Full wwPDB EM Validation Report ⓘ

Jun 3, 2024 – 01:22 pm BST

PDB ID	:	8CBK
EMDB ID	:	EMD-16543
Title	:	Structure of human mitochondrial RNase P in complex with mitochondrial pre-tRNA-His(5,Ser)
Authors	:	MEYNIER, V.; HARDWICK, S.; CATALA, M.; ROSKE, J.; OERUM, S.; CHIRGADZE, D.; BARRAUD, P.; LUISI, B.; TISNE, C.
Deposited on	:	2023-01-25
Resolution	:	2.76 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:

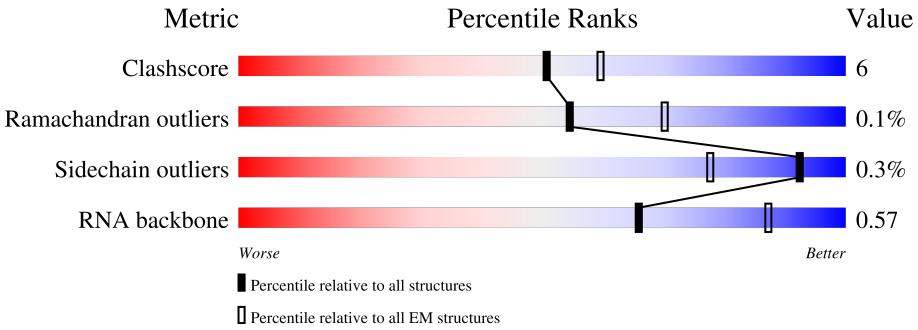
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.76 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
RNA backbone	4643	859

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	261	93% 5% •
1	B	261	93% 5% •
1	C	261	92% 6% •
1	D	261	90% 8% •
2	E	533	59% 29% • 12%
3	F	408	• 75% 10% 16%
4	T	93	• 61% 31% 8%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16221 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 3-hydroxyacyl-CoA dehydrogenase type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	255	Total	C	N	O	S	0	0
			1848	1164	325	351	8		
1	B	255	Total	C	N	O	S	0	0
			1848	1164	325	351	8		
1	C	255	Total	C	N	O	S	0	0
			1848	1164	325	351	8		
1	D	255	Total	C	N	O	S	0	0
			1848	1164	325	351	8		

- Molecule 2 is a protein called Mitochondrial ribonuclease P catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	470	Total	C	N	O	S	0	0
			3814	2432	662	699	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	479	ALA	ASP	engineered mutation	UNP O15091

- Molecule 3 is a protein called tRNA methyltransferase 10 homolog C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	343	Total	C	N	O	S	0	0
			2832	1804	490	521	17		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	18	MET	-	initiating methionine	UNP Q7L0Y3
F	19	HIS	-	expression tag	UNP Q7L0Y3
F	20	HIS	-	expression tag	UNP Q7L0Y3
F	21	HIS	-	expression tag	UNP Q7L0Y3

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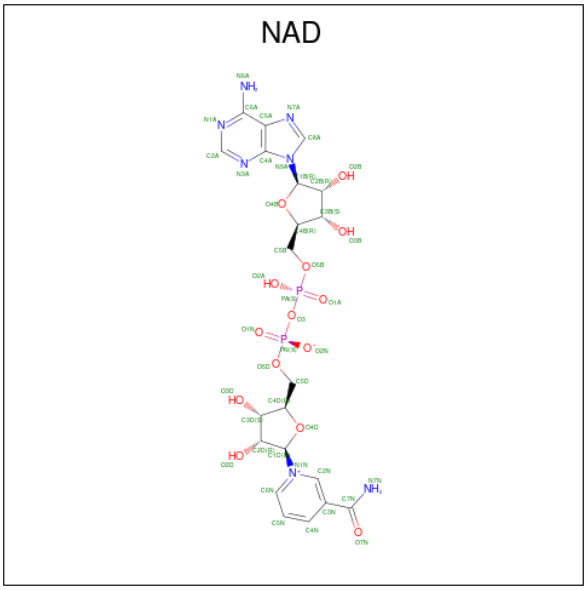
Chain	Residue	Modelled	Actual	Comment	Reference
F	22	HIS	-	expression tag	UNP Q7L0Y3
F	23	HIS	-	expression tag	UNP Q7L0Y3
F	24	HIS	-	expression tag	UNP Q7L0Y3
F	25	SER	-	expression tag	UNP Q7L0Y3
F	26	SER	-	expression tag	UNP Q7L0Y3
F	27	GLY	-	expression tag	UNP Q7L0Y3
F	28	VAL	-	expression tag	UNP Q7L0Y3
F	29	ASP	-	expression tag	UNP Q7L0Y3
F	30	LEU	-	expression tag	UNP Q7L0Y3
F	31	GLY	-	expression tag	UNP Q7L0Y3
F	32	THR	-	expression tag	UNP Q7L0Y3
F	33	GLU	-	expression tag	UNP Q7L0Y3
F	34	ASN	-	expression tag	UNP Q7L0Y3
F	35	LEU	-	expression tag	UNP Q7L0Y3
F	36	TYR	-	expression tag	UNP Q7L0Y3
F	37	PHE	-	expression tag	UNP Q7L0Y3
F	38	GLN	-	expression tag	UNP Q7L0Y3
F	39	SER	-	expression tag	UNP Q7L0Y3
F	404	ALA	-	expression tag	UNP Q7L0Y3
F	405	GLU	-	expression tag	UNP Q7L0Y3
F	406	ASN	-	expression tag	UNP Q7L0Y3
F	407	LEU	-	expression tag	UNP Q7L0Y3
F	408	TYR	-	expression tag	UNP Q7L0Y3
F	409	PHE	-	expression tag	UNP Q7L0Y3
F	410	GLN	-	expression tag	UNP Q7L0Y3
F	411	SER	-	expression tag	UNP Q7L0Y3
F	412	HIS	-	expression tag	UNP Q7L0Y3
F	413	HIS	-	expression tag	UNP Q7L0Y3
F	414	HIS	-	expression tag	UNP Q7L0Y3
F	415	HIS	-	expression tag	UNP Q7L0Y3
F	416	HIS	-	expression tag	UNP Q7L0Y3
F	417	HIS	-	expression tag	UNP Q7L0Y3
F	418	ASP	-	expression tag	UNP Q7L0Y3
F	419	TYR	-	expression tag	UNP Q7L0Y3
F	420	LYS	-	expression tag	UNP Q7L0Y3
F	421	ASP	-	expression tag	UNP Q7L0Y3
F	422	ASP	-	expression tag	UNP Q7L0Y3
F	423	ASP	-	expression tag	UNP Q7L0Y3
F	424	ASP	-	expression tag	UNP Q7L0Y3
F	425	LYS	-	expression tag	UNP Q7L0Y3

- Molecule 4 is a RNA chain called Mitochondrial Precursor tRNA-His(5,Ser).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	93	Total	C	N	O	P	0	0
			1971	884	346	648	93		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

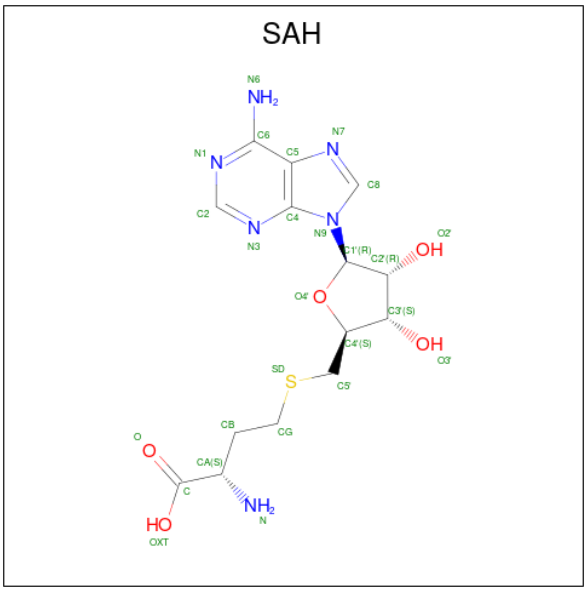


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	B	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	C	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	D	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	E	1	Total	Zn	0
			1	1	

- Molecule 7 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	F	1	Total	C	N	O	S	0
			26	14	6	5	1	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	T	1	Total	Mg	0
			1	1	

- Molecule 9 is water.

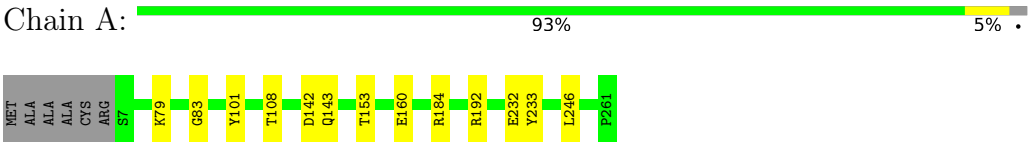
Mol	Chain	Residues	Atoms		AltConf
9	A	6	Total	O	0
			6	6	
9	B	1	Total	O	0
			1	1	
9	F	1	Total	O	0
			1	1	

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.

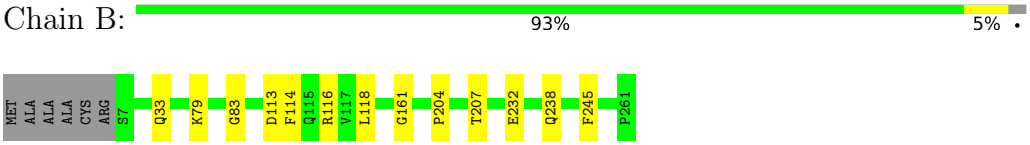
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase type-2

Chain A:



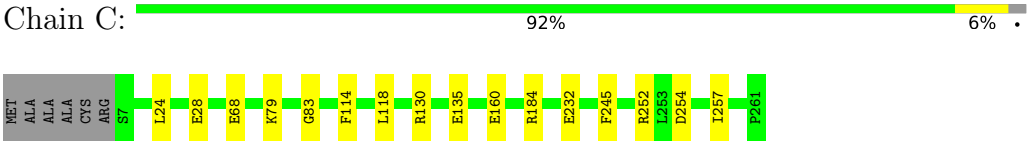
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase type-2

Chain B:



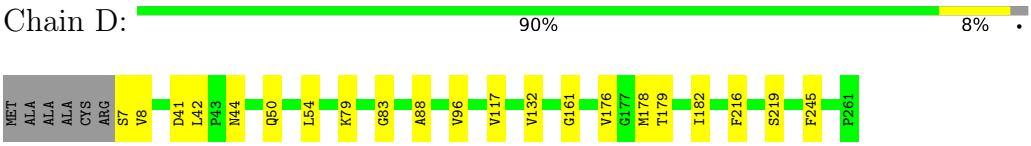
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase type-2

Chain C:



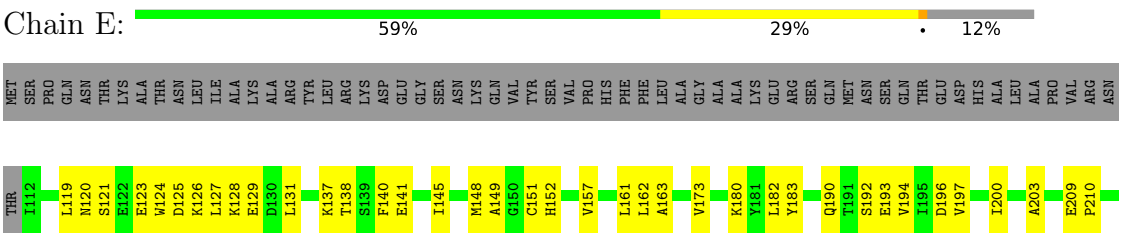
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase type-2

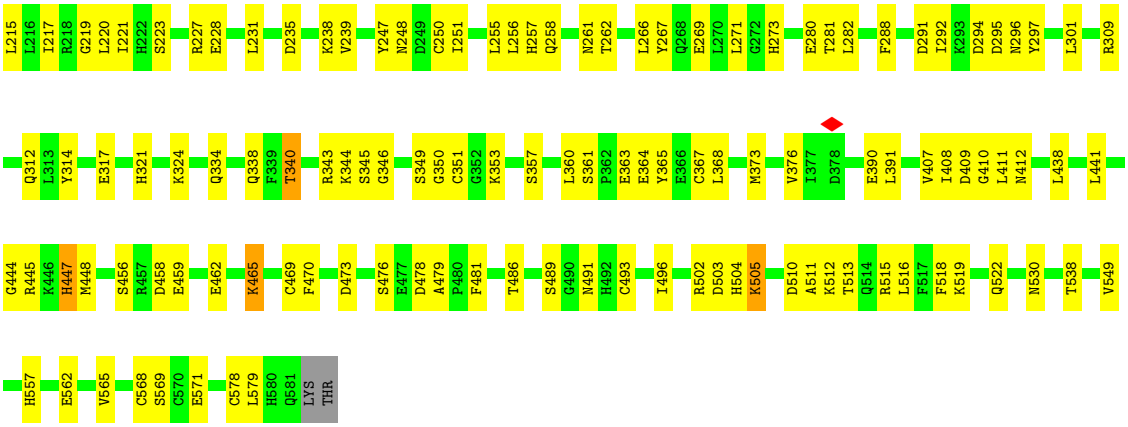
Chain D:



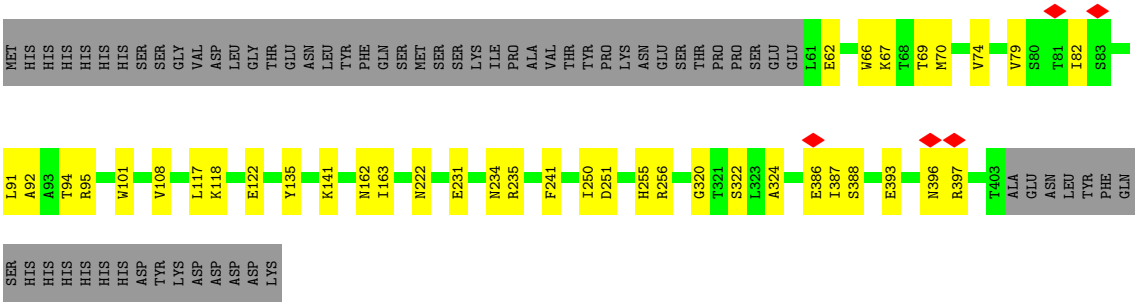
- Molecule 2: Mitochondrial ribonuclease P catalytic subunit

Chain E:

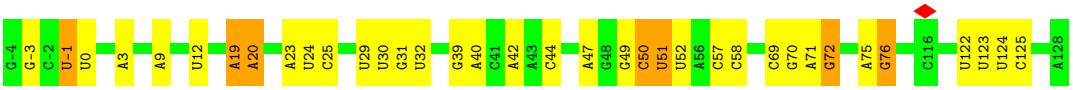




• Molecule 3: tRNA methyltransferase 10 homolog C



• Molecule 4: Mitochondrial Precursor tRNA-His(5,Ser)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81396	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48.52	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	36.551	Depositor
Minimum map value	-15.422	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	1.029	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	312.96, 312.96, 312.96	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.652, 0.652, 0.652	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, NAD, SAH, MG

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	0.25	0/1874	0.47	0/2541
1	B	0.26	0/1874	0.47	0/2541
1	C	0.25	0/1874	0.47	0/2541
1	D	0.26	0/1874	0.48	0/2541
2	E	0.26	0/3901	0.49	0/5271
3	F	0.27	0/2886	0.47	0/3877
4	T	0.20	0/2199	0.73	0/3411
All	All	0.25	0/16482	0.53	0/22723

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1848	0	1896	8	0
1	B	1848	0	1896	8	0
1	C	1848	0	1896	10	0
1	D	1848	0	1896	12	0
2	E	3814	0	3784	119	0
3	F	2832	0	2885	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	1971	0	1001	16	0
5	A	44	0	26	0	0
5	B	44	0	26	0	0
5	C	44	0	26	0	0
5	D	44	0	26	0	0
6	E	1	0	0	0	0
7	F	26	0	19	1	0
8	T	1	0	0	0	0
9	A	6	0	0	0	0
9	B	1	0	0	0	0
9	F	1	0	0	0	0
All	All	16221	0	15377	185	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 6.

All (185) 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)
2:E:557:HIS:CD2	2:E:578:CYS:SG	2.75	0.80
4:T:19:A:HO2'	4:T:20:A:P	2.05	0.79
4:T:19:A:O2'	4:T:20:A:OP1	2.04	0.75
2:E:119:LEU:HD12	2:E:123:GLU:OE2	1.90	0.72
3:F:162:ASN:OD1	3:F:163:ILE:N	2.25	0.69
2:E:203:ALA:HB1	3:F:74:VAL:HG22	1.73	0.69
1:B:204:PRO:O	1:B:207:THR:HG22	1.94	0.68
2:E:196:ASP:OD1	2:E:197:VAL:N	2.26	0.68
2:E:410:GLY:O	2:E:412:ASN:N	2.26	0.68
2:E:445:ARG:NH1	2:E:473:ASP:O	2.27	0.68
2:E:447:HIS:CD2	2:E:448:MET:N	2.61	0.68
2:E:183:TYR:HA	2:E:215:LEU:HD22	1.74	0.68
2:E:518:PHE:O	2:E:522:GLN:NE2	2.27	0.68
2:E:193:GLU:N	2:E:193:GLU:OE1	2.27	0.67
1:C:184:ARG:NH1	1:D:161:GLY:O	2.29	0.66
2:E:281:THR:OG1	2:E:282:LEU:N	2.29	0.65
2:E:447:HIS:CD2	4:T:-1:U:C4	2.85	0.65
2:E:343:ARG:O	2:E:346:GLY:N	2.29	0.65
3:F:141:LYS:NZ	4:T:19:A:OP1	2.30	0.65
2:E:309:ARG:O	2:E:515:ARG:NH1	2.28	0.65
2:E:151:CYS:O	2:E:152:HIS:ND1	2.29	0.65
2:E:295:ASP:OD1	2:E:296:ASN:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:396:ASN:OD1	3:F:397:ARG:N	2.30	0.64
1:B:33:GLN:OE1	1:B:238:GLN:NE2	2.30	0.64
2:E:390:GLU:N	2:E:390:GLU:OE1	2.32	0.63
2:E:269:GLU:OE2	2:E:273:HIS:NE2	2.31	0.63
2:E:571:GLU:N	2:E:571:GLU:OE1	2.31	0.63
4:T:75:A:N6	4:T:76:G:O6	2.33	0.62
1:D:96:VAL:HG12	1:D:117:VAL:HG21	1.82	0.61
2:E:568:CYS:SG	2:E:569:SER:N	2.74	0.61
2:E:163:ALA:HB2	3:F:66:TRP:HE3	1.65	0.61
2:E:203:ALA:CB	3:F:74:VAL:HG22	2.31	0.61
3:F:386:GLU:OE1	3:F:386:GLU:N	2.34	0.61
2:E:489:SER:OG	2:E:493:CYS:SG	2.46	0.61
3:F:70:MET:O	3:F:74:VAL:HG23	2.02	0.60
2:E:255:LEU:HD12	2:E:256:LEU:N	2.15	0.60
2:E:409:ASP:OD2	2:E:410:GLY:N	2.35	0.59
2:E:363:GLU:N	2:E:363:GLU:OE1	2.31	0.59
2:E:196:ASP:OD1	2:E:197:VAL:HG13	2.03	0.58
2:E:391:LEU:HD23	2:E:481:PHE:HE1	1.69	0.58
2:E:510:ASP:OD1	2:E:511:ALA:N	2.36	0.58
2:E:410:GLY:C	2:E:412:ASN:H	2.05	0.57
1:D:50:GLN:O	1:D:54:LEU:HD23	2.04	0.57
2:E:223:SER:O	2:E:257:HIS:NE2	2.36	0.56
1:D:176:VAL:O	1:D:179:THR:HG22	2.05	0.56
2:E:409:ASP:HB2	2:E:496:ILE:O	2.06	0.55
2:E:182:LEU:HD21	2:E:197:VAL:HB	1.88	0.55
3:F:79:VAL:O	3:F:82:ILE:HG22	2.06	0.55
2:E:340:THR:HG21	2:E:578:CYS:HB2	1.90	0.54
2:E:197:VAL:HA	2:E:200:ILE:HD12	1.91	0.52
2:E:145:ILE:HG21	2:E:180:LYS:HB3	1.91	0.52
2:E:317:GLU:O	2:E:321:HIS:ND1	2.43	0.52
2:E:334:GLN:OE1	2:E:334:GLN:N	2.36	0.52
2:E:360:LEU:O	2:E:491:ASN:ND2	2.42	0.52
2:E:120:ASN:O	2:E:123:GLU:HG3	2.09	0.52
1:C:254:ASP:HB2	1:C:257:ILE:HG22	1.91	0.51
1:C:79:LYS:NZ	1:C:135:GLU:OE2	2.34	0.51
2:E:256:LEU:O	2:E:258:GLN:NE2	2.42	0.51
2:E:137:LYS:O	2:E:138:THR:HG22	2.11	0.51
2:E:217:ILE:O	2:E:221:ILE:HG23	2.10	0.51
2:E:469:CYS:SG	2:E:470:PHE:N	2.84	0.51
4:T:39:G:C2	4:T:40:A:C8	2.97	0.51
2:E:409:ASP:CG	2:E:412:ASN:HB2	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ASN:OD1	1:D:44:ASN:O	2.28	0.51
1:D:7:SER:OG	1:D:8:VAL:N	2.45	0.50
1:A:79:LYS:O	1:A:83:GLY:N	2.45	0.50
2:E:119:LEU:HD12	2:E:123:GLU:CD	2.32	0.50
3:F:66:TRP:HA	3:F:69:THR:HG22	1.93	0.50
2:E:220:LEU:HD12	2:E:223:SER:OG	2.12	0.50
2:E:297:TYR:O	2:E:301:LEU:HD13	2.12	0.50
2:E:447:HIS:CG	4:T:-1:U:C4	3.00	0.49
2:E:157:VAL:O	2:E:161:LEU:HD23	2.13	0.49
2:E:228:GLU:OE1	2:E:228:GLU:N	2.40	0.49
3:F:222:ASN:HD22	3:F:222:ASN:N	2.10	0.49
1:C:24:LEU:O	1:C:28:GLU:HG3	2.11	0.49
2:E:510:ASP:O	2:E:513:THR:OG1	2.25	0.49
1:A:101:TYR:HD1	1:A:108:THR:HG1	1.61	0.48
2:E:291:ASP:OD1	2:E:292:ILE:N	2.45	0.48
2:E:340:THR:CG2	2:E:578:CYS:HB2	2.43	0.48
2:E:456:SER:OG	2:E:459:GLU:OE1	2.27	0.48
3:F:393:GLU:O	3:F:396:ASN:OD1	2.32	0.48
1:B:232:GLU:OE1	1:C:245:PHE:HB2	2.13	0.48
2:E:350:GLY:O	2:E:351:CYS:SG	2.72	0.48
4:T:71:A:C2'	4:T:72:G:H5'	2.44	0.48
2:E:373:MET:O	2:E:376:VAL:HG12	2.14	0.47
3:F:118:LYS:O	3:F:122:GLU:OE1	2.33	0.47
1:C:68:GLU:OE1	1:C:130:ARG:NH2	2.43	0.47
2:E:344:LYS:O	2:E:345:SER:CB	2.63	0.47
3:F:66:TRP:CD1	3:F:67:LYS:HE3	2.50	0.47
1:A:160:GLU:O	1:A:160:GLU:HG3	2.15	0.47
2:E:200:ILE:HG23	3:F:70:MET:SD	2.54	0.47
1:B:114:PHE:O	1:B:118:LEU:HD13	2.13	0.47
2:E:121:SER:O	2:E:124:TRP:CD1	2.67	0.47
2:E:235:ASP:HA	2:E:238:LYS:NZ	2.30	0.47
2:E:445:ARG:NH2	2:E:476:SER:O	2.45	0.47
2:E:128:LYS:HG3	2:E:140:PHE:CZ	2.50	0.47
2:E:503:ASP:OD1	2:E:504:HIS:N	2.48	0.47
3:F:62:GLU:O	3:F:66:TRP:CE3	2.67	0.47
1:D:41:ASP:OD1	1:D:42:LEU:N	2.43	0.47
2:E:578:CYS:C	2:E:579:LEU:HD22	2.35	0.47
2:E:294:ASP:OD1	2:E:295:ASP:N	2.48	0.46
2:E:512:LYS:O	2:E:516:LEU:HD13	2.14	0.46
2:E:163:ALA:HB2	3:F:66:TRP:CE3	2.46	0.46
2:E:312:GLN:NE2	2:E:314:TYR:CZ	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:410:GLY:C	2:E:412:ASN:N	2.68	0.46
1:C:160:GLU:OE2	1:C:252:ARG:NH2	2.48	0.46
1:D:88:ALA:HB2	1:D:132:VAL:HG11	1.98	0.46
2:E:458:ASP:OD1	2:E:459:GLU:N	2.49	0.46
2:E:364:GLU:HA	2:E:367:CYS:SG	2.56	0.46
1:D:216:PHE:O	1:D:219:SER:OG	2.26	0.45
2:E:239:VAL:HG23	3:F:94:THR:HG22	1.98	0.45
2:E:502:ARG:NH2	4:T:3:A:OP2	2.50	0.45
1:A:153:THR:OG1	1:A:233:TYR:OH	2.33	0.45
2:E:407:VAL:C	2:E:408:ILE:HD12	2.37	0.45
1:A:142:ASP:OD1	1:A:143:GLN:N	2.45	0.45
2:E:408:ILE:HD12	2:E:408:ILE:N	2.31	0.45
2:E:408:ILE:HD13	2:E:441:LEU:O	2.17	0.45
1:B:79:LYS:O	1:B:83:GLY:N	2.50	0.44
3:F:234:ASN:OD1	3:F:241:PHE:N	2.46	0.44
2:E:364:GLU:O	2:E:368:LEU:HD13	2.18	0.44
2:E:438:LEU:H	2:E:438:LEU:HD23	1.82	0.44
2:E:458:ASP:OD1	2:E:459:GLU:OE1	2.35	0.44
2:E:267:TYR:CZ	2:E:271:LEU:HD11	2.52	0.44
2:E:351:CYS:SG	2:E:353:LYS:HG2	2.58	0.44
2:E:478:ASP:OD1	2:E:479:ALA:N	2.49	0.44
3:F:95:ARG:NE	3:F:117:LEU:HD11	2.33	0.44
2:E:340:THR:HG1	2:E:349:SER:CB	2.30	0.44
2:E:196:ASP:O	2:E:200:ILE:HG13	2.18	0.44
2:E:261:ASN:OD1	2:E:262:THR:N	2.51	0.43
2:E:357:SER:O	2:E:519:LYS:NZ	2.51	0.43
2:E:227:ARG:O	2:E:231:LEU:HD13	2.18	0.43
4:T:24:U:C2	4:T:25:C:C5	3.06	0.43
1:D:178:MET:CE	1:D:182:ILE:HD11	2.48	0.43
2:E:247:TYR:HA	2:E:250:CYS:SG	2.59	0.43
2:E:338:GLN:OE1	2:E:338:GLN:N	2.51	0.43
2:E:209:GLU:OE1	2:E:210:PRO:O	2.36	0.43
2:E:562:GLU:OE2	2:E:565:VAL:N	2.50	0.43
2:E:365:TYR:OH	2:E:486:THR:O	2.33	0.43
3:F:231:GLU:OE1	3:F:235:ARG:NH2	2.48	0.43
3:F:250:ILE:O	3:F:255:HIS:ND1	2.52	0.42
3:F:387:ILE:HG13	3:F:388:SER:N	2.34	0.42
4:T:122:U:H2'	4:T:123:U:C6	2.54	0.42
2:E:194:VAL:HA	2:E:197:VAL:HG22	2.01	0.42
3:F:322:SER:HB3	7:F:501:SAH:OXT	2.19	0.42
4:T:71:A:O2'	4:T:72:G:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:190:GLN:O	2:E:194:VAL:HG23	2.19	0.42
2:E:192:SER:OG	2:E:193:GLU:OE1	2.36	0.42
2:E:125:ASP:O	2:E:129:GLU:OE1	2.37	0.42
2:E:248:ASN:ND2	2:E:280:GLU:OE1	2.48	0.42
2:E:361:SER:OG	2:E:363:GLU:OE1	2.23	0.42
2:E:462:GLU:O	2:E:465:LYS:HG3	2.20	0.42
1:B:245:PHE:HB2	1:C:232:GLU:OE1	2.20	0.42
2:E:123:GLU:O	2:E:126:LYS:HG2	2.20	0.42
2:E:127:LEU:O	2:E:131:LEU:HD13	2.19	0.42
2:E:530:ASN:N	2:E:538:THR:OG1	2.52	0.42
2:E:148:MET:O	2:E:149:ALA:HB3	2.19	0.42
3:F:101:TRP:HB3	3:F:108:VAL:HG11	2.02	0.42
4:T:50:C:H2'	4:T:51:U:N1	2.35	0.42
1:A:232:GLU:OE2	1:D:245:PHE:HB2	2.20	0.42
4:T:124:U:H2'	4:T:125:C:C6	2.54	0.42
2:E:194:VAL:HG11	2:E:219:GLY:C	2.41	0.41
2:E:321:HIS:O	2:E:324:LYS:HG2	2.21	0.41
1:C:114:PHE:CE2	1:C:118:LEU:HD11	2.55	0.41
2:E:444:GLY:N	2:E:470:PHE:O	2.54	0.41
2:E:447:HIS:CG	4:T:-1:U:N3	2.89	0.41
1:B:113:ASP:OD1	1:B:116:ARG:NH2	2.54	0.41
1:C:79:LYS:O	1:C:83:GLY:N	2.53	0.41
3:F:251:ASP:O	3:F:256:ARG:NH2	2.54	0.41
1:A:192:ARG:NH1	1:A:246:LEU:O	2.49	0.41
2:E:193:GLU:O	2:E:197:VAL:HG22	2.21	0.41
2:E:255:LEU:HD13	2:E:288:PHE:HB2	2.01	0.41
2:E:182:LEU:CD2	2:E:197:VAL:HG21	2.51	0.41
2:E:409:ASP:CG	2:E:412:ASN:CB	2.89	0.41
2:E:502:ARG:O	2:E:505:LYS:HG3	2.21	0.41
3:F:135:TYR:OH	4:T:42:A:OP1	2.28	0.41
1:A:184:ARG:NH1	1:B:161:GLY:O	2.46	0.41
1:D:79:LYS:O	1:D:83:GLY:N	2.53	0.41
2:E:140:PHE:CD2	2:E:141:GLU:OE1	2.74	0.41
2:E:447:HIS:CD2	2:E:447:HIS:C	2.93	0.41
3:F:91:LEU:HD12	3:F:92:ALA:N	2.37	0.40
2:E:251:ILE:HG22	2:E:266:LEU:HD23	2.02	0.40
2:E:255:LEU:O	2:E:288:PHE:CZ	2.74	0.40
2:E:162:LEU:HD21	2:E:173:VAL:HG21	2.02	0.40
2:E:309:ARG:NE	2:E:549:VAL:O	2.54	0.40
3:F:320:GLY:O	3:F:324:ALA:N	2.45	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	253/261 (97%)	247 (98%)	6 (2%)	0	100	100
1	B	253/261 (97%)	247 (98%)	6 (2%)	0	100	100
1	C	253/261 (97%)	245 (97%)	8 (3%)	0	100	100
1	D	253/261 (97%)	247 (98%)	6 (2%)	0	100	100
2	E	468/533 (88%)	432 (92%)	35 (8%)	1 (0%)	47	69
3	F	341/408 (84%)	330 (97%)	11 (3%)	0	100	100
All	All	1821/1985 (92%)	1748 (96%)	72 (4%)	1 (0%)	54	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	411	LEU

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	192/195 (98%)	192 (100%)	0	100	100
1	B	192/195 (98%)	192 (100%)	0	100	100
1	C	192/195 (98%)	192 (100%)	0	100	100
1	D	192/195 (98%)	192 (100%)	0	100	100
2	E	421/480 (88%)	417 (99%)	4 (1%)	76	85
3	F	313/374 (84%)	313 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1502/1634 (92%)	1498 (100%)	4 (0%)	92 95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	340	THR
2	E	447	HIS
2	E	465	LYS
2	E	505	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	312	GLN
2	E	447	HIS
2	E	522	GLN
3	F	222	ASN
3	F	348	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	T	89/93 (95%)	22 (24%)	2 (2%)

All (22) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	T	-3	G
4	T	-1	U
4	T	0	U
4	T	9	A
4	T	12	U
4	T	20	A
4	T	23	A
4	T	29	U
4	T	30	U
4	T	32	U
4	T	44	C
4	T	47	A

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Mol	Chain	Res	Type
4	T	49	G
4	T	50	C
4	T	51	U
4	T	52	U
4	T	57	C
4	T	58	C
4	T	69	C
4	T	70	G
4	T	72	G
4	T	76	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	T	19	A
4	T	31	G

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
7	SAH	F	501	-	24,28,28	0.88	2 (8%)	25,40,40	0.92	1 (4%)
5	NAD	C	301	-	42,48,48	0.84	2 (4%)	50,73,73	0.95	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAD	D	301	-	42,48,48	1.22	3 (7%)	50,73,73	1.01	4 (8%)
5	NAD	B	301	-	42,48,48	0.81	1 (2%)	50,73,73	0.88	3 (6%)
5	NAD	A	301	-	42,48,48	0.83	2 (4%)	50,73,73	0.98	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SAH	F	501	-	-	6/11/31/31	0/3/3/3
5	NAD	C	301	-	-	12/26/62/62	0/5/5/5
5	NAD	D	301	-	-	11/26/62/62	0/5/5/5
5	NAD	B	301	-	-	10/26/62/62	0/5/5/5
5	NAD	A	301	-	-	10/26/62/62	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	301	NAD	C2N-C3N	-4.81	1.31	1.39
5	D	301	NAD	C4N-C3N	-3.79	1.32	1.39
7	F	501	SAH	OXT-C	-2.48	1.22	1.30
5	C	301	NAD	C4N-C3N	-2.17	1.35	1.39
5	C	301	NAD	C8A-N7A	-2.14	1.30	1.34
5	A	301	NAD	C8A-N7A	-2.14	1.30	1.34
7	F	501	SAH	C8-N7	-2.07	1.31	1.34
5	A	301	NAD	C2N-C3N	-2.04	1.35	1.39
5	D	301	NAD	C8A-N7A	-2.03	1.31	1.34
5	B	301	NAD	C8A-N7A	-2.02	1.31	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	301	NAD	C2N-C3N-C4N	3.10	121.77	118.26
5	D	301	NAD	O4D-C1D-C2D	-2.94	102.63	106.93
5	A	301	NAD	PN-O3-PA	-2.89	122.90	132.83
5	C	301	NAD	O4D-C1D-C2D	-2.80	102.84	106.93
5	B	301	NAD	O4B-C1B-C2B	-2.71	102.97	106.93
5	B	301	NAD	PN-O3-PA	-2.69	123.61	132.83
5	C	301	NAD	PN-O3-PA	-2.68	123.61	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	301	NAD	O4D-C1D-C2D	-2.56	103.18	106.93
5	A	301	NAD	C6N-N1N-C2N	-2.45	119.74	121.97
5	B	301	NAD	C5A-C6A-N6A	2.22	123.72	120.35
5	C	301	NAD	O4B-C1B-C2B	-2.17	103.75	106.93
5	C	301	NAD	C2N-C3N-C4N	2.09	120.63	118.26
5	A	301	NAD	C3N-C2N-N1N	2.09	122.47	120.43
5	A	301	NAD	O4B-C1B-C2B	-2.08	103.89	106.93
5	D	301	NAD	PN-O3-PA	-2.05	125.80	132.83
5	D	301	NAD	C5A-C6A-N6A	2.04	123.45	120.35
7	F	501	SAH	CB-CG-SD	-2.01	108.79	113.31

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	NAD	C5B-O5B-PA-O1A
5	A	301	NAD	C5D-O5D-PN-O3
5	B	301	NAD	C5B-O5B-PA-O1A
5	B	301	NAD	PN-O3-PA-O5B
5	B	301	NAD	C5D-O5D-PN-O1N
5	B	301	NAD	O4D-C1D-N1N-C2N
5	C	301	NAD	C5B-O5B-PA-O1A
5	C	301	NAD	O4D-C1D-N1N-C2N
5	C	301	NAD	O4D-C1D-N1N-C6N
5	C	301	NAD	C2D-C1D-N1N-C6N
5	D	301	NAD	C5B-O5B-PA-O1A
5	D	301	NAD	C5D-O5D-PN-O3
7	F	501	SAH	N-CA-CB-CG
7	F	501	SAH	C-CA-CB-CG
5	B	301	NAD	C3D-C4D-C5D-O5D
5	D	301	NAD	O4B-C4B-C5B-O5B
5	B	301	NAD	O4D-C4D-C5D-O5D
5	C	301	NAD	O4D-C4D-C5D-O5D
5	C	301	NAD	C3D-C4D-C5D-O5D
5	D	301	NAD	C3B-C4B-C5B-O5B
7	F	501	SAH	O-C-CA-CB
7	F	501	SAH	OXT-C-CA-CB
5	A	301	NAD	O4B-C4B-C5B-O5B
5	A	301	NAD	PN-O3-PA-O5B
5	C	301	NAD	PN-O3-PA-O5B
5	D	301	NAD	PN-O3-PA-O5B
5	A	301	NAD	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
5	B	301	NAD	C5B-O5B-PA-O3
5	C	301	NAD	C5B-O5B-PA-O3
7	F	501	SAH	OXT-C-CA-N
5	A	301	NAD	C5B-O5B-PA-O2A
5	A	301	NAD	C5D-O5D-PN-O1N
5	D	301	NAD	C5B-O5B-PA-O2A
5	D	301	NAD	C5D-O5D-PN-O1N
7	F	501	SAH	CB-CG-SD-C5'
5	A	301	NAD	C3B-C4B-C5B-O5B
5	A	301	NAD	C3D-C4D-C5D-O5D
5	D	301	NAD	O4D-C4D-C5D-O5D
5	D	301	NAD	C3D-C4D-C5D-O5D
5	A	301	NAD	C5B-O5B-PA-O3
5	B	301	NAD	C2D-C1D-N1N-C6N
5	C	301	NAD	C2D-C1D-N1N-C2N
5	D	301	NAD	C5B-O5B-PA-O3
5	B	301	NAD	PA-O3-PN-O2N
5	D	301	NAD	C4B-C5B-O5B-PA
5	C	301	NAD	C5B-O5B-PA-O2A
5	C	301	NAD	C5D-O5D-PN-O1N
5	B	301	NAD	O4B-C4B-C5B-O5B
5	C	301	NAD	O4B-C4B-C5B-O5B

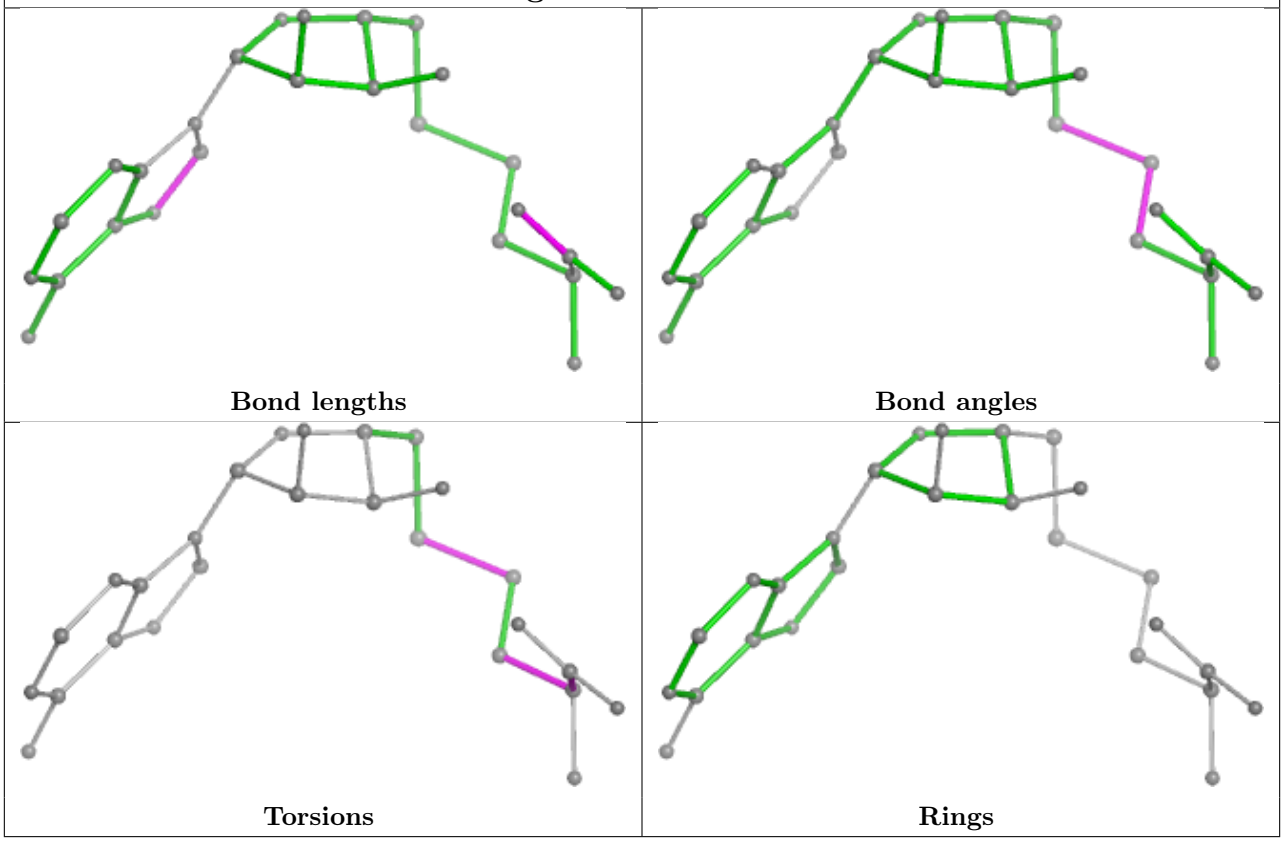
There are no ring outliers.

1 monomer is involved in 1 short contact:

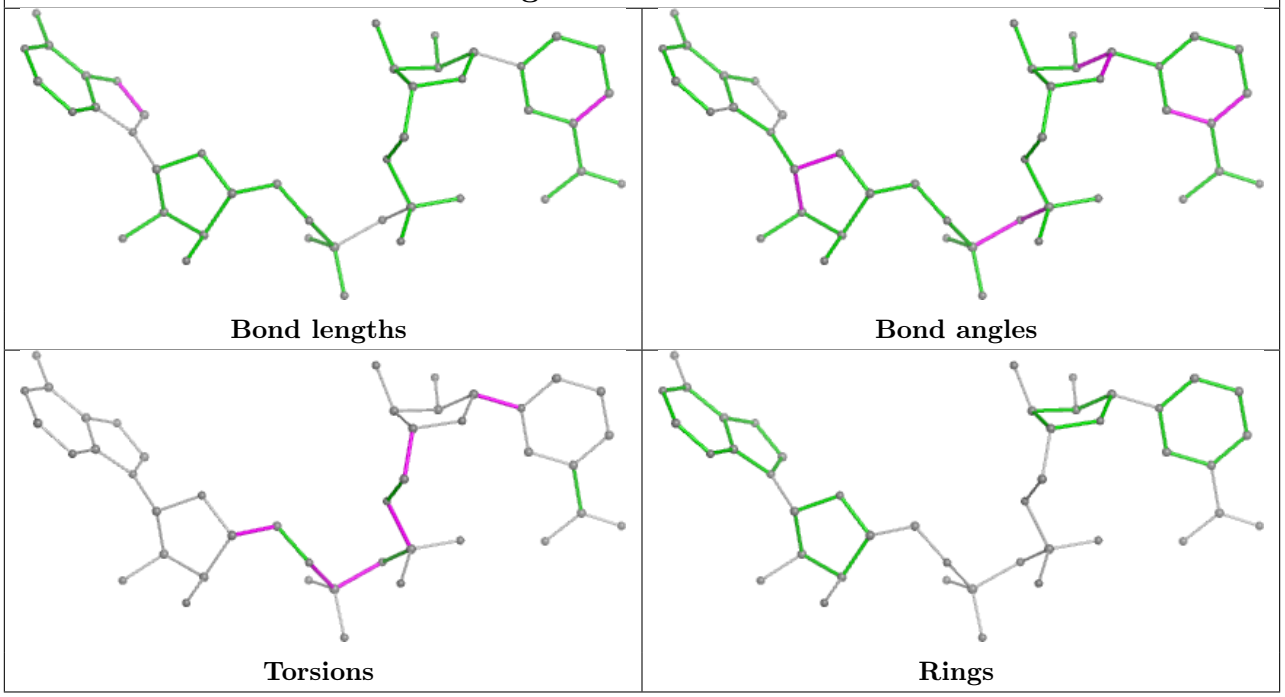
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	501	SAH	1	0

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.

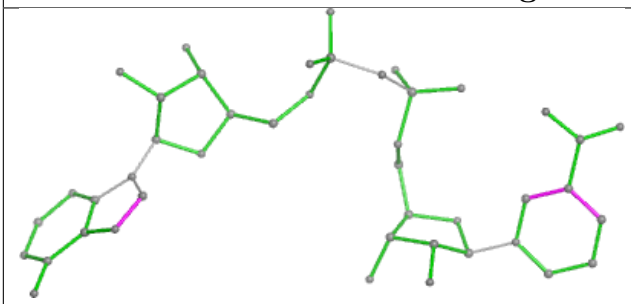
Ligand SAH F 501



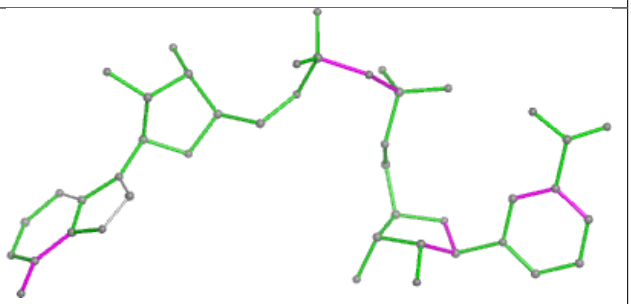
Ligand NAD C 301



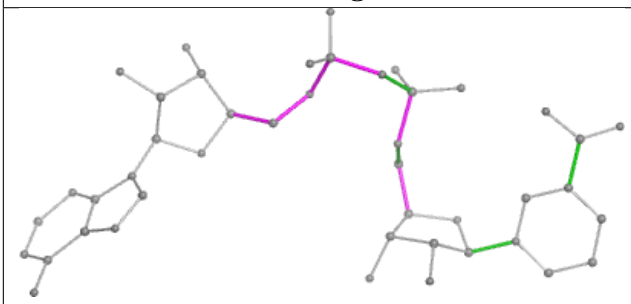
Ligand NAD D 301



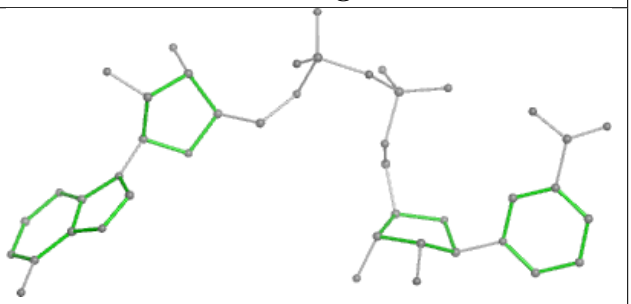
Bond lengths



Bond angles

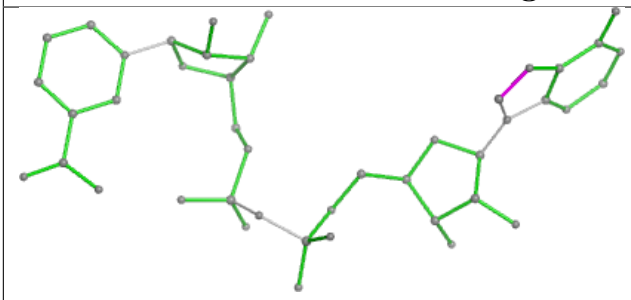


Torsions

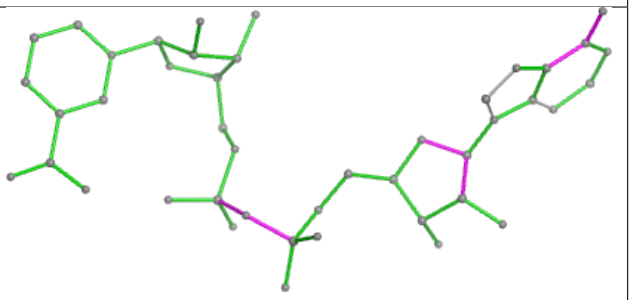


Rings

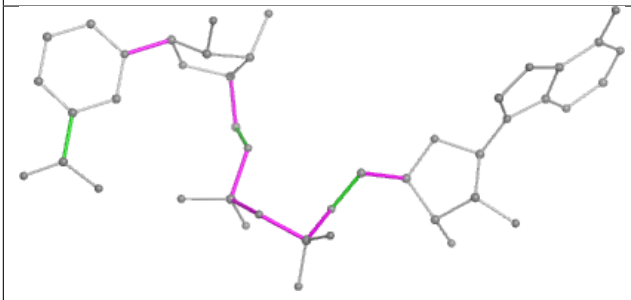
Ligand NAD B 301



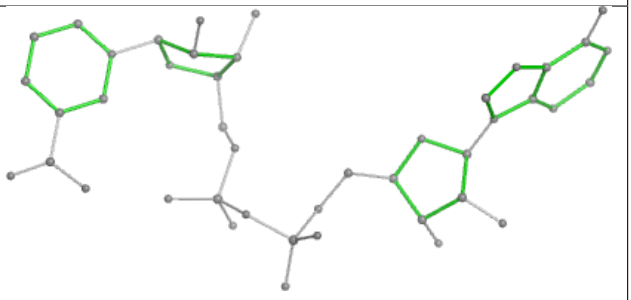
Bond lengths



Bond angles

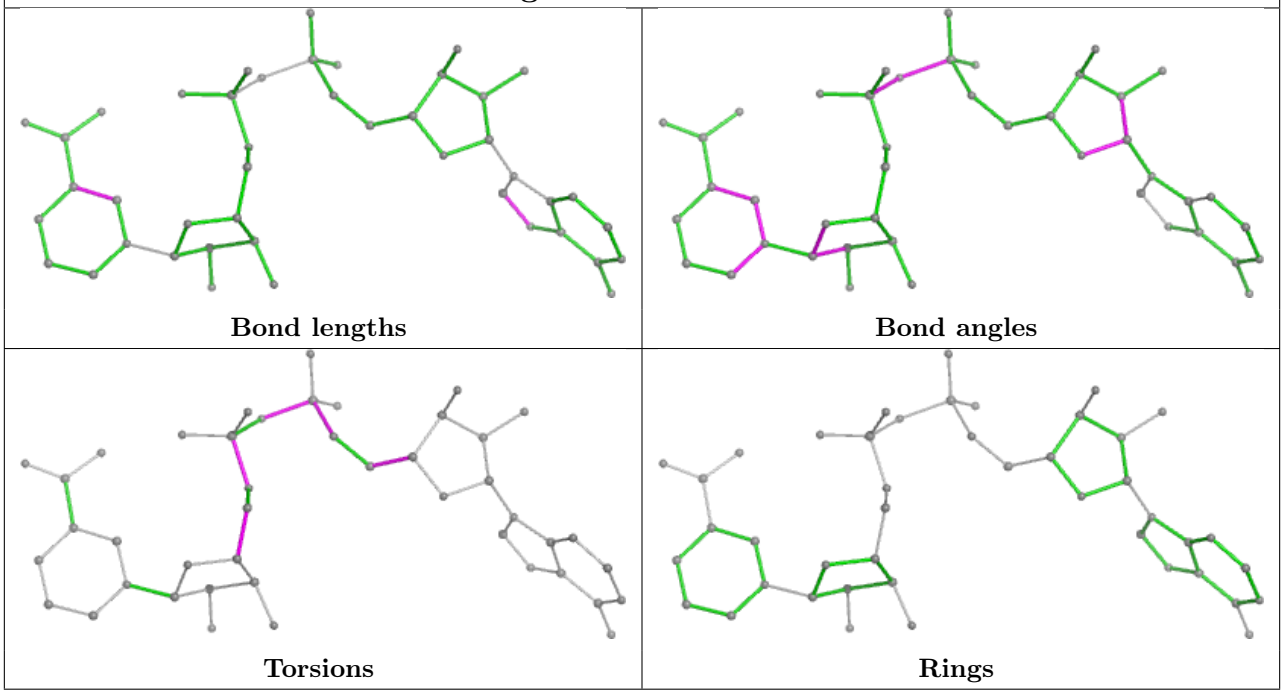


Torsions



Rings

Ligand NAD A 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	T	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	107:G	O3'	116:C	P	17.38
1	T	15:A	O3'	19:A	P	11.77
1	T	52:U	O3'	56:A	P	8.58
1	T	76:G	O3'	103:C	P	5.38

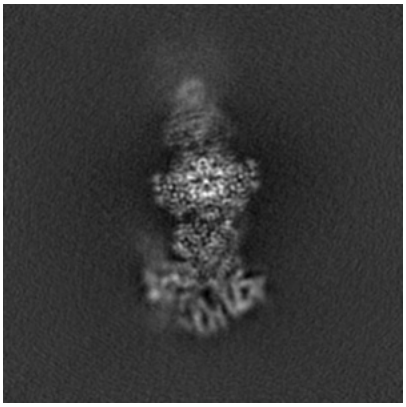
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16543. These allow visual inspection of the internal detail of the map and identification of artifacts.

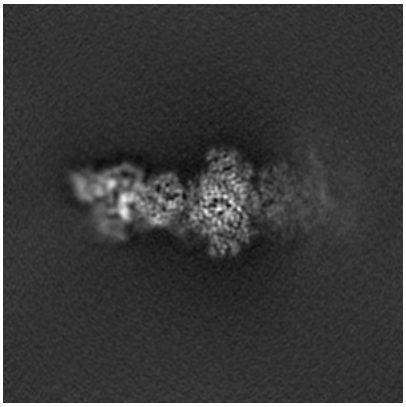
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

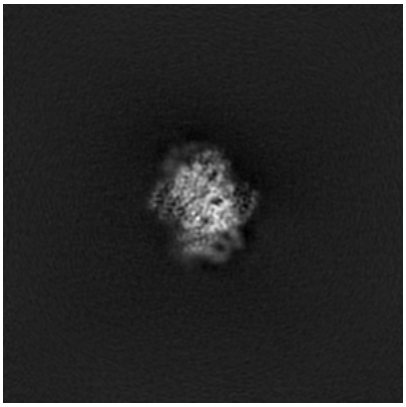
6.1.1 Primary map



X



Y

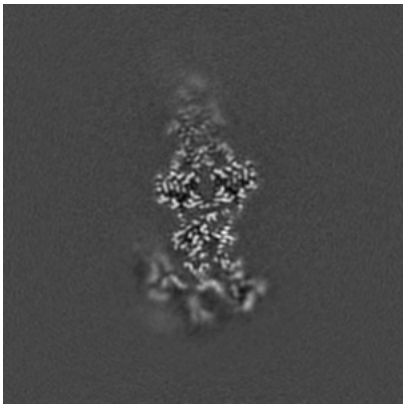


Z

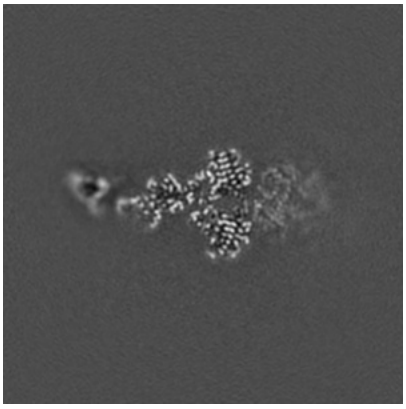
The images above show the map projected in three orthogonal directions.

6.2 Central slices

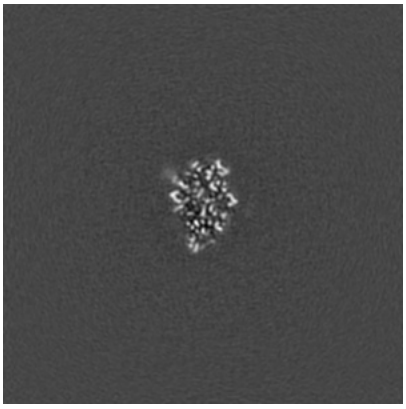
6.2.1 Primary map



X Index: 240



Y Index: 240

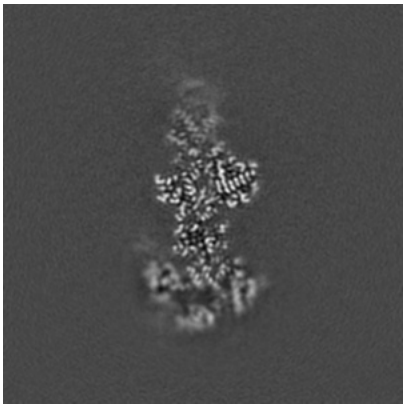


Z Index: 240

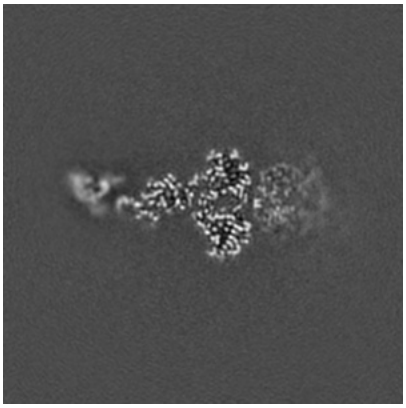
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

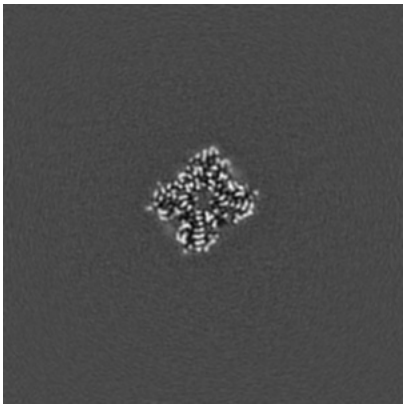
6.3.1 Primary map



X Index: 247



Y Index: 237

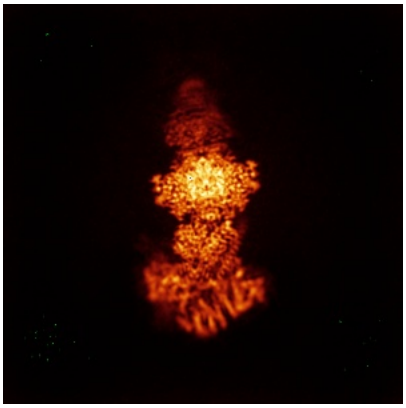


Z Index: 260

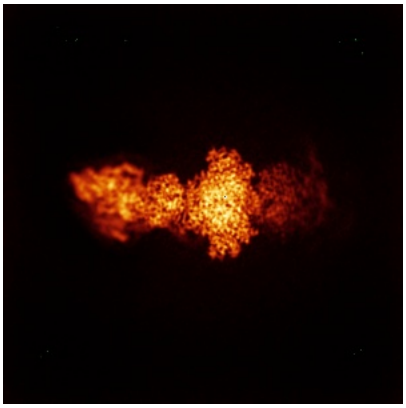
The images above show the largest variance slices of the map in three orthogonal directions.

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

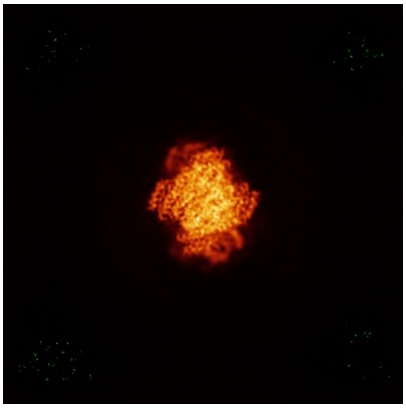
6.4.1 Primary map



X



Y

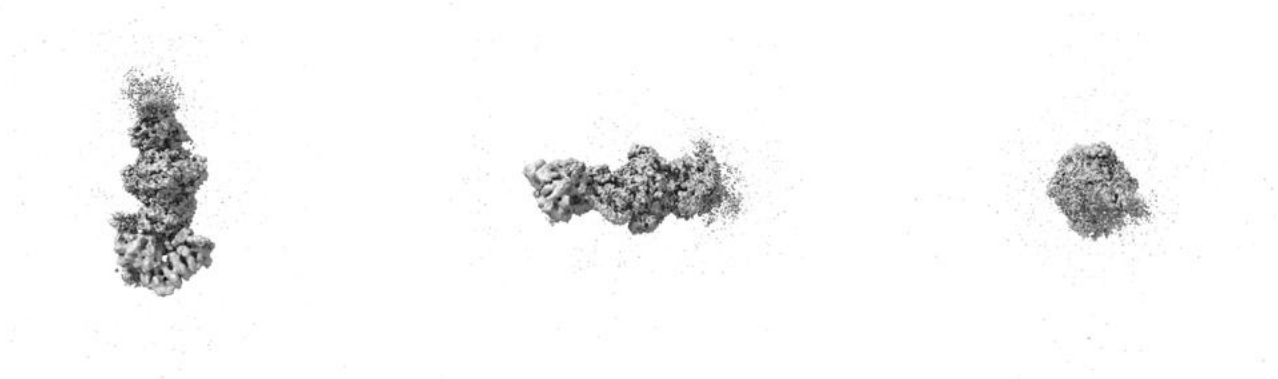


Z

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

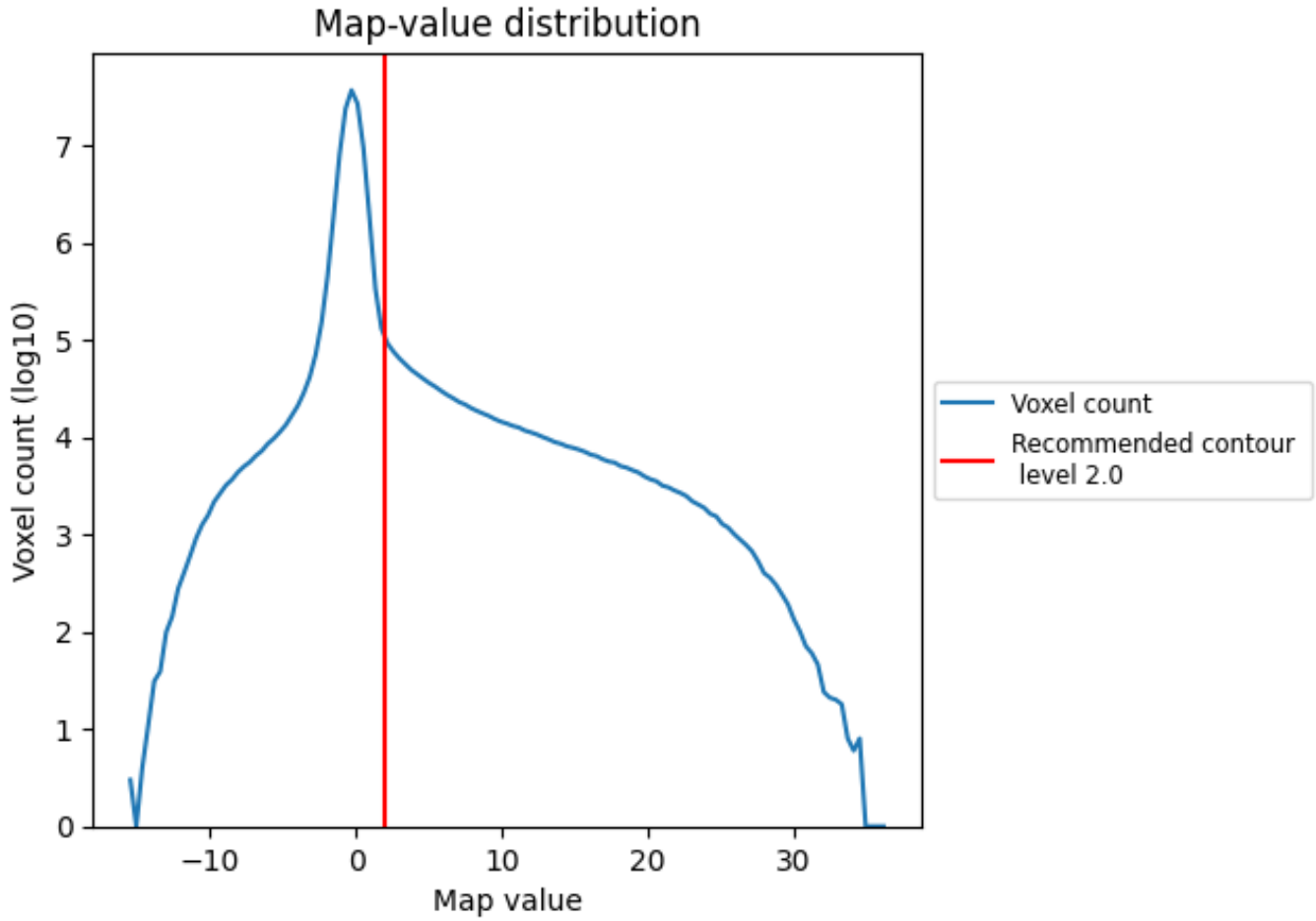
6.6 Mask visualisation (i)

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

7 Map analysis

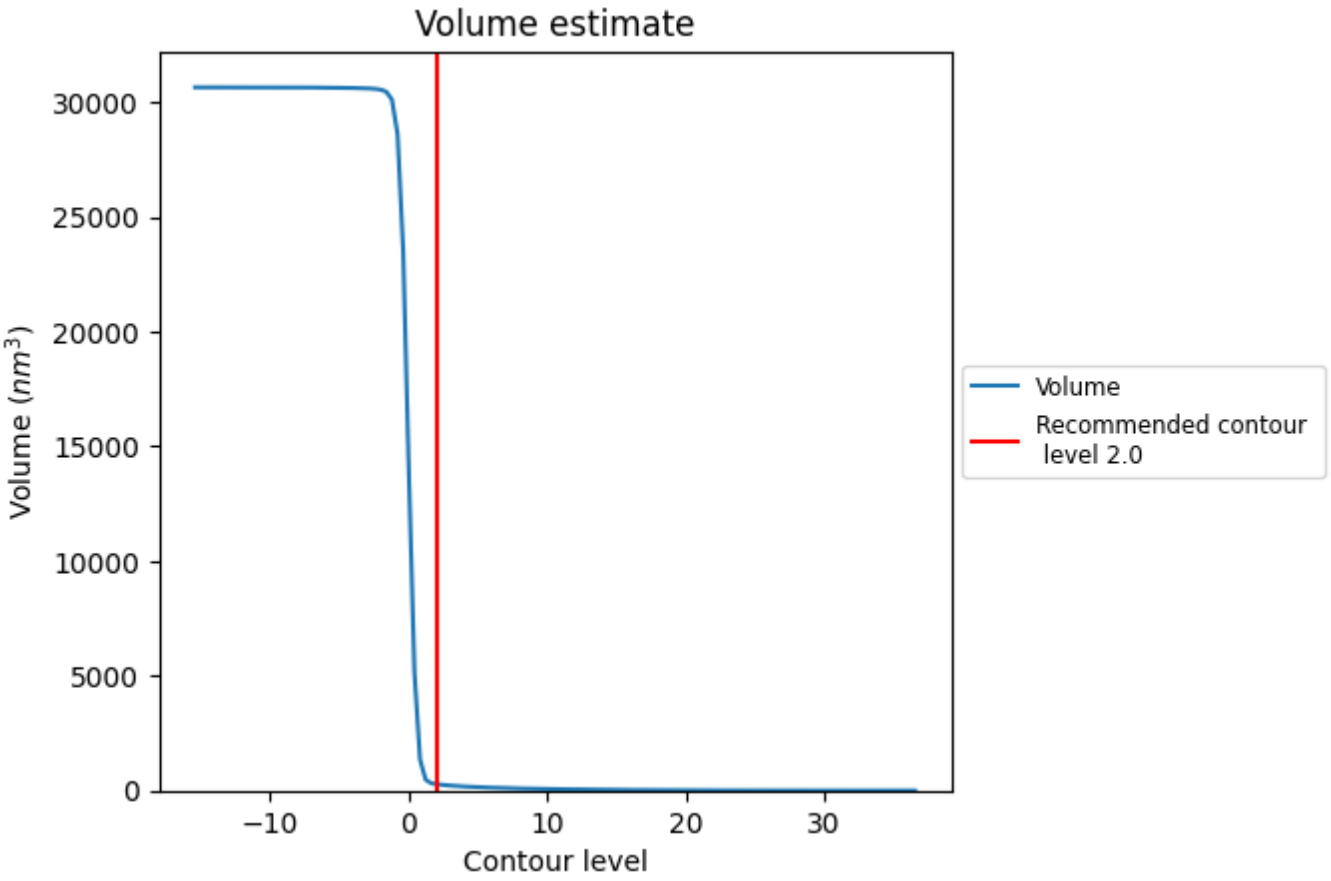
This section contains the results of statistical analysis of the map.

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.

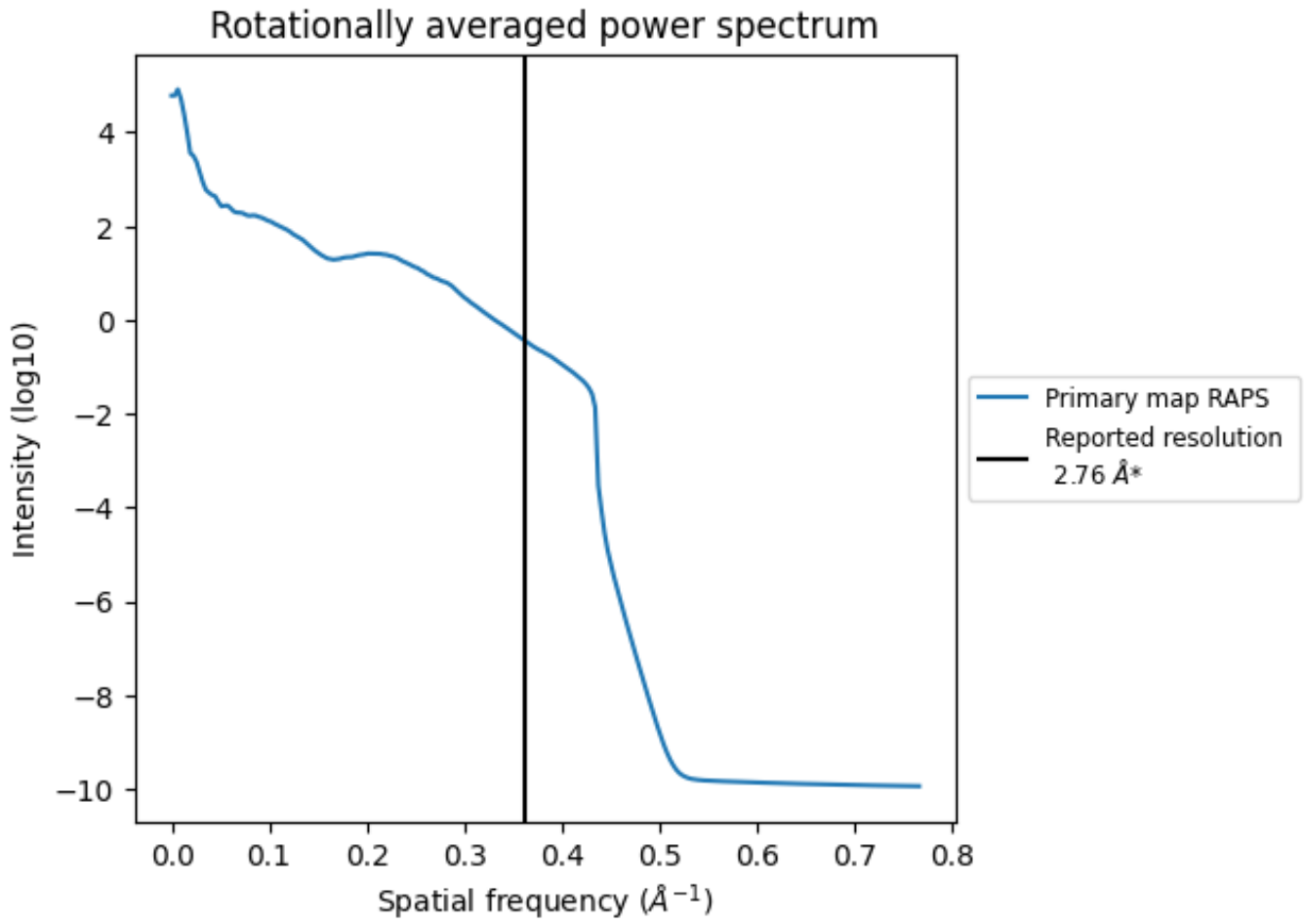
7.2 Volume estimate



The volume at the recommended contour level is 278 nm^3; this corresponds to an approximate mass of 251 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 0.362 Å^{-1}

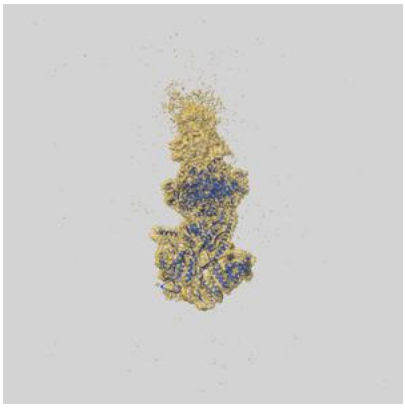
8 Fourier-Shell correlation (i)

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

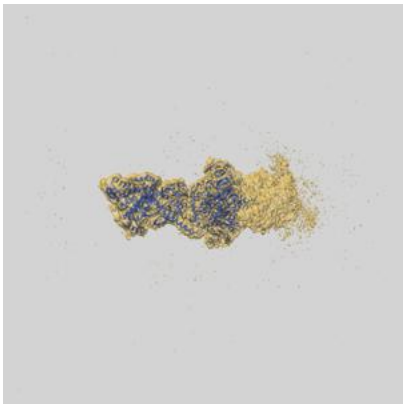
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16543 and PDB model 8CBK. Per-residue inclusion information can be found in section 3 on page 7.

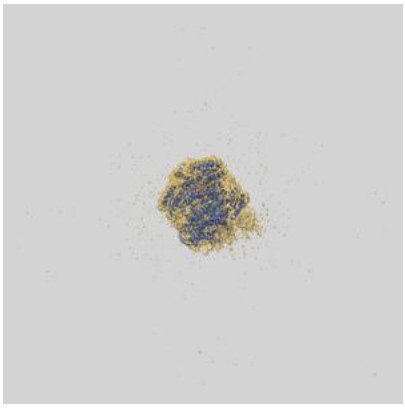
9.1 Map-model overlay



X



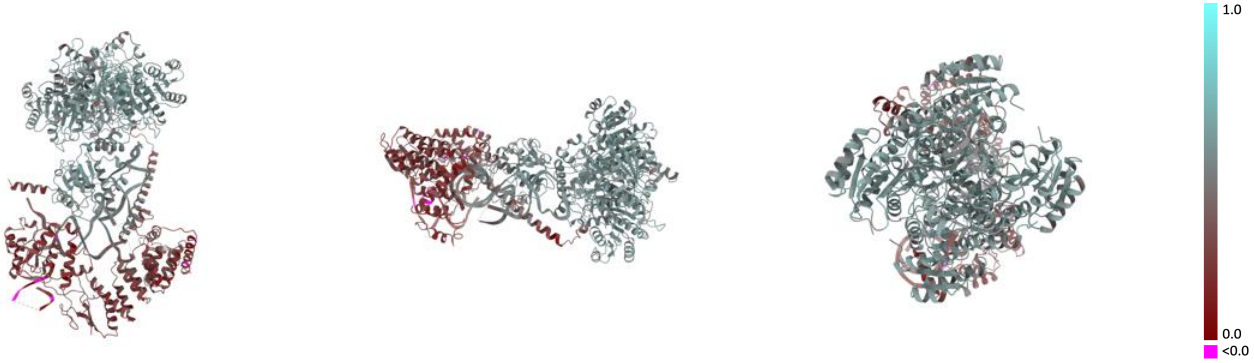
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 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

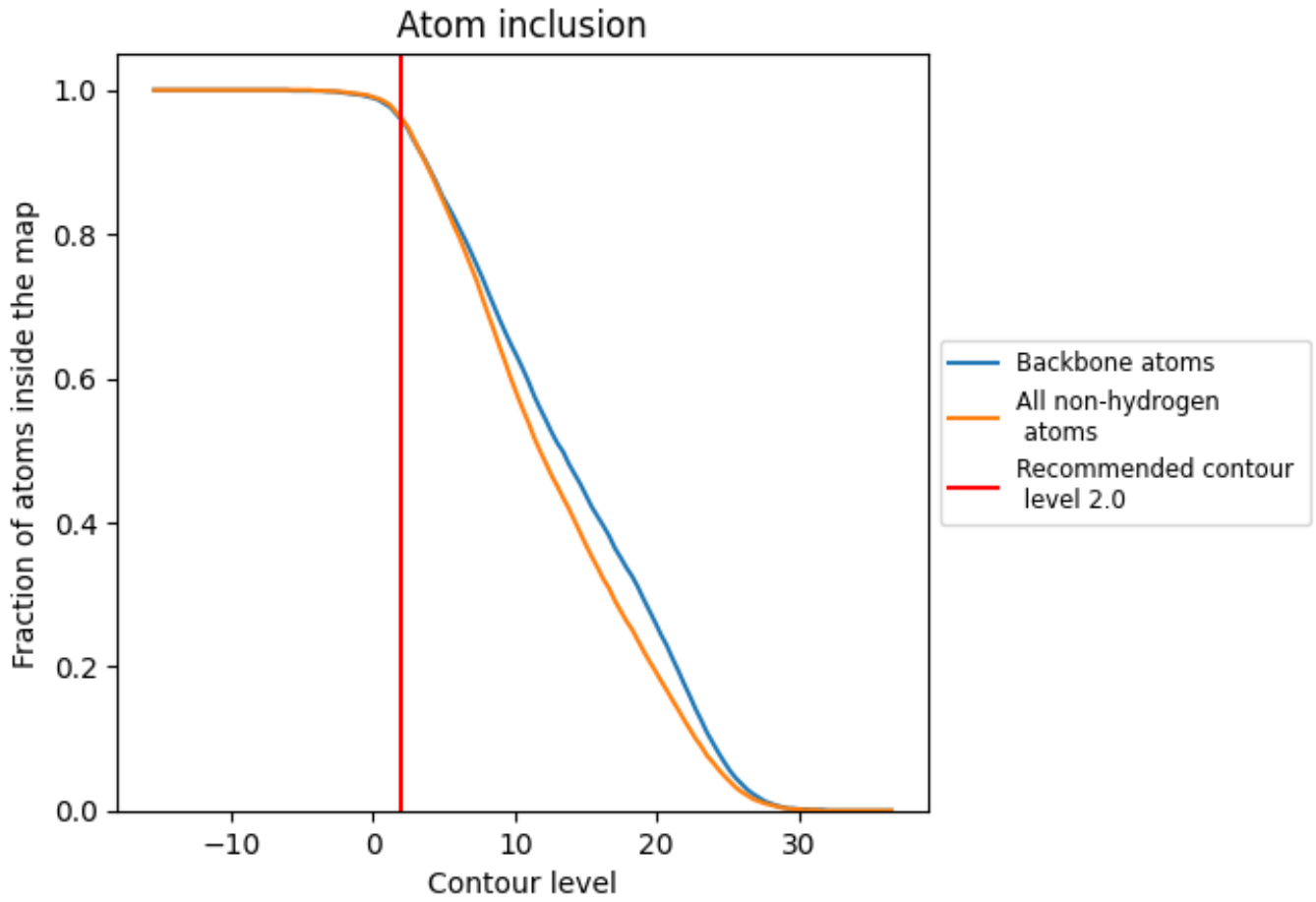
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.4520
A	0.9900	0.5640
B	0.9930	0.5580
C	0.9920	0.5630
D	0.9920	0.5630
E	0.9200	0.2620
F	0.9440	0.4570
T	0.9560	0.3870