH1	2.37	0.57
1:A:709:TYR:OH	4:G:468:LEU:O	2.03	0.57
6:N:38:DG:N1	7:T:-37:DG:C2	2.72	0.57
1:A:841:MET:O	1:A:846:LYS:NZ	2.37	0.56
4:G:452:VAL:O	4:G:452:VAL:HG13	2.05	0.56
3:D:96:ARG:O	3:D:96:ARG:HG2	2.04	0.56
6:N:-25:DC:C2'	6:N:-24:DT:C7	2.66	0.56
3:E:335:ILE:HD11	3:E:362:PHE:CE2	2.40	0.56
7:T:55:DA:H2"	7:T:56:DC:C5	2.41	0.56
2:B:320:ARG:NH1	2:B:354:SER:O	2.39	0.56
1:A:871:TYR:OH	4:G:98:GLU:OE1	2.23	0.56
6:N:-62:DT:C6	6:N:-61:DT:H72	2.41	0.56
6:N:-61:DT:C2'	6:N:-60:DT:H71	2.36	0.55
6:N:70:DG:H1	7:T:-70:DC:H42	1.55	0.55
1:A:1140:ALA:HB1	1:A:1144:ILE:HB	1.86	0.55
2:B:236:VAL:HG22	2:B:376:ILE:CD1	2.36	0.55
4:G:106:SER:O	4:G:108:VAL:HG23	2.06	0.55
1:A:689:LEU:HD13	1:A:689:LEU:O	2.06	0.55
1:A:1144:ILE:HG12	1:A:1256:LEU:HD11	1.89	0.55
1:A:1303:ILE:HG12	1:A:1314:ILE:HD12	1.88	0.55
4:G:275:CYS:CB	4:G:278:CYS:SG	2.95	0.55
6:N:53:DC:C2'	6:N:54:DT:H71	2.37	0.55
1:A:1284:ILE:O	1:A:1288:LEU:HD13	2.06	0.55
3:E:353:GLN:N	3:E:353:GLN:OE1	2.40	0.55
2:B:55:TYR:CD1	2:B:334:LEU:HD22	2.41	0.55
3:D:304:LEU:HD23	3:D:394:TYR:CE1	2.41	0.55
3:E:355:LEU:O	3:E:359:THR:OG1	2.23	0.55
4:G:500:LYS:O	4:G:502:ASN:N	2.40	0.55
6:N:-55:DT:H2"	6:N:-54:DC:C5	2.42	0.55
3:D:305:GLN:N	3:D:394:TYR:OH	2.39	0.54
3:D:79:ILE:CD1	3:D:92:VAL:HG21	2.38	0.54
7:T:-40:DG:C2	7:T:-39:DT:N3	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:35:DC:H2"	7:T:36:DC:C5	2.42	0.54
1:A:945:THR:HG22	1:A:949:ILE:CD1	2.37	0.54
6:N:59:DA:H2	7:T:-58:DG:N2	1.92	0.54
7:T:-69:DA:H2"	7:T:-68:DG:C8	2.42	0.54
1:A:872:ASP:O	1:A:875:ARG:N	2.40	0.54
2:B:191:ASP:N	2:B:191:ASP:OD1	2.41	0.54
1:A:796:ILE:HD13	4:G:395:ILE:HD13	1.89	0.54
2:B:134:LEU:HD23	2:B:304:PRO:HB3	1.90	0.54
1:A:1156:GLU:N	1:A:1156:GLU:OE2	2.41	0.54
2:B:2:VAL:HG22	2:B:370:ASP:OD1	2.08	0.54
4:F:350:GLN:O	4:F:352:GLN:NE2	2.39	0.54
6:N:12:DG:C2	7:T:-11:DG:C2	2.96	0.54
7:T:25:DG:H21	7:T:26:DG:N2	1.93	0.54
4:G:475:TYR:CE1	4:G:491:VAL:HG22	2.42	0.53
3:E:83:GLY:N	7:T:12:DT:OP1	2.33	0.53
4:G:122:LYS:C	4:G:122:LYS:HD2	2.28	0.53
6:N:-75:DG:C2	7:T:76:DG:C2	2.96	0.53
6:N:-61:DT:H2'	6:N:-60:DT:H71	1.90	0.53
1:A:720:PHE:O	1:A:724:VAL:HG22	2.07	0.53
1:A:1003:SER:N	1:A:1006:ASP:OD2	2.39	0.53
3:E:248:LEU:HB3	3:E:249:PRO:HD2	1.90	0.53
1:A:1254:HIS:O	1:A:1258:THR:HG22	2.08	0.53
6:N:-62:DT:H2'	6:N:-61:DT:H72	1.90	0.52
6:N:70:DG:H22	7:T:-70:DC:H42	1.58	0.52
2:B:29:VAL:HB	2:B:122:ILE:HG21	1.91	0.52
6:N:-6:DG:C2	6:N:-5:DG:C2	2.97	0.52
4:F:326:PHE:HB3	4:F:341:PHE:CZ	2.45	0.52
1:A:1259:ASP:O	1:A:1260:ALA:HB2	2.09	0.52
3:D:254:VAL:HG21	3:D:289:PHE:CE2	2.44	0.52
6:N:73:DA:C4	6:N:74:DT:C4	2.98	0.52
2:B:325:GLU:OE2	2:B:325:GLU:HA	2.10	0.52
3:E:273:GLY:C	4:G:512:ILE:HD11	2.30	0.52
6:N:-56:DG:H2"	6:N:-55:DT:C7	2.40	0.52
3:D:226:ILE:HD12	3:D:227:LYS:N	2.25	0.52
3:D:383:ASP:OD1	3:D:383:ASP:N	2.42	0.52
3:E:240:THR:O	3:E:243:LYS:NZ	2.27	0.52
1:A:756:LYS:HE2	3:D:389:ASN:HB3	1.92	0.51
1:A:954:SER:CB	4:G:425:LEU:HD21	2.40	0.51
1:A:1291:ARG:NH2	1:A:1298:GLU:O	2.39	0.51
1:A:889:VAL:HB	4:G:96:LEU:HD13	1.91	0.51
1:A:1259:ASP:O	1:A:1260:ALA:CB	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:ARG:NH1	4:G:179:SER:OG	2.44	0.51
3:E:232:LEU:HD12	3:E:233:VAL:N	2.25	0.51
6:N:-68:DT:H2"	6:N:-67:DT:H71	1.91	0.51
6:N:-43:DA:H61	7:T:43:DT:H3	1.59	0.51
2:B:327:GLY:O	2:B:332:VAL:O	2.29	0.51
4:F:278:CYS:HA	4:F:279:PRO:CG	2.40	0.51
6:N:-88:DC:H2'	6:N:-87:DT:H71	1.93	0.51
7:T:-84:DA:H2'	7:T:-83:DT:H71	1.93	0.51
7:T:69:DC:H2"	7:T:70:DG:C8	2.46	0.51
3:E:228:LEU:HD13	3:E:366:LEU:HD11	1.92	0.51
4:F:278:CYS:CA	4:F:279:PRO:CG	2.88	0.51
3:D:109:LYS:O	3:D:113:ASN:OD1	2.28	0.51
4:G:550:ASP:O	4:G:553:ASP:OD1	2.29	0.51
4:G:557:LYS:O	4:G:561:VAL:HG23	2.10	0.51
6:N:83:DA:H2'	6:N:84:DT:H71	1.92	0.51
6:N:-62:DT:H2"	6:N:-61:DT:C7	2.41	0.51
3:D:77:PHE:N	3:D:92:VAL:O	2.41	0.50
3:E:274:SER:N	4:G:512:ILE:HD11	2.26	0.50
1:A:863:TYR:OH	1:A:884:HIS:NE2	2.23	0.50
3:E:261:TYR:O	3:E:265:VAL:HG23	2.11	0.50
4:F:265:ALA:O	4:F:350:GLN:N	2.44	0.50
4:F:316:MET:N	4:F:316:MET:SD	2.85	0.50
4:G:379:ILE:O	4:G:379:ILE:HD12	2.12	0.50
3:D:92:VAL:HG11	3:D:97:ILE:HB	1.94	0.50
3:E:302:GLU:OE2	3:E:305:GLN:NE2	2.44	0.50
4:G:183:SER:O	4:G:185:ILE:HG23	2.11	0.50
1:A:796:ILE:C	1:A:796:ILE:HD12	2.32	0.50
3:D:228:LEU:HD13	3:D:332:LEU:HD11	1.94	0.50
3:E:346:THR:HG23	4:F:338:LYS:HZ2	1.77	0.50
4:F:323:GLU:HA	4:F:341:PHE:CE2	2.47	0.50
6:N:-64:DT:H2'	6:N:-63:DT:H71	1.93	0.50
6:N:-59:DT:H3	7:T:59:DA:H61	1.59	0.50
1:A:879:ILE:HD11	4:G:84:LEU:HD13	1.93	0.50
1:A:1148:PHE:O	1:A:1152:THR:HG23	2.12	0.50
4:G:509:LEU:HD22	4:G:509:LEU:H	1.77	0.50
6:N:12:DG:N2	7:T:-11:DG:C4	2.80	0.50
2:B:44:ARG:NH2	2:B:310:GLY:O	2.42	0.49
3:E:223:GLN:HA	3:E:223:GLN:OE1	2.12	0.49
1:A:818:ASP:OD2	2:B:346:TYR:OH	2.29	0.49
1:A:834:ILE:O	1:A:838:ILE:HG12	2.12	0.49
3:D:90:GLU:OE2	3:D:96:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:38:DG:N3	7:T:-37:DG:N2	2.50	0.49
6:N:62:DG:C6	6:N:63:DG:C6	2.99	0.49
2:B:148:GLY:HA2	2:B:166:ILE:HD11	1.93	0.49
4:G:102:ILE:HD12	4:G:103:SER:N	2.28	0.49
6:N:-64:DT:C2'	6:N:-63:DT:H71	2.41	0.49
1:A:863:TYR:HH	1:A:884:HIS:CE1	2.23	0.49
2:B:175:ARG:O	2:B:176:TYR:CD2	2.66	0.49
4:G:392:GLY:H	4:G:396:THR:HG21	1.77	0.49
6:N:73:DA:N9	6:N:74:DT:H72	2.27	0.49
3:D:265:VAL:HG12	3:D:278:LEU:HD12	1.95	0.49
3:E:17:PHE:N	3:E:96:ARG:O	2.37	0.49
1:A:889:VAL:O	1:A:890:THR:HB	2.13	0.49
2:B:17:ASP:OD1	2:B:19:ARG:NE	2.46	0.48
4:G:440:CYS:SG	4:G:443:CYS:N	2.86	0.48
6:N:-58:DC:H2"	6:N:-57:DT:H72	1.95	0.48
1:A:670:GLU:OE1	1:A:670:GLU:N	2.30	0.48
2:B:2:VAL:HG23	2:B:373:MET:HE2	1.96	0.48
2:B:109:ASP:OD1	2:B:110:CYS:N	2.46	0.48
3:D:289:PHE:HE1	3:D:293:LEU:HD13	1.78	0.48
3:E:248:LEU:HB3	3:E:249:PRO:CD	2.44	0.48
3:E:254:VAL:HG21	3:E:289:PHE:CE2	2.48	0.48
4:G:181:ILE:O	4:G:182:ARG:HG2	2.12	0.48
1:A:822:GLU:OE1	2:B:46:ARG:CZ	2.61	0.48
4:G:542:ILE:HG23	4:G:547:ILE:HD11	1.95	0.48
1:A:1181:ALA:HA	1:A:1186:LEU:HB2	1.94	0.48
1:A:1204:TYR:O	1:A:1204:TYR:CD1	2.67	0.48
1:A:1258:THR:O	1:A:1258:THR:CG2	2.60	0.48
4:F:339:LEU:O	4:F:343:ILE:HG12	2.13	0.48
4:G:278:CYS:HB3	4:G:306:CYS:SG	2.53	0.48
6:N:83:DA:C2'	6:N:84:DT:H71	2.44	0.48
1:A:796:ILE:HG22	4:G:386:LEU:HD11	1.95	0.48
2:B:321:THR:O	2:B:325:GLU:N	2.47	0.48
3:D:236:TRP:CE3	4:G:372:TYR:CG	3.02	0.48
4:F:339:LEU:HD12	4:F:339:LEU:H	1.79	0.48
6:N:56:DG:N2	7:T:-55:DG:C2	2.82	0.48
1:A:706:VAL:O	1:A:710:LEU:N	2.44	0.47
2:B:220:GLU:OE2	2:B:222:ARG:NH1	2.47	0.47
6:N:73:DA:H2"	6:N:74:DT:H73	1.96	0.47
1:A:1283:GLN:O	1:A:1287:ARG:HG3	2.14	0.47
3:D:266:SER:HA	3:D:269:LEU:HD12	1.96	0.47
4:F:279:PRO:N	4:F:279:PRO:HG3	2.07	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:ILE:CG1	1:A:1316:TYR:HB2	2.45	0.47
1:A:1267:ALA:O	1:A:1271:LYS:HG2	2.14	0.47
2:B:123:SER:OG	2:B:165:ASP:OD2	2.32	0.47
3:D:92:VAL:HG22	3:D:96:ARG:NE	2.28	0.47
6:N:8:DG:C2'	6:N:9:DT:H71	2.44	0.47
6:N:-88:DC:C2'	6:N:-87:DT:H71	2.45	0.47
3:D:252:VAL:HG11	3:D:373:TYR:CE2	2.50	0.47
3:E:352:CYS:O	3:E:355:LEU:HD23	2.14	0.47
4:G:122:LYS:HD2	4:G:122:LYS:O	2.15	0.47
1:A:689:LEU:HD13	1:A:689:LEU:C	2.35	0.47
2:B:210:LYS:O	2:B:211:TYR:HB3	2.13	0.47
6:N:-62:DT:C2'	6:N:-61:DT:C7	2.92	0.47
6:N:4:DG:H2"	6:N:5:DT:C6	2.50	0.47
7:T:-74:DA:C2'	7:T:-73:DT:H71	2.43	0.47
4:G:440:CYS:HB2	4:G:466:CYS:SG	2.53	0.47
1:A:1181:ALA:O	1:A:1185:ASP:N	2.48	0.47
1:A:1241:THR:O	1:A:1241:THR:OG1	2.32	0.47
4:G:512:ILE:HG22	4:G:513:GLY:N	2.29	0.47
4:G:402:ASN:N	4:G:403:PRO:HD3	2.30	0.47
6:N:8:DG:H2'	6:N:9:DT:H71	1.97	0.47
6:N:73:DA:C6	7:T:-72:DA:N1	2.82	0.47
1:A:796:ILE:HD12	1:A:796:ILE:O	2.15	0.47
1:A:945:THR:HG23	1:A:1146:ILE:HG13	1.97	0.47
1:A:1242:ILE:O	1:A:1246:THR:HG22	2.14	0.46
3:D:345:THR:HG22	4:G:342:ASN:HD22	1.80	0.46
2:B:363:VAL:HG22	2:B:363:VAL:O	2.13	0.46
3:D:38:TYR:HE2	3:D:61:LEU:HD12	1.81	0.46
3:E:36:LYS:HG3	3:E:36:LYS:O	2.15	0.46
4:F:326:PHE:O	4:F:326:PHE:CD1	2.68	0.46
2:B:330:ASN:N	2:B:330:ASN:OD1	2.48	0.46
4:F:326:PHE:CD2	4:F:341:PHE:CZ	3.03	0.46
4:G:84:LEU:CD2	4:G:96:LEU:HD11	2.45	0.46
6:N:-81:DG:H2'	6:N:-80:DT:H71	1.97	0.46
6:N:-65:DT:C6	6:N:-64:DT:H72	2.51	0.46
2:B:324:PHE:O	2:B:328:LEU:HB2	2.15	0.46
4:G:354:PRO:HG2	4:G:357:ILE:HD11	1.97	0.46
4:G:557:LYS:N	4:G:557:LYS:CD	2.79	0.46
1:A:1029:ILE:HD12	1:A:1029:ILE:H	1.81	0.46
6:N:12:DG:N2	7:T:-11:DG:C2	2.84	0.46
1:A:897:ARG:NH2	4:G:98:GLU:OE2	2.49	0.46
1:A:701:ASP:N	1:A:701:ASP:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:321:VAL:HG21	3:D:324:ARG:NH1	2.30	0.46
4:G:506:TYR:CZ	4:G:514:TYR:OH	2.68	0.46
1:A:867:ILE:HG21	1:A:879:ILE:CG2	2.46	0.45
1:A:969:PRO:O	1:A:970:LYS:HB3	2.17	0.45
2:B:187:VAL:HG12	2:B:274:ASP:HB3	1.98	0.45
4:G:474:VAL:O	4:G:475:TYR:C	2.55	0.45
2:B:174:LEU:HD22	2:B:202:ARG:CZ	2.46	0.45
7:T:-40:DG:C2	7:T:-39:DT:C2	3.04	0.45
4:F:338:LYS:O	4:F:341:PHE:HB2	2.16	0.45
4:G:305:GLU:OE2	4:G:347:ASN:N	2.48	0.45
4:G:395:ILE:H	4:G:395:ILE:HG13	1.60	0.45
6:N:43:DA:N6	7:T:-44:DA:N6	2.64	0.45
6:N:76:DG:C4	6:N:77:DC:C5	3.05	0.45
6:N:-25:DC:H2"	6:N:-24:DT:C5	2.46	0.45
4:G:507:GLU:OE1	4:G:507:GLU:HA	2.17	0.45
1:A:697:LEU:HD22	1:A:701:ASP:HB2	1.98	0.45
1:A:968:THR:HB	1:A:969:PRO:HD3	1.99	0.45
1:A:1184:LEU:HB2	1:A:1186:LEU:HD13	1.99	0.45
3:D:335:ILE:HG21	3:D:363:LEU:HD21	1.99	0.45
6:N:56:DG:C2	7:T:-55:DG:N2	2.85	0.45
2:B:92:ASP:OD1	2:B:92:ASP:N	2.49	0.45
3:E:272:PRO:HG2	4:G:552:PHE:CE1	2.52	0.45
7:T:70:DG:H2"	7:T:71:DA:N7	2.31	0.45
3:E:368:MET:N	3:E:368:MET:HE2	2.31	0.44
6:N:4:DG:C2	7:T:-3:DG:N2	2.85	0.44
1:A:974:GLN:O	1:A:975:LEU:HD23	2.18	0.44
4:G:440:CYS:CB	4:G:466:CYS:SG	3.05	0.44
3:E:127:LYS:O	3:E:131:LEU:HD23	2.17	0.44
4:G:359:GLU:C	4:G:359:GLU:OE2	2.56	0.44
7:T:37:DC:H2"	7:T:38:DT:C6	2.52	0.44
1:A:665:GLU:HG2	4:G:552:PHE:HD2	1.83	0.44
1:A:1295:SER:N	1:A:1298:GLU:OE2	2.42	0.44
2:B:109:ASP:OD1	2:B:109:ASP:C	2.55	0.44
3:D:337:VAL:HG22	3:D:337:VAL:O	2.18	0.44
4:G:176:THR:HG23	4:G:176:THR:O	2.16	0.44
4:G:542:ILE:HD11	4:G:546:SER:HB2	1.99	0.44
1:A:922:LYS:NZ	4:G:126:GLU:O	2.51	0.44
7:T:20:DG:H2"	7:T:21:DC:O5'	2.18	0.44
3:D:22:MET:SD	3:D:98:ARG:NH1	2.90	0.44
1:A:970:LYS:H	1:A:971:PRO:HD2	1.82	0.44
2:B:274:ASP:HA	2:B:279:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:233:VAL:HA	3:D:236:TRP:HD1	1.82	0.44
7:T:-68:DG:H4'	7:T:-67:DA:OP1	2.18	0.44
1:A:773:MET:SD	1:A:773:MET:C	2.97	0.43
1:A:879:ILE:O	1:A:882:ALA:N	2.50	0.43
3:D:368:MET:O	3:D:368:MET:CE	2.66	0.43
4:G:443:CYS:O	4:G:445:THR:N	2.46	0.43
6:N:72:DT:H2"	6:N:73:DA:OP2	2.18	0.43
2:B:220:GLU:OE1	2:B:222:ARG:N	2.36	0.43
2:B:252:GLU:HB2	2:B:253:PRO:HD3	2.00	0.43
3:E:248:LEU:O	3:E:249:PRO:C	2.56	0.43
4:G:475:TYR:HE1	4:G:491:VAL:HG22	1.84	0.43
7:T:45:DC:H2"	7:T:46:DT:C5	2.52	0.43
2:B:213:GLU:OE2	2:B:213:GLU:HA	2.18	0.43
2:B:246:THR:HG21	2:B:362:ASN:HD21	1.82	0.43
4:G:408:ASP:O	4:G:412:GLY:N	2.51	0.43
6:N:26:DA:C2	7:T:-25:DA:C2	3.06	0.43
1:A:900:GLN:O	1:A:903:GLU:HG3	2.18	0.43
7:T:-43:DT:C2	7:T:-42:DT:C5	3.05	0.43
3:E:97:ILE:O	3:E:98:ARG:NH1	2.35	0.43
4:G:316:MET:HE3	4:G:320:LYS:HE3	2.01	0.43
4:G:542:ILE:HD11	4:G:546:SER:CB	2.49	0.43
6:N:46:DG:N2	7:T:-45:DA:C2	2.87	0.43
7:T:-72:DA:H2"	7:T:-71:DT:C6	2.54	0.43
7:T:-44:DA:C4	7:T:-43:DT:C5	3.07	0.43
1:A:1178:VAL:HG23	1:A:1179:THR:H	1.83	0.43
1:A:1315:GLN:O	1:A:1316:TYR:C	2.57	0.43
2:B:166:ILE:HG21	2:B:182:TYR:CE1	2.54	0.43
2:B:174:LEU:O	2:B:202:ARG:NH2	2.50	0.43
3:E:289:PHE:HE1	3:E:293:LEU:HD13	1.81	0.43
4:G:124:LYS:O	4:G:128:LEU:HG	2.19	0.43
3:D:77:PHE:HE2	3:D:97:ILE:HG21	1.84	0.42
4:G:393:GLN:N	4:G:396:THR:HB	2.34	0.42
1:A:811:GLU:OE2	2:B:315:MET:O	2.37	0.42
1:A:867:ILE:HG21	1:A:879:ILE:HG21	2.00	0.42
4:G:393:GLN:O	4:G:394:SER:HB3	2.19	0.42
4:G:440:CYS:SG	4:G:442:TYR:N	2.92	0.42
7:T:-7:DG:H2"	7:T:-6:DT:H71	2.00	0.42
1:A:693:SER:HA	4:G:554:LYS:HG2	2.01	0.42
3:D:92:VAL:HG13	3:D:96:ARG:CD	2.49	0.42
3:D:340:GLU:OE2	3:D:340:GLU:O	2.37	0.42
3:D:347:MET:HE1	3:D:352:CYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:401:TYR:C	4:G:403:PRO:HD3	2.39	0.42
4:G:520:ILE:CG2	4:G:542:ILE:HG22	2.46	0.42
6:N:74:DT:C4	6:N:75:DC:N4	2.88	0.42
7:T:-84:DA:C2'	7:T:-83:DT:H71	2.48	0.42
3:E:358:GLN:OE1	3:E:358:GLN:HA	2.19	0.42
6:N:14:DT:O2	7:T:-13:DA:C2	2.73	0.42
1:A:984:ILE:HG23	1:A:1204:TYR:OH	2.19	0.42
1:A:990:CYS:SG	1:A:1036:HIS:NE2	2.93	0.42
2:B:45:ILE:HG23	2:B:145:TYR:O	2.19	0.42
3:D:236:TRP:CZ3	4:G:372:TYR:CD1	3.07	0.42
2:B:134:LEU:HD21	2:B:305:MET:N	2.34	0.42
2:B:315:MET:O	2:B:316:ARG:HB2	2.20	0.42
2:B:332:VAL:O	2:B:332:VAL:CG1	2.67	0.42
4:G:121:GLU:OE1	4:G:121:GLU:N	2.48	0.42
4:G:393:GLN:O	4:G:394:SER:CB	2.68	0.42
7:T:11:DG:C2'	7:T:12:DT:H71	2.48	0.42
1:A:794:GLY:HA2	4:G:460:LEU:HD23	2.02	0.42
1:A:914:LYS:O	1:A:918:GLU:HG2	2.20	0.42
1:A:960:THR:O	1:A:963:LYS:HB3	2.20	0.42
1:A:1191:LEU:HD21	1:A:1227:SER:HA	2.02	0.42
2:B:180:VAL:HG12	2:B:181:LEU:N	2.34	0.42
3:D:17:PHE:CD1	3:D:22:MET:HE1	2.55	0.42
3:D:235:ASP:OD2	3:D:333:ARG:NE	2.53	0.42
3:E:288:TYR:O	3:E:292:CYS:SG	2.76	0.42
3:E:346:THR:HG23	4:F:338:LYS:HZ3	1.82	0.42
3:E:346:THR:H	4:F:338:LYS:HD3	1.85	0.42
4:F:336:PHE:O	4:F:340:LEU:HG	2.20	0.42
1:A:668:PHE:CD2	1:A:719:TRP:CZ3	3.08	0.41
1:A:765:MET:CG	1:A:765:MET:O	2.68	0.41
1:A:874:GLU:HG2	1:A:875:ARG:H	1.85	0.41
1:A:1146:ILE:N	1:A:1146:ILE:HD13	2.35	0.41
4:G:316:MET:O	4:G:316:MET:SD	2.78	0.41
4:G:458:LYS:HG3	4:G:464:TRP:HB2	2.01	0.41
6:N:85:DC:H2'	6:N:86:DT:H71	2.02	0.41
1:A:865:LYS:NZ	2:B:31:ASN:O	2.46	0.41
1:A:945:THR:HG22	1:A:949:ILE:HD11	2.01	0.41
1:A:993:ASP:OD1	1:A:993:ASP:C	2.59	0.41
2:B:204:MET:SD	2:B:258:ILE:HG23	2.61	0.41
2:B:261:TRP:CD1	2:B:384:LYS:HG3	2.55	0.41
4:G:332:ASN:N	4:G:332:ASN:OD1	2.53	0.41
1:A:675:TYR:OH	1:A:712:SER:OG	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:12:GLY:O	3:D:27:ILE:HD12	2.20	0.41
3:D:240:THR:HG21	4:G:370:GLY:O	2.20	0.41
3:E:275:GLN:HA	3:E:275:GLN:OE1	2.21	0.41
4:G:108:VAL:HG22	4:G:114:PRO:HD3	2.02	0.41
1:A:764:PHE:C	1:A:766:PRO:HD3	2.40	0.41
1:A:1207:VAL:HG12	1:A:1228:LEU:HD11	2.01	0.41
2:B:298:VAL:HG12	2:B:305:MET:HE2	2.02	0.41
3:D:76:CYS:HA	3:D:92:VAL:O	2.20	0.41
4:G:275:CYS:HB2	4:G:278:CYS:SG	2.59	0.41
1:A:962:LYS:O	1:A:966:TRP:HB3	2.20	0.41
3:D:254:VAL:HG21	3:D:289:PHE:CZ	2.56	0.41
4:G:542:ILE:CD1	4:G:546:SER:OG	2.68	0.41
2:B:363:VAL:HG21	4:G:398:LEU:HD22	2.02	0.41
3:E:296:MET:SD	3:E:296:MET:N	2.94	0.41
3:E:364:VAL:O	3:E:368:MET:HE3	2.20	0.41
6:N:-72:DT:H2"	6:N:-71:DT:O5'	2.21	0.41
4:G:495:GLN:H	4:G:519:ASN:HD21	1.69	0.41
6:N:76:DG:C5	6:N:77:DC:C4	3.08	0.41
1:A:676:ILE:O	1:A:676:ILE:HG22	2.21	0.41
1:A:770:ARG:HB3	1:A:775:TRP:CE3	2.55	0.41
1:A:1020:LEU:HD11	1:A:1270:VAL:HG22	2.03	0.41
2:B:42:PRO:O	2:B:45:ILE:HD12	2.21	0.41
2:B:236:VAL:HG22	2:B:376:ILE:HD11	2.02	0.41
2:B:270:GLN:NE2	2:B:310:GLY:HA3	2.36	0.41
4:G:389:THR:HB	4:G:393:GLN:HB2	2.03	0.41
4:G:500:LYS:O	4:G:503:GLN:N	2.52	0.41
4:G:557:LYS:N	4:G:557:LYS:HD3	2.36	0.41
6:N:-56:DG:H2"	6:N:-55:DT:C5	2.56	0.41
1:A:696:ILE:O	4:G:474:VAL:CG1	2.69	0.41
2:B:135:ASN:ND2	2:B:172:GLU:OE1	2.53	0.41
2:B:288:MET:HE1	2:B:353:LEU:O	2.21	0.41
2:B:343:TYR:O	2:B:347:TYR:HE2	2.03	0.41
2:B:350:ASP:O	2:B:352:LYS:N	2.53	0.41
4:F:326:PHE:CD1	4:F:326:PHE:C	2.94	0.41
4:G:366:THR:HG22	4:G:367:GLY:N	2.36	0.41
6:N:73:DA:C1'	6:N:74:DT:H72	2.49	0.41
1:A:668:PHE:CD1	1:A:668:PHE:C	2.94	0.41
2:B:45:ILE:HG12	2:B:145:TYR:O	2.20	0.41
3:E:293:LEU:HD22	3:E:322:PRO:HB3	2.02	0.41
4:G:508:PRO:HA	4:G:514:TYR:OH	2.21	0.41
1:A:929:ASP:OD1	2:B:359:ASN:ND2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:299:TYR:OH	4:F:353:LEU:HD11	2.21	0.40
4:G:357:ILE:H	4:G:357:ILE:HG12	1.78	0.40
1:A:699:LEU:HD21	1:A:724:VAL:HB	2.03	0.40
2:B:288:MET:HG3	2:B:355:VAL:HG22	2.03	0.40
3:E:247:ARG:NH1	3:E:249:PRO:O	2.54	0.40
4:G:475:TYR:CD1	4:G:491:VAL:HG22	2.56	0.40
7:T:9:DG:C5	7:T:10:DC:C4	3.09	0.40
1:A:872:ASP:O	1:A:874:GLU:N	2.55	0.40
2:B:370:ASP:O	2:B:374:THR:OG1	2.25	0.40
4:F:312:ILE:HG22	4:F:315:SER:H	1.85	0.40
4:G:129:TRP:O	4:G:130:ASN:HB3	2.22	0.40
1:A:822:GLU:OE1	2:B:46:ARG:NE	2.54	0.40
2:B:210:LYS:HD2	2:B:283:CYS:SG	2.61	0.40
2:B:244:ASP:N	2:B:244:ASP:OD1	2.54	0.40
3:D:92:VAL:HG12	3:D:93:GLY:O	2.22	0.40
3:E:362:PHE:CD1	3:E:362:PHE:O	2.74	0.40
1:A:970:LYS:H	1:A:971:PRO:CD	2.35	0.40
1:A:1273:ARG:HD2	1:A:1273:ARG:HA	1.97	0.40
3:E:20:PRO:O	3:E:111:LEU:HD13	2.22	0.40
3:E:292:CYS:HB3	3:E:296:MET:SD	2.62	0.40
4:G:396:THR:C	4:G:398:LEU:H	2.25	0.40
7:T:-43:DT:C2'	7:T:-42:DT:C7	3.00	0.40
7:T:20:DG:H4'	7:T:21:DC:OP1	2.22	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	539/1536 (35%)	478 (89%)	57 (11%)	4 (1%)	22	53
2	B	383/433 (88%)	348 (91%)	32 (8%)	3 (1%)	19	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	D	283/401 (71%)	272 (96%)	10 (4%)	1 (0%)	34 66
3	E	247/401 (62%)	238 (96%)	9 (4%)	0	100 100
4	F	85/684 (12%)	83 (98%)	2 (2%)	0	100 100
4	G	357/684 (52%)	301 (84%)	52 (15%)	4 (1%)	14 41
5	H	1/5 (20%)	1 (100%)	0	0	100 100
8	a	98/136 (72%)	96 (98%)	1 (1%)	1 (1%)	15 44
8	e	98/136 (72%)	97 (99%)	1 (1%)	0	100 100
9	b	79/103 (77%)	79 (100%)	0	0	100 100
9	f	76/103 (74%)	75 (99%)	1 (1%)	0	100 100
10	c	101/130 (78%)	100 (99%)	1 (1%)	0	100 100
10	g	103/130 (79%)	100 (97%)	3 (3%)	0	100 100
11	d	93/123 (76%)	90 (97%)	3 (3%)	0	100 100
11	h	91/123 (74%)	90 (99%)	1 (1%)	0	100 100
12	x	1/7 (14%)	1 (100%)	0	0	100 100
All	All	2635/5135 (51%)	2449 (93%)	173 (7%)	13 (0%)	32 61

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	970	LYS
1	A	1260	ALA
2	B	316	ARG
4	G	102	ILE
4	G	394	SER
2	B	176	TYR
1	A	759	PRO
8	a	37	LYS
4	G	510	GLN
1	A	1139	PHE
2	B	211	TYR
4	G	511	LYS
3	D	271	SER

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	508/1391 (36%)	472 (93%)	36 (7%)	14 39
2	B	326/367 (89%)	312 (96%)	14 (4%)	29 62
3	D	263/359 (73%)	244 (93%)	19 (7%)	14 38
3	E	233/359 (65%)	214 (92%)	19 (8%)	11 33
4	F	85/653 (13%)	77 (91%)	8 (9%)	8 26
4	G	349/653 (53%)	318 (91%)	31 (9%)	9 28
5	H	1/1 (100%)	1 (100%)	0	100 100
8	a	87/110 (79%)	83 (95%)	4 (5%)	27 60
8	e	87/110 (79%)	87 (100%)	0	100 100
9	b	66/79 (84%)	64 (97%)	2 (3%)	41 75
9	f	63/79 (80%)	62 (98%)	1 (2%)	62 88
10	c	82/102 (80%)	80 (98%)	2 (2%)	49 81
10	g	83/102 (81%)	82 (99%)	1 (1%)	71 92
11	d	81/103 (79%)	77 (95%)	4 (5%)	25 57
11	h	79/103 (77%)	75 (95%)	4 (5%)	24 55
12	x	1/1 (100%)	1 (100%)	0	100 100
All	All	2394/4572 (52%)	2249 (94%)	145 (6%)	22 48

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	701	ASP
1	A	723	PHE
1	A	754	SER
1	A	774	CYS
1	A	775	TRP
1	A	776	GLU
1	A	793	SER
1	A	812	GLU
1	A	860	MET
1	A	871	TYR
1	A	873	LYS
1	A	886	HIS

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Mol	Chain	Res	Type
1	A	897	ARG
1	A	906	ARG
1	A	920	GLU
1	A	954	SER
1	A	962	LYS
1	A	967	LEU
1	A	968	THR
1	A	972	LYS
1	A	978	ASP
1	A	1006	ASP
1	A	1009	ARG
1	A	1036	HIS
1	A	1162	LYS
1	A	1165	ASN
1	A	1169	THR
1	A	1171	GLU
1	A	1178	VAL
1	A	1212	ARG
1	A	1250	VAL
1	A	1259	ASP
1	A	1291	ARG
1	A	1311	HIS
1	A	1315	GLN
1	A	1317	ILE
2	B	20	ARG
2	B	44	ARG
2	B	90	THR
2	B	101	SER
2	B	114	ASP
2	B	123	SER
2	B	133	ARG
2	B	134	LEU
2	B	139	CYS
2	B	150	HIS
2	B	172	GLU
2	B	306	MET
2	B	330	ASN
2	B	341	ASN
3	D	13	ARG
3	D	24	GLU
3	D	37	MET
3	D	38	TYR

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Mol	Chain	Res	Type
3	D	77	PHE
3	D	78	PHE
3	D	90	GLU
3	D	96	ARG
3	D	113	ASN
3	D	222	LEU
3	D	227	LYS
3	D	236	TRP
3	D	251	ASP
3	D	289	PHE
3	D	292	CYS
3	D	293	LEU
3	D	352	CYS
3	D	355	LEU
3	D	367	LEU
3	E	24	GLU
3	E	37	MET
3	E	77	PHE
3	E	80	HIS
3	E	107	MET
3	E	114	GLU
3	E	116	LYS
3	E	236	TRP
3	E	263	HIS
3	E	264	GLU
3	E	277	GLN
3	E	289	PHE
3	E	296	MET
3	E	304	LEU
3	E	322	PRO
3	E	324	ARG
3	E	353	GLN
3	E	355	LEU
3	E	362	PHE
4	F	262	PHE
4	F	285	LEU
4	F	308	PHE
4	F	326	PHE
4	F	336	PHE
4	F	339	LEU
4	F	356	TYR
4	F	358	LYS

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Mol	Chain	Res	Type
4	G	113	LEU
4	G	129	TRP
4	G	163	ASN
4	G	166	ASP
4	G	175	MET
4	G	180	ASN
4	G	182	ARG
4	G	187	TRP
4	G	271	SER
4	G	276	ASP
4	G	313	ASN
4	G	346	HIS
4	G	357	ILE
4	G	359	GLU
4	G	379	ILE
4	G	391	TYR
4	G	395	ILE
4	G	396	THR
4	G	406	HIS
4	G	417	CYS
4	G	425	LEU
4	G	430	HIS
4	G	440	CYS
4	G	476	LYS
4	G	502	ASN
4	G	506	TYR
4	G	509	LEU
4	G	511	LYS
4	G	514	TYR
4	G	517	ASN
4	G	554	LYS
8	a	76	GLN
8	a	83	ARG
8	a	115	LYS
8	a	120	MET
9	b	35	ARG
9	b	79	LYS
10	c	76	THR
10	c	101	THR
11	d	30	ARG
11	d	31	LYS
11	d	44	GLN

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Mol	Chain	Res	Type
11	d	84	SER
9	f	35	ARG
10	g	118	LYS
11	h	30	ARG
11	h	44	GLN
11	h	83	ARG
11	h	113	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	848	ASN
1	A	965	HIS
1	A	1150	HIS
1	A	1252	HIS
2	B	291	HIS
4	G	116	ASN
4	G	519	ASN
8	a	39	HIS
9	b	75	HIS
9	f	75	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	ML3	e	36	8	10,11,12	2.41	1 (10%)	10,14,16	1.08	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	ML3	a	36	8	10,11,12	2.41	1 (10%)	10,14,16	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ML3	e	36	8	-	3/8/10/12	-
8	ML3	a	36	8	-	2/8/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	36	ML3	CA-N	-7.04	1.26	1.48
8	e	36	ML3	CA-N	-7.01	1.27	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	e	36	ML3	CB-SG-CD	2.59	110.04	102.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	a	36	ML3	N-CA-CB-SG
8	a	36	ML3	C-CA-CB-SG
8	e	36	ML3	N-CA-CB-SG
8	e	36	ML3	C-CA-CB-SG
8	e	36	ML3	SG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

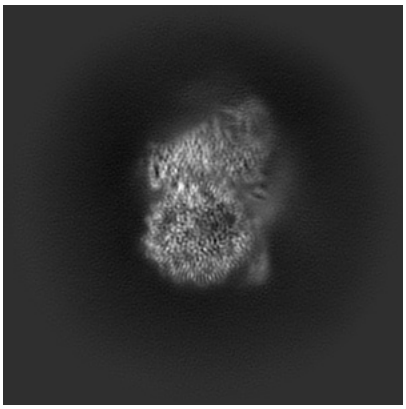
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41449. These allow visual inspection of the internal detail of the map and identification of artifacts.

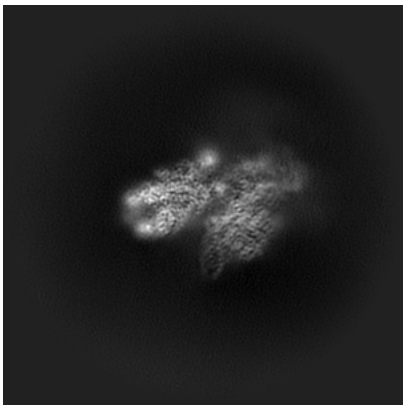
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

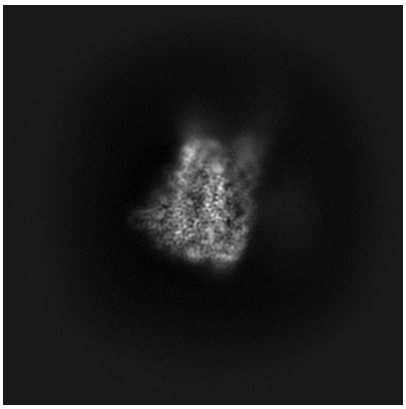
6.1.1 Primary map



X

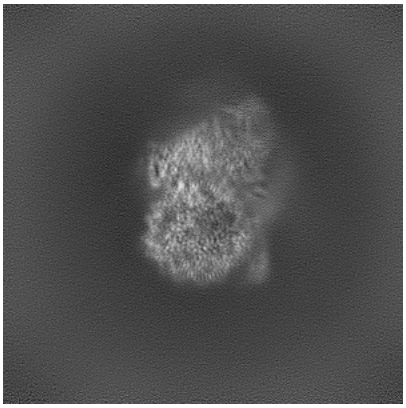


Y

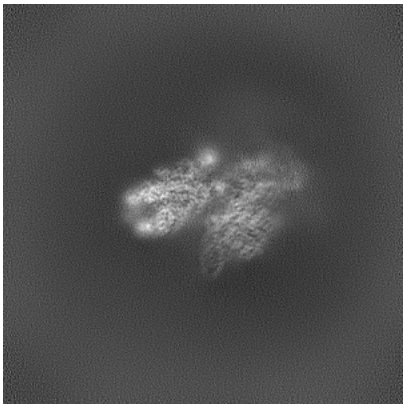


Z

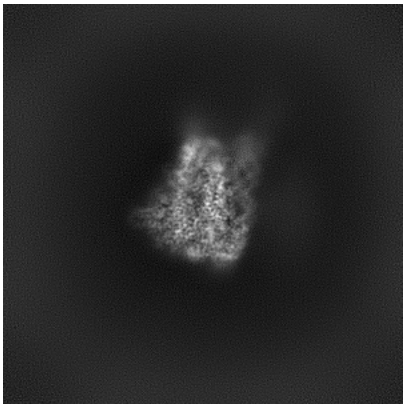
6.1.2 Raw map



X



Y

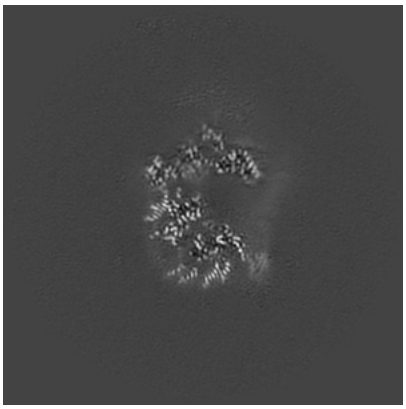


Z

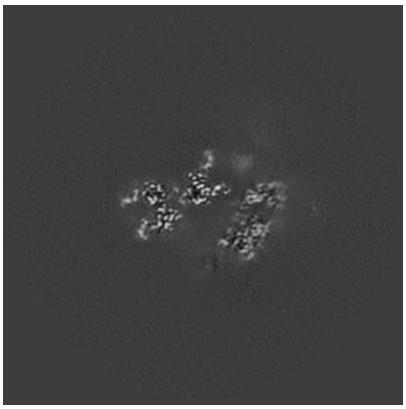
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

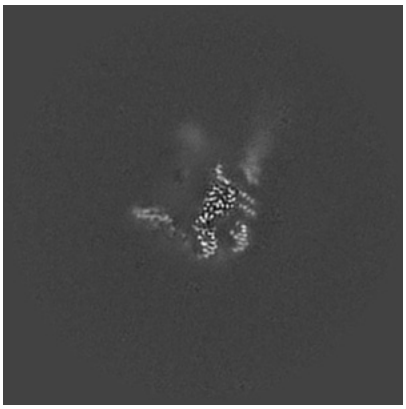
6.2.1 Primary map



X Index: 225

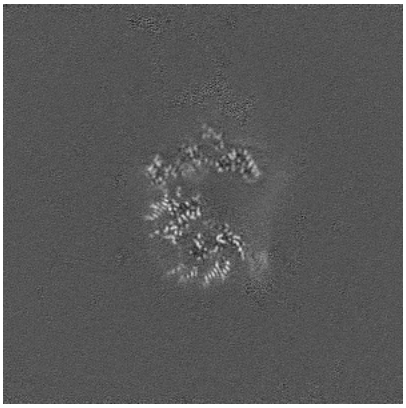


Y Index: 225

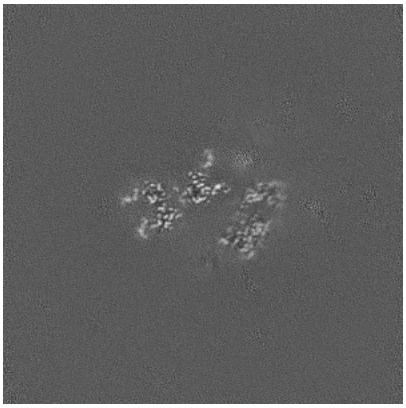


Z Index: 225

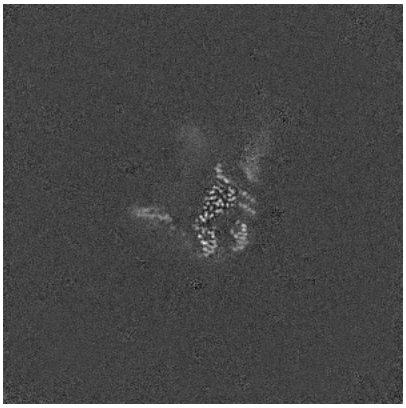
6.2.2 Raw map



X Index: 225



Y Index: 225

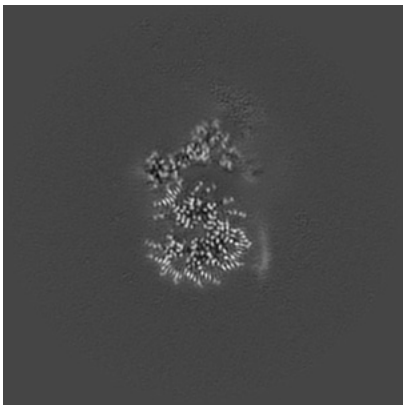


Z Index: 225

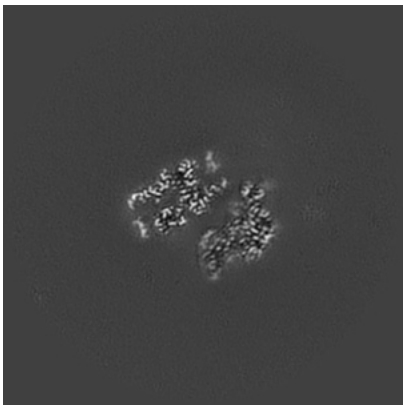
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

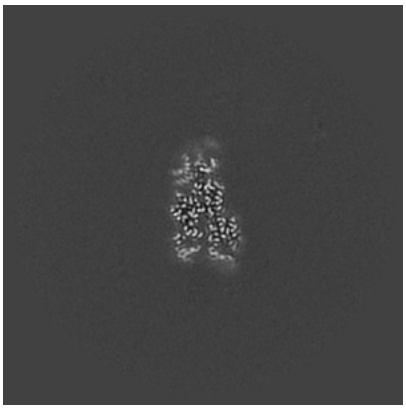
6.3.1 Primary map



X Index: 234

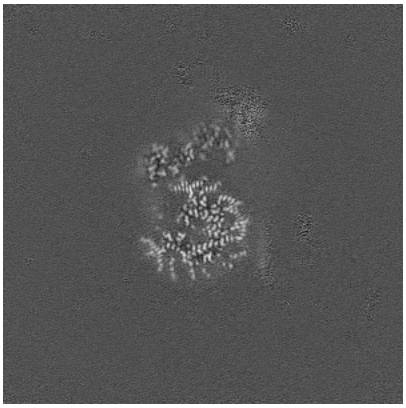


Y Index: 208

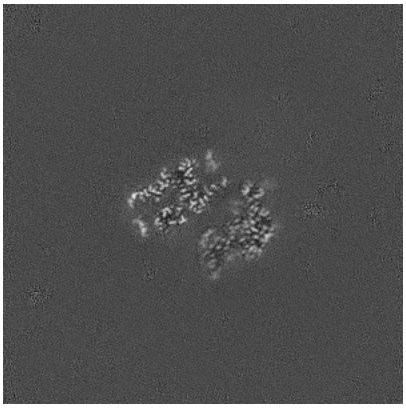


Z Index: 178

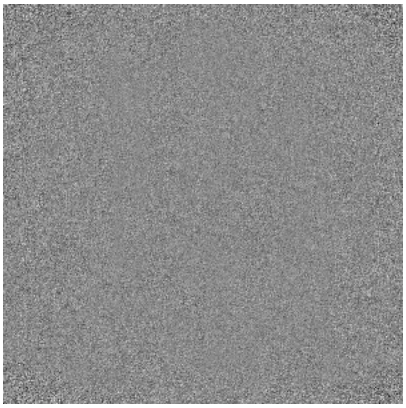
6.3.2 Raw map



X Index: 241



Y Index: 208

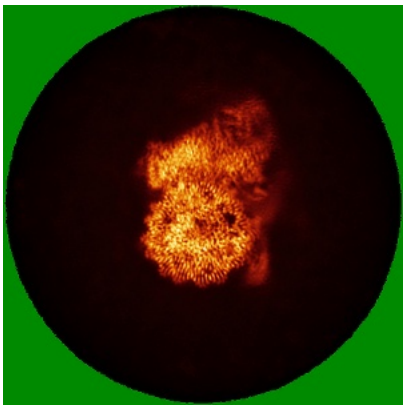


Z Index: 0

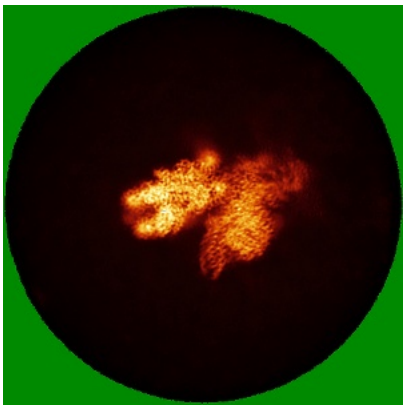
The images above show the largest variance slices of the map in three orthogonal directions.

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

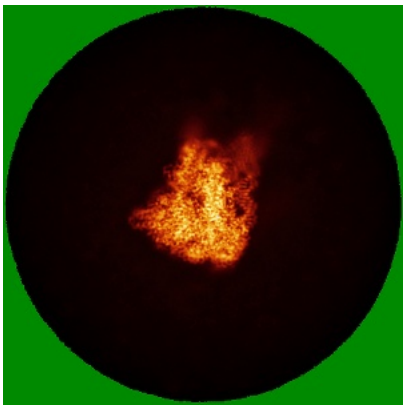
6.4.1 Primary map



X

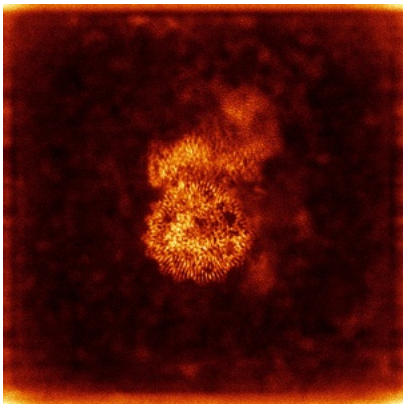


Y

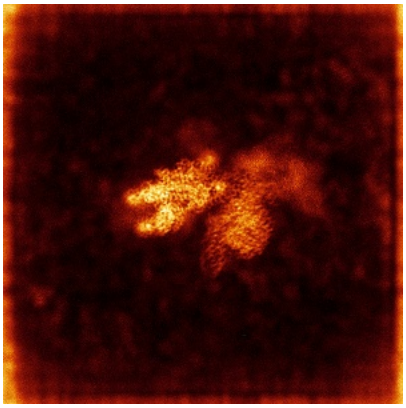


Z

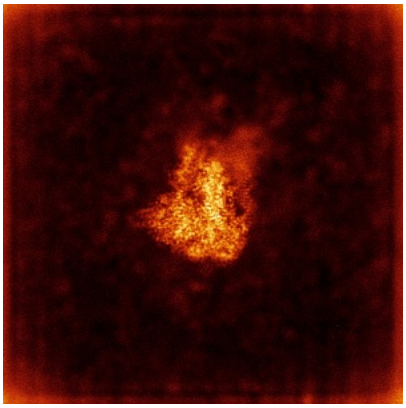
6.4.2 Raw map



X



Y

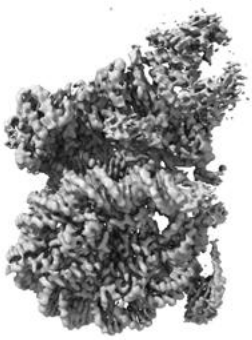


Z

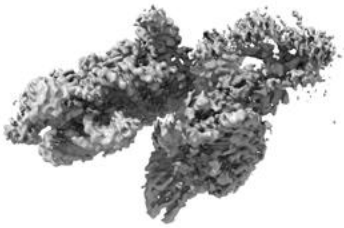
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

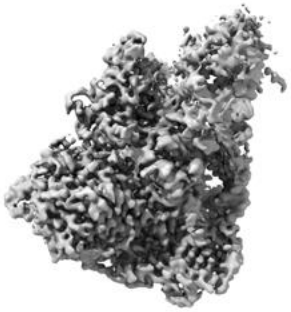
6.5.1 Primary map



X



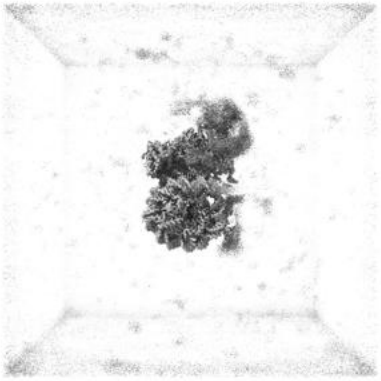
Y



Z

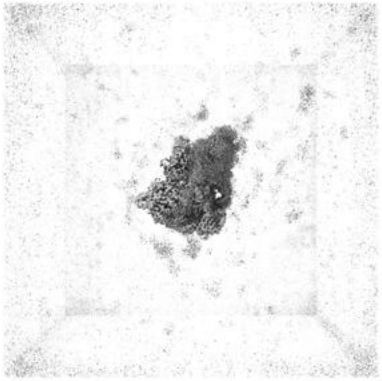
The images above show the 3D surface view of the map at the recommended contour level 0.07768. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X

Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

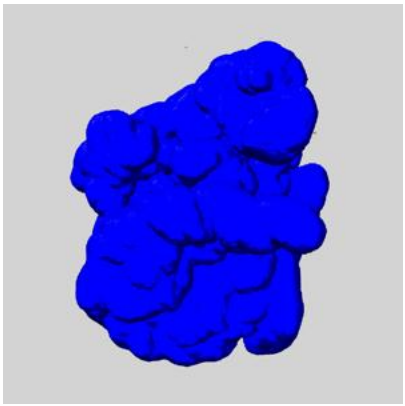
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

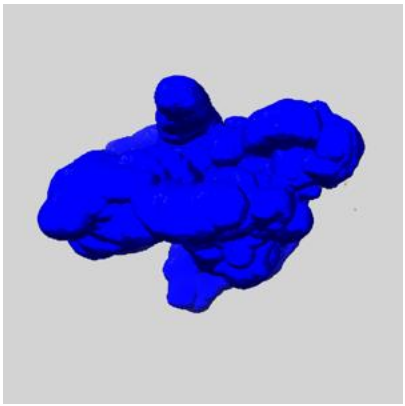
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

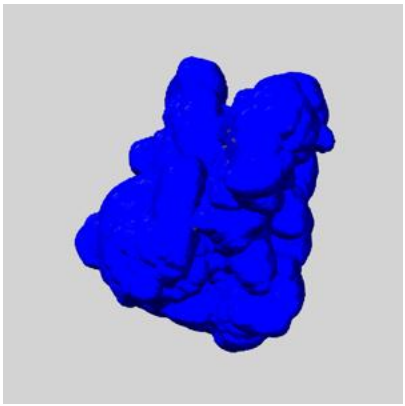
6.6.1 emd_41449_msk_1.map (i)



X



Y

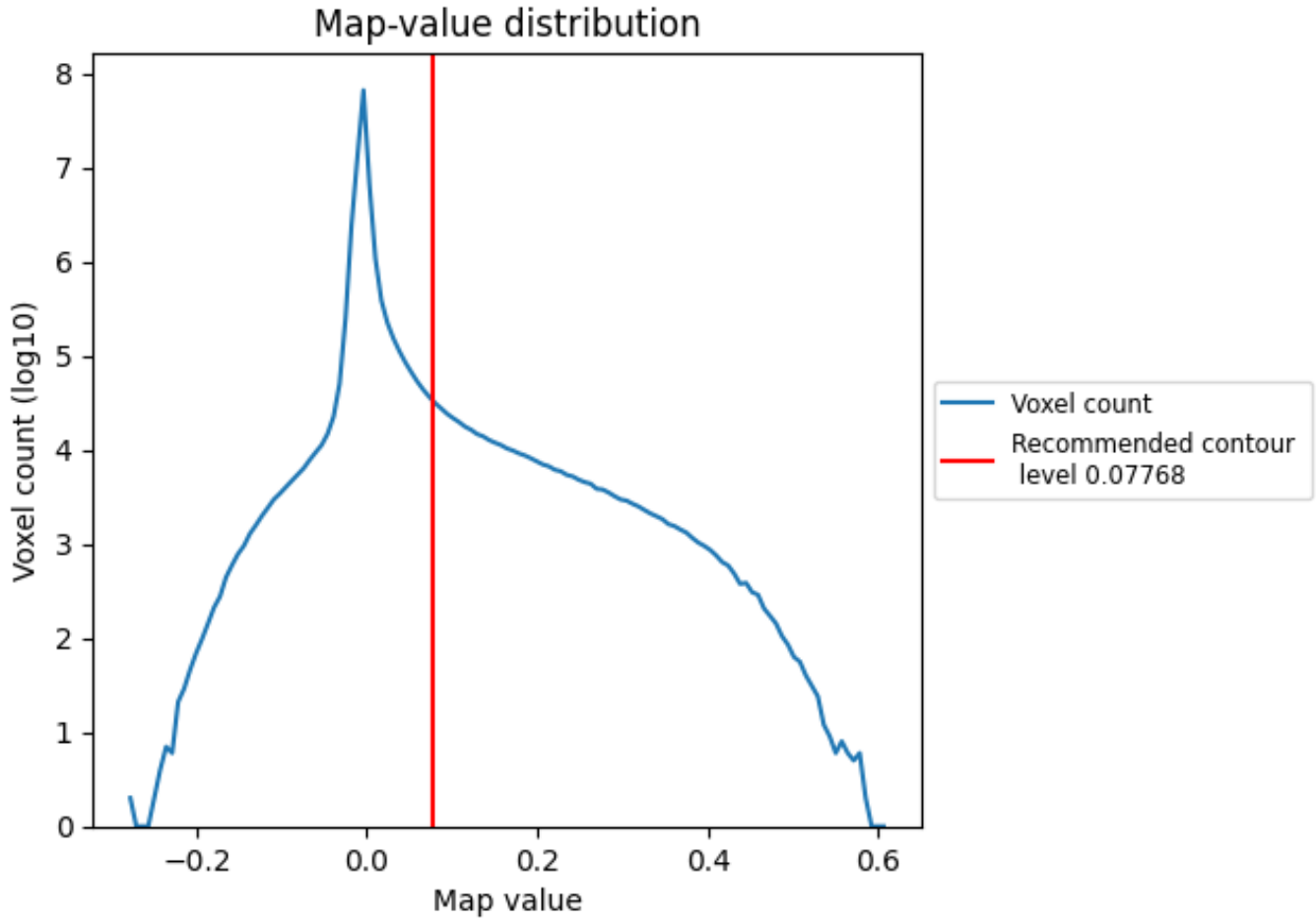


Z

7 Map analysis

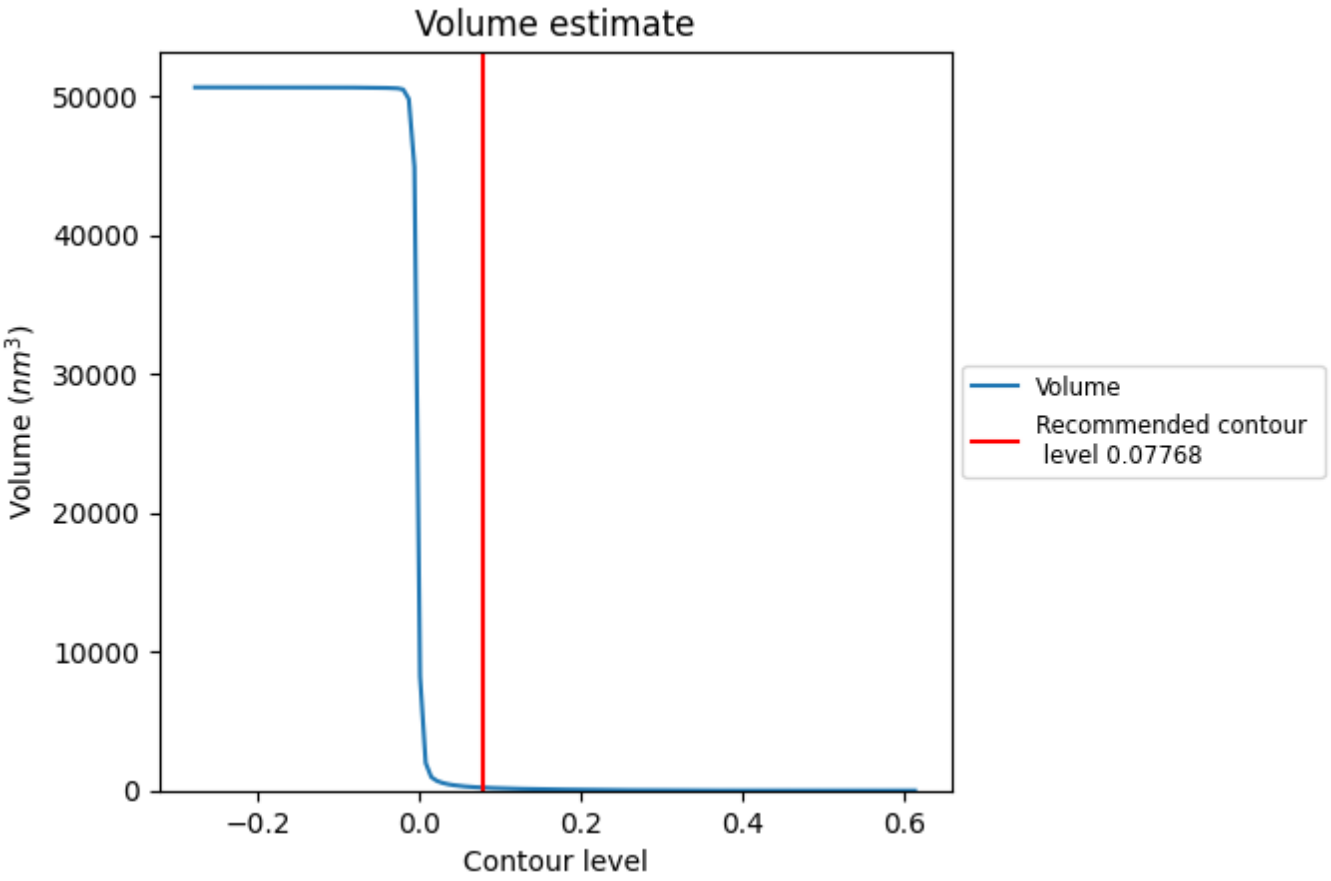
This section contains the results of statistical analysis of the map.

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.

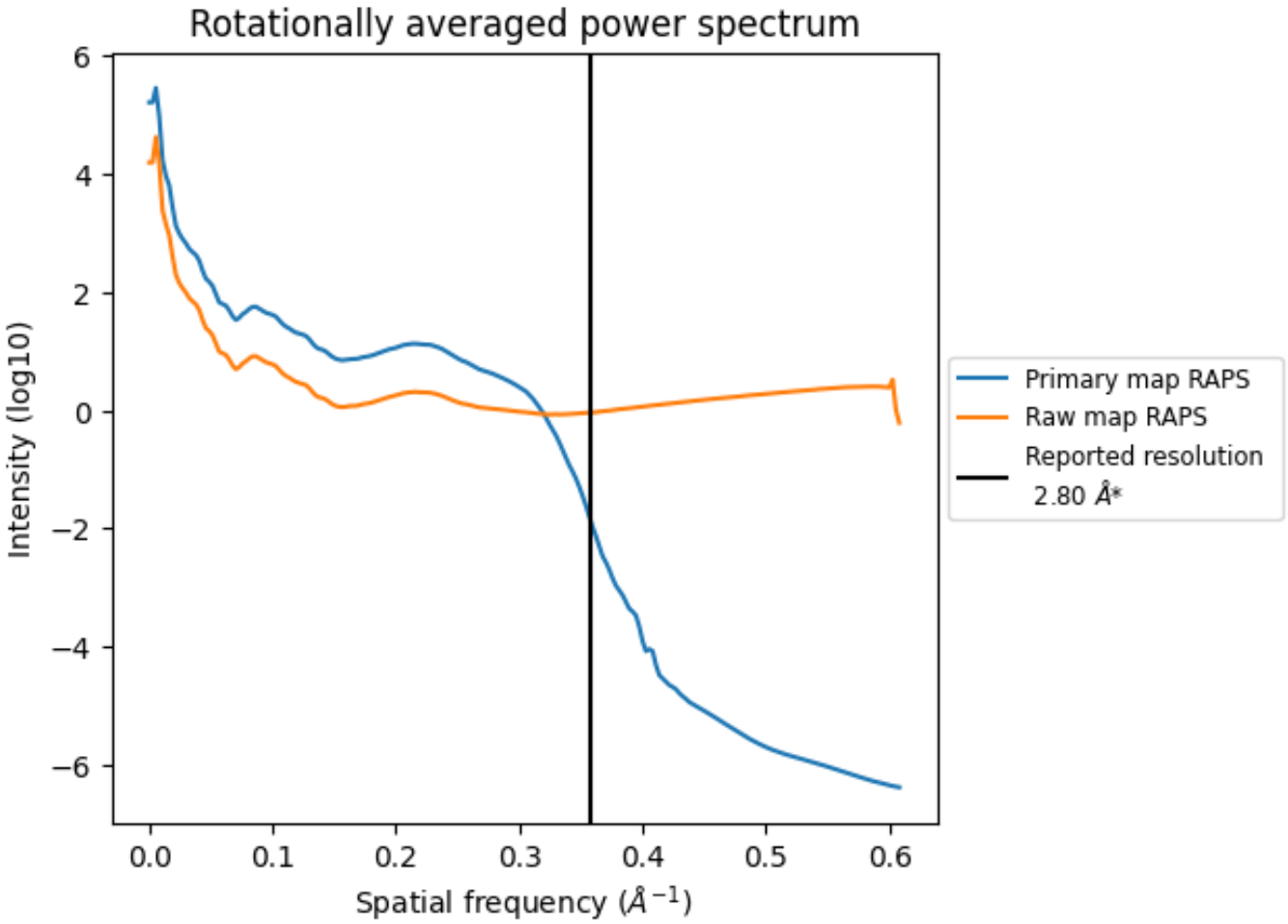
7.2 Volume estimate



The volume at the recommended contour level is 215 nm^3; this corresponds to an approximate mass of 194 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)

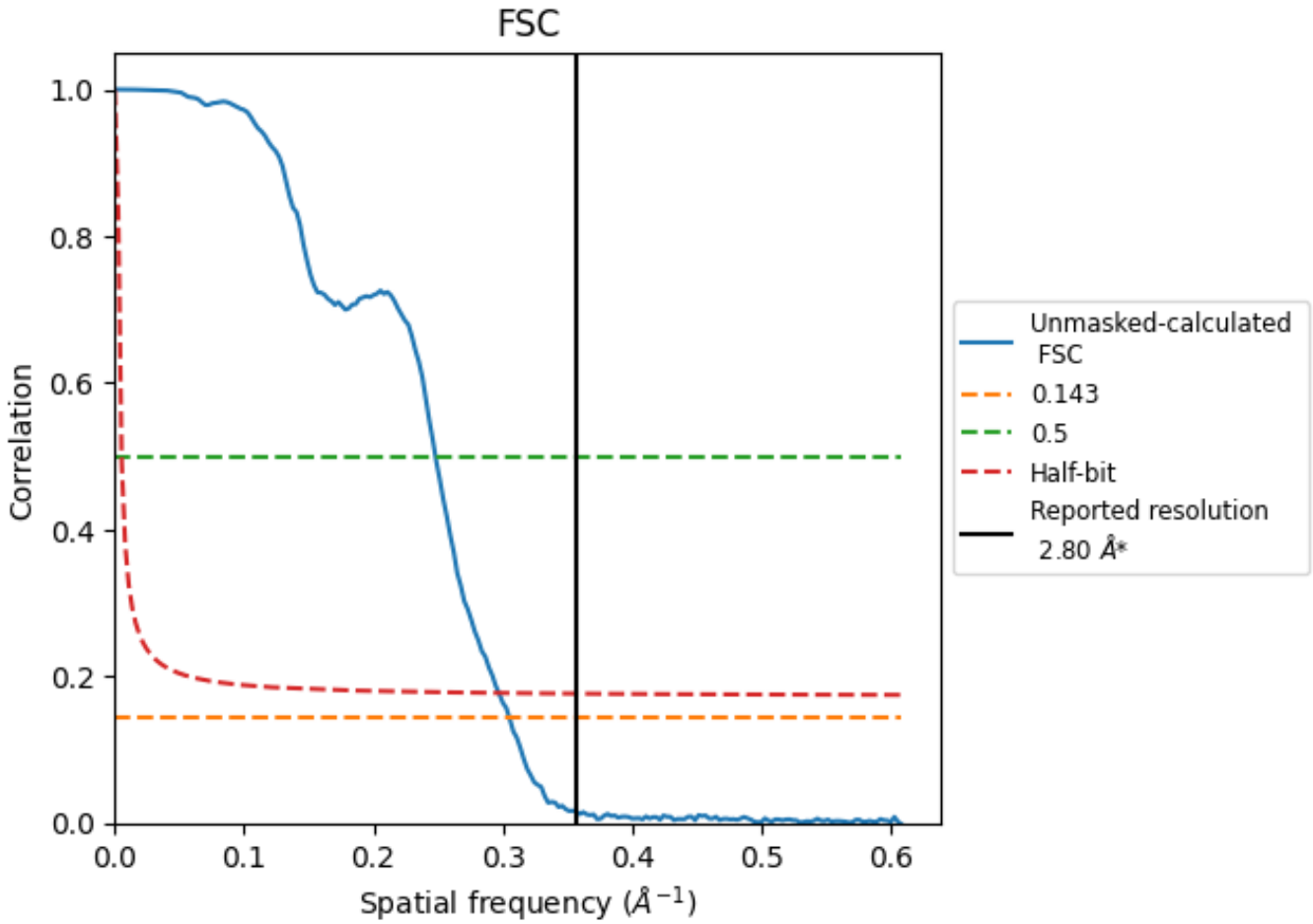


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

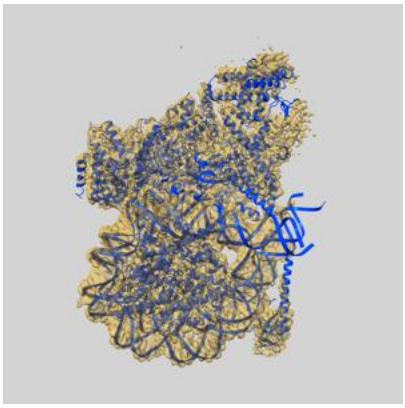
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.28	4.03	3.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 2.8 by more than 10 %

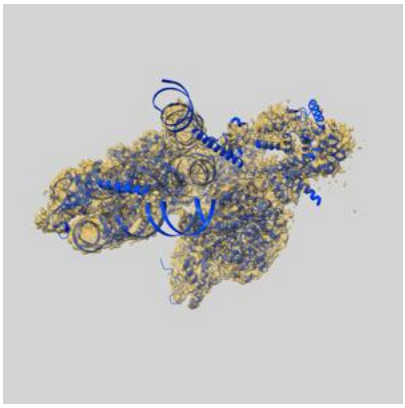
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41449 and PDB model 8TOF. Per-residue inclusion information can be found in section 3 on page 7.

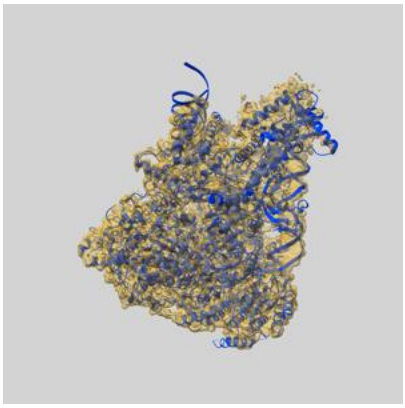
9.1 Map-model overlay



X



Y



Z

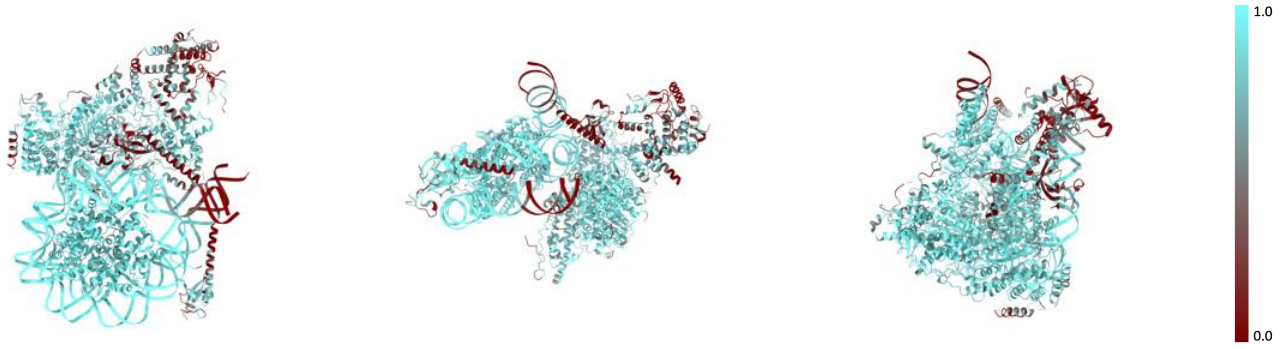
The images above show the 3D surface view of the map at the recommended contour level 0.07768 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

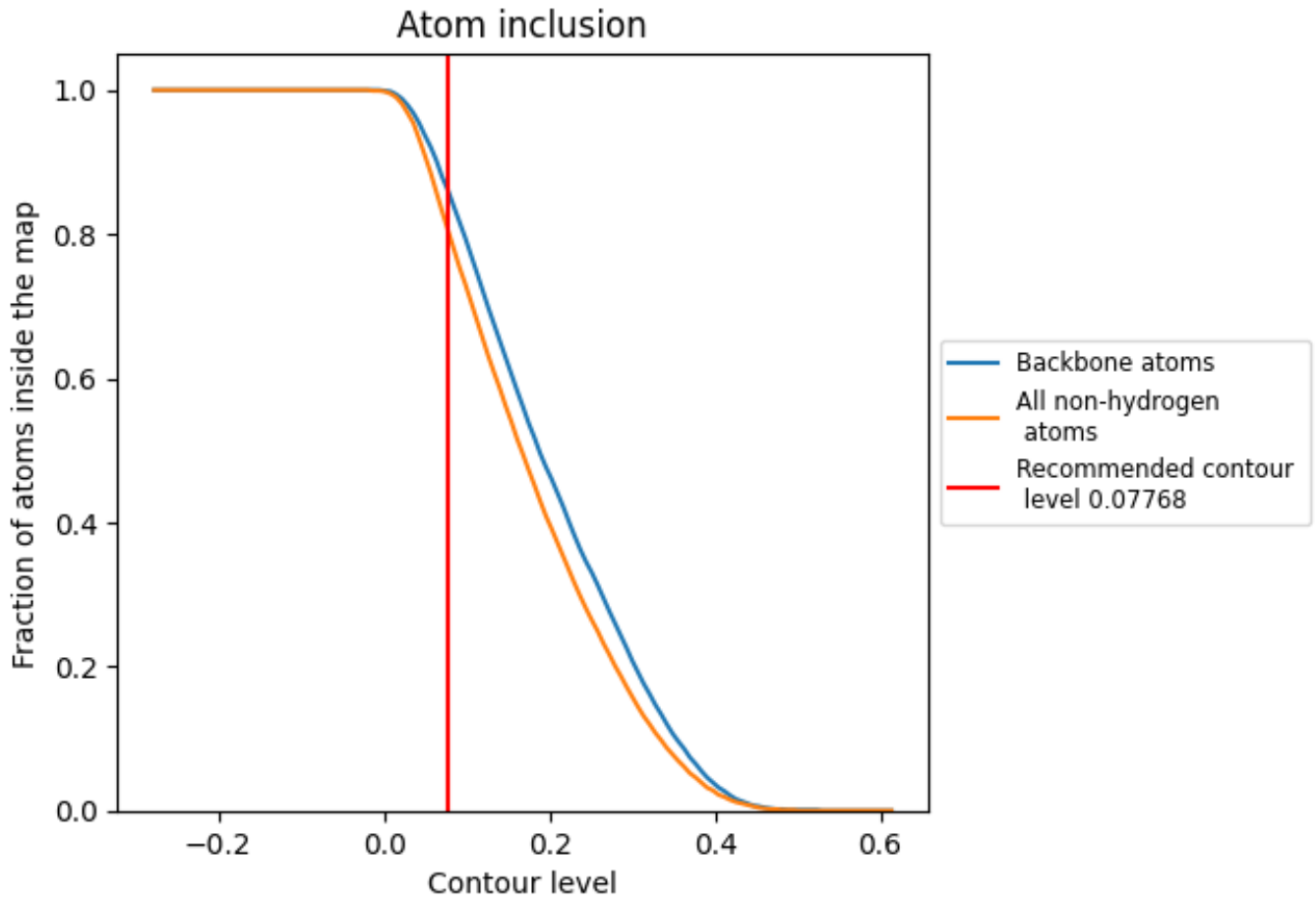
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.07768).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.07768) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.4640
A	0.8090	0.4690
B	0.9270	0.5460
D	0.7460	0.4060
E	0.3420	0.2070
F	0.3550	0.1550
G	0.7130	0.4160
H	0.6550	0.5430
N	0.8750	0.4780
T	0.8620	0.4700
a	0.9290	0.5780
b	0.9310	0.5850
c	0.9680	0.5890
d	0.9410	0.5660
e	0.9500	0.5780
f	0.9770	0.5940
g	0.9630	0.5870
h	0.9620	0.5740
x	0.4360	0.4010