Full wwPDB EM Validation Report ⓘ

Mar 19, 2024 – 03:48 PM JST

PDB ID	:	5ZR1
EMDB ID	:	EMD-6941
Title	:	Saccharomyces Cerevisiae Origin Recognition Complex Bound to a 72-bp Origin DNA containing ACS and B1 element
Authors	:	Li, N.; Lam, W.H.; Zhai, Y.; Cheng, J.; Cheng, E.; Zhao, Y.; Gao, N.; Tye, B.K.
Deposited on	:	2018-04-21
Resolution	:	3.00 Å(reported)

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

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

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

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

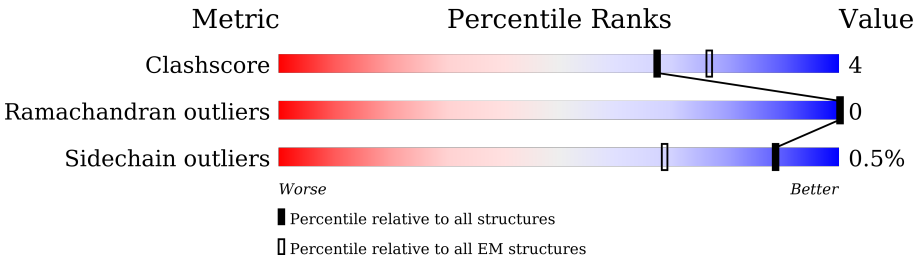
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	914	47% 7% 46%
2	B	620	51% 9% 40%
3	C	616	16% 83% 12% 5%
4	D	529	71% 12% 17%
5	E	479	13% 86% 10%
6	F	435	7% 34% 63%
7	G	72	54% 43%
8	H	72	57% 43%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 22260 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 Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	494	3958	2527	676	736	19	0	0

- Molecule 2 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	374	3041	1954	509	561	17	0	0

- Molecule 3 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	583	4822	3108	795	903	16	0	0

- Molecule 4 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	438	3572	2288	606	665	13	0	0

- Molecule 5 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	460	3758	2436	610	698	14	0	0

- Molecule 6 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	160	1335	858	225	240	12	0	0

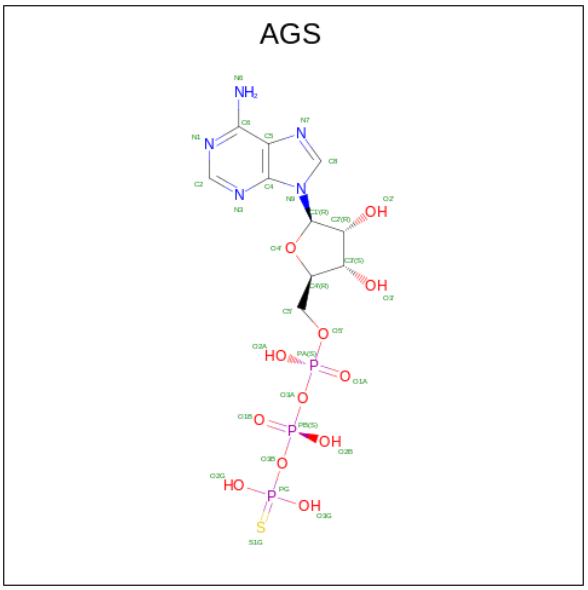
- Molecule 7 is a DNA chain called 72bp-oring DNA, ACS305, T-rich.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	41	Total	C	N	O	P	0	0
			831	407	118	266	40		

- Molecule 8 is a DNA chain called 72bp-oring DNA, ACS305, A-rich.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	41	Total	C	N	O	P	0	0
			847	404	178	224	41		

- Molecule 9 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
9	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	

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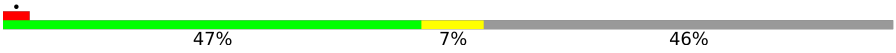
Mol	Chain	Residues	Atoms	AltConf
10	D	1	Total Mg 1 1	0
10	E	1	Total Mg 1 1	0

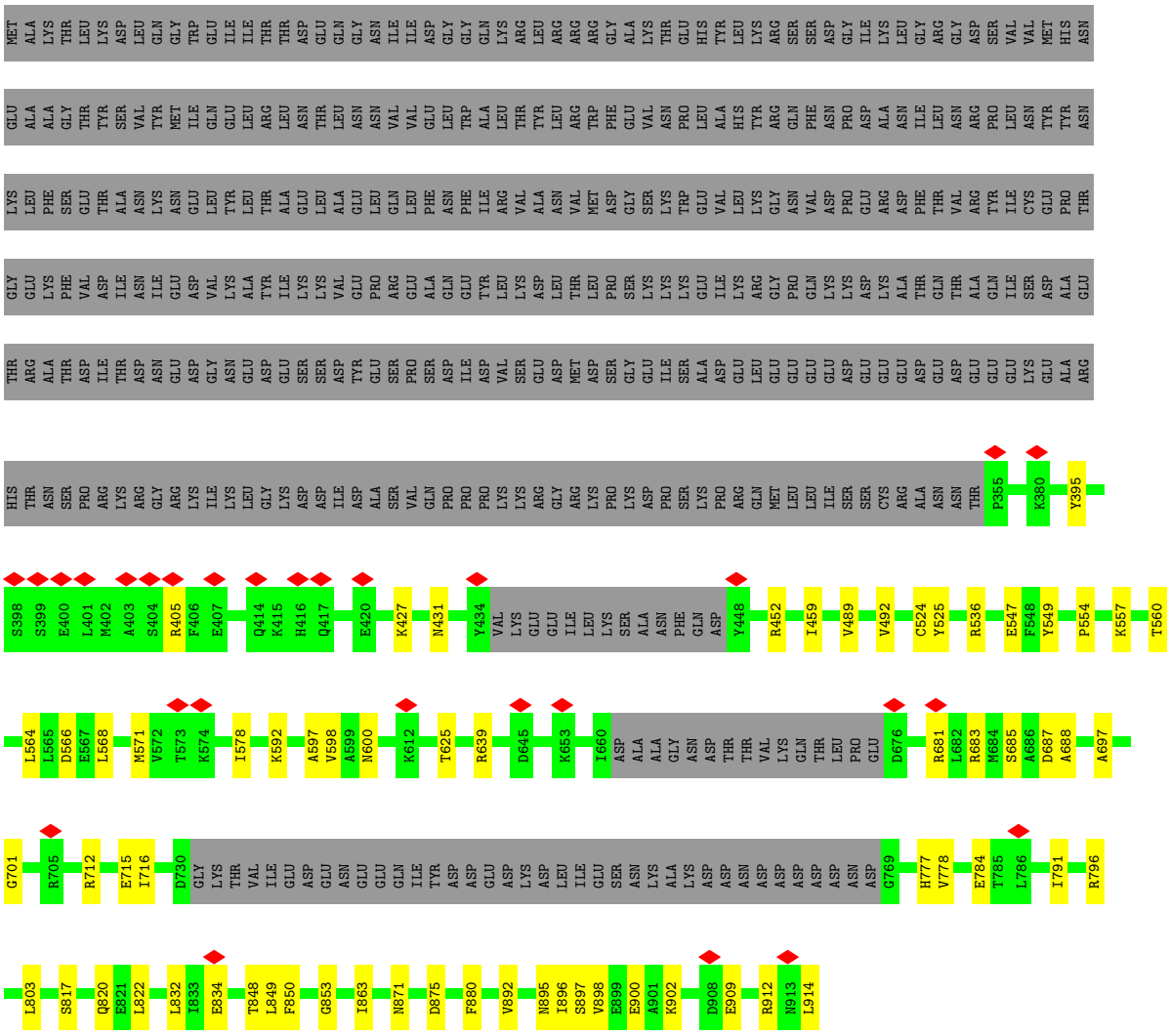
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Origin recognition complex subunit 1

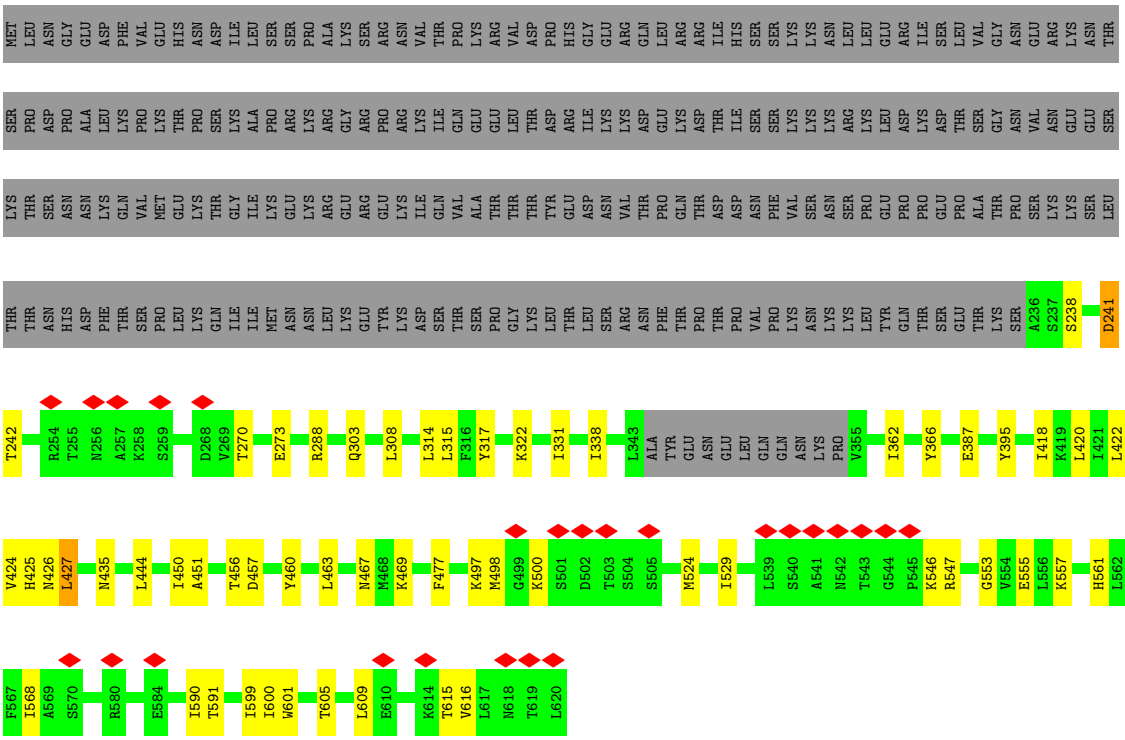
Chain A:





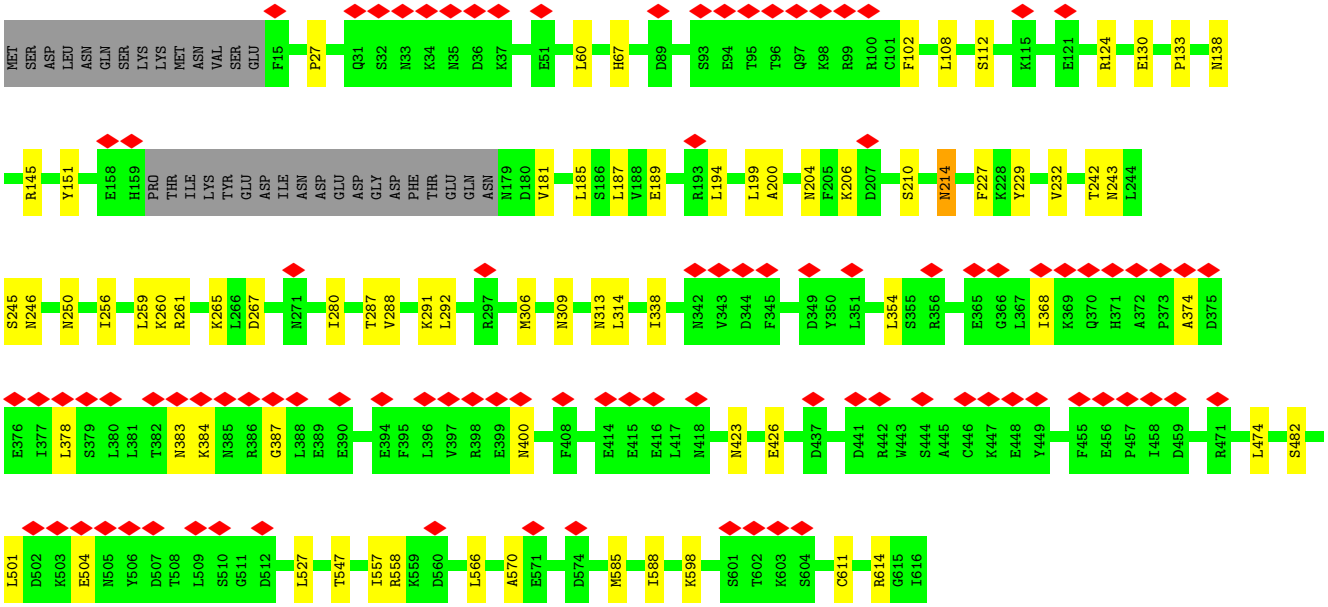
• Molecule 2: Origin recognition complex subunit 2

Chain B:



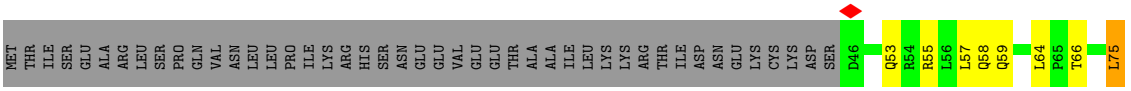
• Molecule 3: Origin recognition complex subunit 3

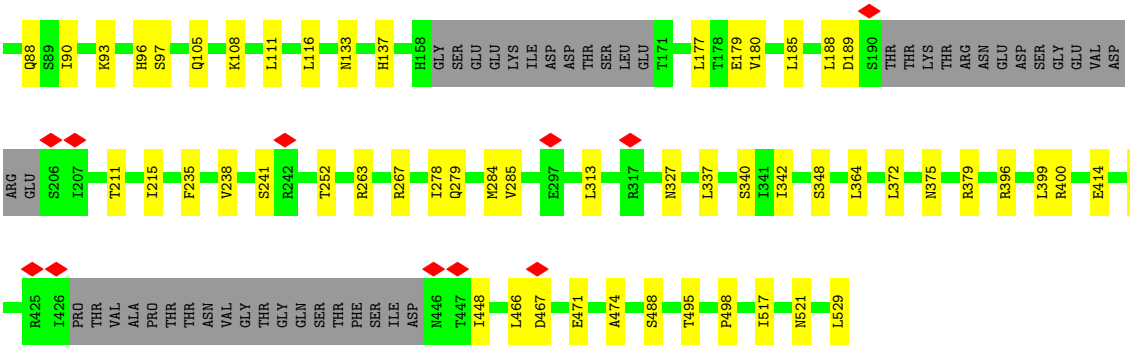
Chain C:



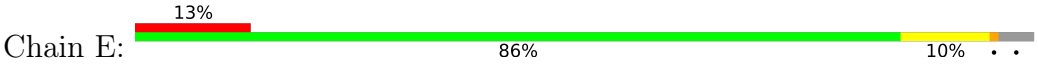
• Molecule 4: Origin recognition complex subunit 4

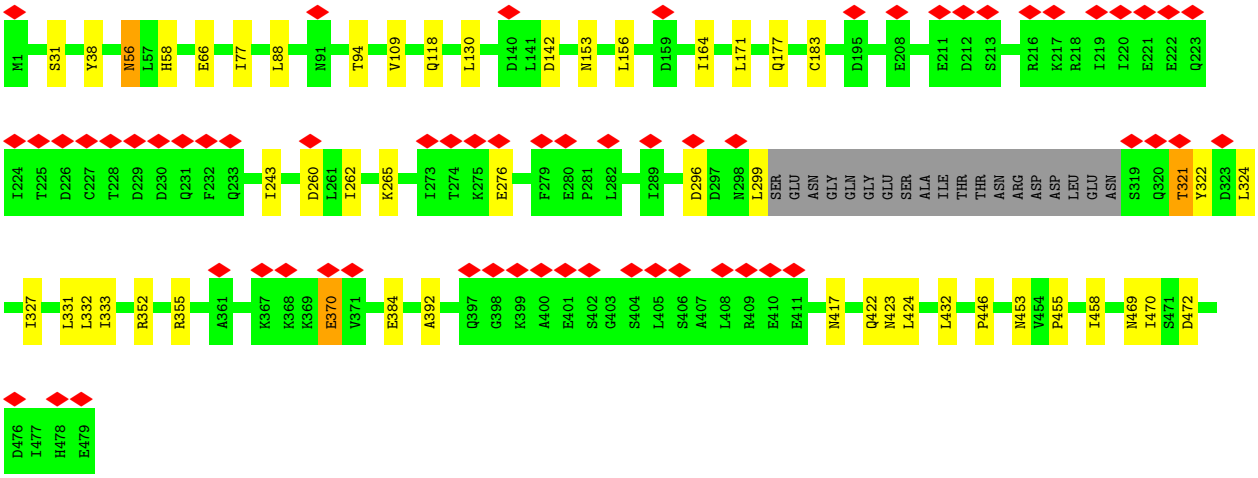
Chain D:



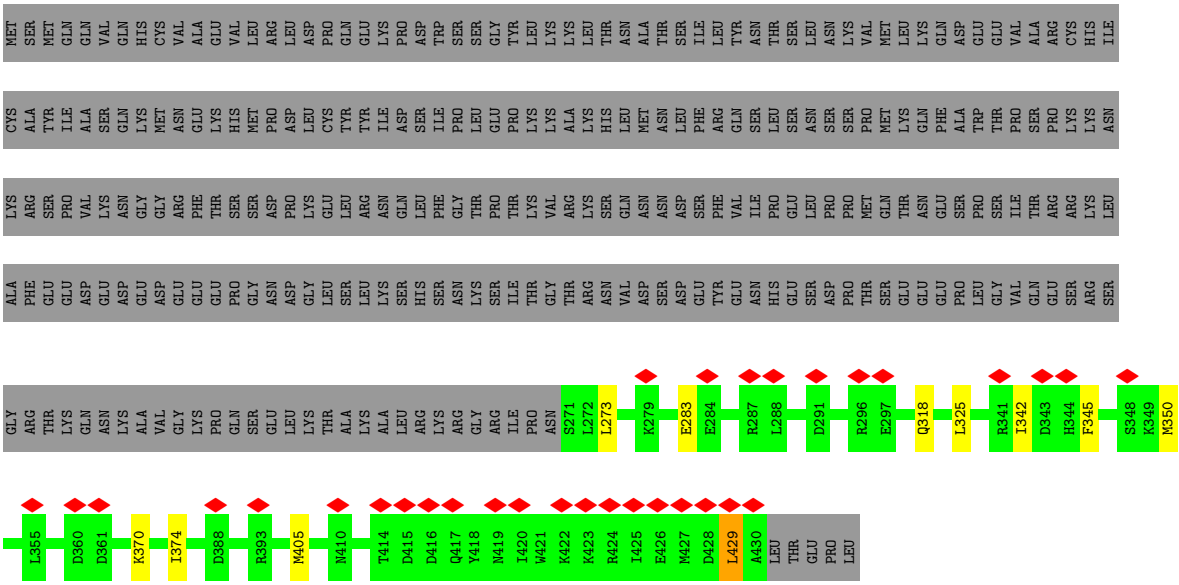


• Molecule 5: Origin recognition complex subunit 5



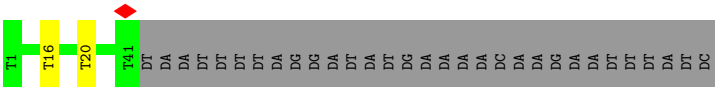


• Molecule 6: Origin recognition complex subunit 6



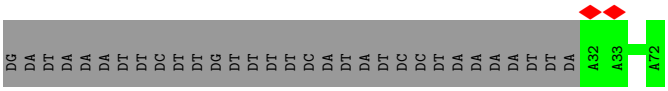
• Molecule 7: 72bp-oring DNA, ACS305, T-rich

Chain G:



• Molecule 8: 72bp-oring DNA, ACS305, A-rich

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	164857	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 ($e^-/Å^2$)	52.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.443	Depositor
Minimum map value	-0.200	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	269.312, 269.312, 269.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.32	0/4020	0.60	1/5407 (0.0%)
2	B	0.34	0/3107	0.62	4/4193 (0.1%)
3	C	0.33	0/4927	0.60	2/6652 (0.0%)
4	D	0.34	0/3634	0.59	2/4909 (0.0%)
5	E	0.36	0/3844	0.62	2/5217 (0.0%)
6	F	0.29	0/1357	0.62	1/1828 (0.1%)
7	G	0.73	0/923	1.19	0/1425
8	H	0.75	0/958	0.92	0/1474
All	All	0.38	0/22770	0.66	12/31105 (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	2
3	C	0	1
4	D	0	1
5	E	0	1
All	All	0	5

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	372	LEU	CA-CB-CG	10.05	138.42	115.30
2	B	422	LEU	CA-CB-CG	6.83	131.01	115.30
3	C	60	LEU	CA-CB-CG	6.41	130.04	115.30
1	A	849	LEU	CA-CB-CG	6.06	129.24	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	444	LEU	CA-CB-CG	5.96	129.00	115.30
5	E	370	GLU	CA-CB-CG	5.89	126.37	113.40
2	B	314	LEU	CA-CB-CG	5.71	128.44	115.30
4	D	75	LEU	CA-CB-CG	5.60	128.18	115.30
5	E	331	LEU	CA-CB-CG	5.47	127.88	115.30
6	F	429	LEU	CA-CB-CG	5.29	127.46	115.30
2	B	427	LEU	CA-CB-CG	5.20	127.27	115.30
3	C	194	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	241	ASP	Peptide
2	B	387	GLU	Peptide
3	C	242	THR	Peptide
4	D	66	THR	Peptide
5	E	171	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	3958	0	4070	37	0
2	B	3041	0	3042	34	0
3	C	4822	0	4776	48	0
4	D	3572	0	3632	38	0
5	E	3758	0	3787	32	0
6	F	1335	0	1372	7	0
7	G	831	0	480	2	0
8	H	847	0	457	0	0
9	A	31	0	12	1	0
9	D	31	0	12	2	0
9	E	31	0	12	1	0
10	A	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22260	0	21652	169	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 4.

All (169) 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)
3:C:598:LYS:HG2	5:E:446:PRO:HB3	1.71	0.72
4:D:90:ILE:HA	4:D:211:THR:HG21	1.75	0.68
1:A:897:SER:HB2	1:A:900:GLU:HG2	1.76	0.68
2:B:546:LYS:HG3	7:G:20:DT:H5"	1.76	0.67
3:C:378:LEU:HD11	3:C:383:ASN:HD22	1.61	0.66
1:A:681:ARG:HH12	1:A:683:ARG:HE	1.46	0.64
4:D:108:LYS:NZ	9:D:2001:AGS:S1G	2.72	0.63
1:A:536:ARG:NH2	4:D:179:GLU:OE2	2.32	0.63
2:B:590:ILE:HG12	2:B:600:ILE:HG22	1.80	0.63
3:C:384:LYS:HG3	3:C:387:GLY:H	1.64	0.62
2:B:288:ARG:HH21	3:C:504:GLU:HG2	1.63	0.61
4:D:59:GLN:HG2	4:D:64:LEU:HD11	1.83	0.61
5:E:455:PRO:HD2	5:E:458:ILE:HD12	1.82	0.61
3:C:199:LEU:HB3	3:C:232:VAL:HG12	1.82	0.60
4:D:396:ARG:NH1	4:D:414:GLU:OE2	2.36	0.59
3:C:181:VAL:HG11	3:C:187:LEU:HD13	1.83	0.59
3:C:309:ASN:O	3:C:313:ASN:ND2	2.35	0.59
6:F:325:LEU:HD11	6:F:350:MET:HG2	1.85	0.59
4:D:517:ILE:HG23	4:D:521:ASN:HD22	1.68	0.58
3:C:291:LYS:HD3	3:C:338:ILE:HD12	1.84	0.58
1:A:431:ASN:O	1:A:639:ARG:NH1	2.36	0.58
3:C:288:VAL:HB	3:C:292:LEU:HB2	1.86	0.58
1:A:600:ASN:OD1	4:D:263:ARG:NH1	2.36	0.58
3:C:145:ARG:NH2	7:G:16:DT:OP1	2.32	0.58
4:D:379:ARG:NH1	4:D:466:LEU:O	2.36	0.58
4:D:90:ILE:O	4:D:93:LYS:NZ	2.36	0.57
2:B:615:THR:HG23	2:B:616:VAL:HG23	1.85	0.57
3:C:256:ILE:HG23	5:E:299:LEU:HD22	1.86	0.57
1:A:452:ARG:NH1	1:A:625:THR:O	2.38	0.57
2:B:529:ILE:HG23	2:B:609:LEU:HG	1.87	0.57
2:B:524:MET:HB2	2:B:568:ILE:HG21	1.86	0.57
2:B:395:TYR:O	3:C:145:ARG:NH1	2.38	0.56
1:A:796:ARG:HD2	4:D:279:GLN:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:THR:HG22	2:B:601:TRP:HE1	1.69	0.56
4:D:57:LEU:HD11	4:D:342:ILE:HG23	1.88	0.56
1:A:571:MET:HB3	1:A:578:ILE:HD13	1.88	0.56
1:A:560:THR:HG22	1:A:592:LYS:HB3	1.86	0.56
4:D:75:LEU:HD12	4:D:111:LEU:HD11	1.88	0.56
2:B:241:ASP:OD2	3:C:614:ARG:NH2	2.38	0.55
4:D:379:ARG:HH12	4:D:467:ASP:HB2	1.71	0.55
3:C:501:LEU:HD13	3:C:504:GLU:HB2	1.88	0.55
9:E:2001:AGS:H5'1	9:E:2001:AGS:H8	1.87	0.55
4:D:185:LEU:O	4:D:189:ASP:N	2.39	0.55
1:A:568:LEU:HD22	1:A:597:ALA:HB1	1.90	0.54
5:E:56:ASN:OD1	5:E:56:ASN:N	2.32	0.54
3:C:474:LEU:HD21	6:F:405:MET:HG2	1.89	0.54
1:A:554:PRO:HD2	1:A:557:LYS:HD2	1.91	0.53
2:B:460:TYR:OH	5:E:384:GLU:OE1	2.25	0.53
1:A:871:ASN:ND2	5:E:177:GLN:O	2.41	0.53
2:B:467:ASN:HA	5:E:422:GLN:HE21	1.74	0.53
5:E:94:THR:OG1	5:E:118:GLN:NE2	2.41	0.53
5:E:352:ARG:NH2	5:E:392:ALA:O	2.41	0.53
1:A:909:GLU:OE1	1:A:912:ARG:NH1	2.42	0.53
2:B:366:TYR:HB3	2:B:426:ASN:HD22	1.74	0.52
3:C:185:LEU:HB3	5:E:66:GLU:HB2	1.91	0.52
4:D:340:SER:HB3	4:D:364:LEU:HD22	1.91	0.52
2:B:238:SER:OG	5:E:355:ARG:NH1	2.43	0.52
2:B:498:MET:HG2	3:C:585:MET:HB2	1.92	0.52
1:A:832:LEU:HD21	1:A:914:LEU:HD13	1.91	0.52
1:A:898:VAL:HG12	1:A:902:LYS:HE2	1.90	0.52
2:B:424:VAL:HG11	2:B:427:LEU:HD23	1.92	0.51
4:D:471:GLU:HB3	4:D:474:ALA:HB2	1.92	0.51
3:C:482:SER:HA	5:E:417:ASN:HA	1.92	0.51
2:B:362:ILE:HD12	2:B:425:HIS:HE1	1.76	0.51
4:D:399:LEU:HD23	4:D:529:LEU:HD13	1.94	0.50
2:B:555:GLU:HA	2:B:599:ILE:HA	1.94	0.50
3:C:368:ILE:HD11	6:F:429:LEU:HD12	1.92	0.50
4:D:97:SER:HB3	4:D:238:VAL:HG21	1.93	0.50
3:C:423:ASN:HB2	3:C:426:GLU:HG2	1.94	0.50
5:E:130:LEU:HD22	5:E:164:ILE:HD11	1.91	0.50
3:C:102:PHE:HE2	3:C:259:LEU:HD23	1.76	0.50
1:A:395:TYR:HH	1:A:549:TYR:HH	1.53	0.50
4:D:400:ARG:NH1	4:D:414:GLU:OE1	2.45	0.49
3:C:102:PHE:HD1	3:C:227:PHE:HZ	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:379:ARG:NH1	5:E:38:TYR:OH	2.45	0.49
4:D:422:ILE:HG21	4:D:448:ILE:HD12	1.95	0.49
3:C:112:SER:OG	3:C:206:LYS:O	2.30	0.49
4:D:177:LEU:HA	4:D:180:VAL:HG12	1.94	0.49
9:D:2001:AGS:O2G	9:D:2001:AGS:O2B	2.30	0.49
3:C:246:ASN:O	3:C:250:ASN:ND2	2.46	0.49
2:B:547:ARG:HA	2:B:605:THR:HA	1.95	0.48
6:F:273:LEU:HD12	6:F:318:GLN:HG2	1.96	0.48
1:A:524:CYS:SG	1:A:525:TYR:N	2.87	0.48
3:C:108:LEU:HB2	3:C:267:ASP:HA	1.96	0.48
1:A:716:ILE:HG22	1:A:777:HIS:HD2	1.79	0.47
3:C:260:LYS:NZ	5:E:296:ASP:O	2.47	0.47
1:A:688:ALA:HB1	1:A:778:VAL:HG21	1.95	0.47
3:C:124:ARG:HH11	3:C:200:ALA:HB2	1.78	0.47
1:A:896:ILE:HG13	1:A:897:SER:H	1.78	0.47
3:C:243:ASN:ND2	5:E:321:THR:HG23	2.29	0.47
5:E:322:TYR:HB3	5:E:324:LEU:HG	1.96	0.47
5:E:77:ILE:HG12	5:E:130:LEU:HD21	1.97	0.47
1:A:685:SER:OG	1:A:687:ASP:OD1	2.27	0.46
5:E:333:ILE:HG23	5:E:470:ILE:HD12	1.97	0.46
2:B:463:LEU:HD11	5:E:424:LEU:HD22	1.97	0.46
1:A:427:LYS:HD3	1:A:715:GLU:HB3	1.96	0.46
4:D:188:LEU:O	4:D:241:SER:OG	2.23	0.46
4:D:285:VAL:HG13	4:D:313:LEU:HD22	1.97	0.46
4:D:498:PRO:HD3	5:E:453:ASN:HB2	1.97	0.46
1:A:566:ASP:HA	1:A:598:VAL:HG13	1.98	0.46
6:F:370:LYS:HE3	6:F:374:ILE:HD13	1.98	0.46
1:A:697:ALA:HA	1:A:701:GLY:HA2	1.96	0.46
4:D:53:GLN:NE2	4:D:348:SER:O	2.49	0.46
4:D:88:GLN:HG3	4:D:96:HIS:HE1	1.81	0.46
1:A:848:THR:HA	1:A:853:GLY:H	1.80	0.45
2:B:497:LYS:O	2:B:500:LYS:NZ	2.37	0.45
1:A:875:ASP:HB3	4:D:252:THR:HG21	1.99	0.45
2:B:241:ASP:O	2:B:242:THR:OG1	2.33	0.45
5:E:58:HIS:CE1	5:E:88:LEU:HD11	2.52	0.45
3:C:243:ASN:HD21	3:C:245:SER:HB2	1.82	0.45
4:D:116:LEU:HD11	4:D:215:ILE:HD11	1.99	0.45
2:B:270:THR:HB	2:B:273:GLU:HG2	1.98	0.45
2:B:553:GLY:HA3	2:B:601:TRP:HB3	1.98	0.45
3:C:130:GLU:HG2	3:C:204:ASN:HB3	1.99	0.45
3:C:67:HIS:CD2	3:C:287:THR:HG22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:375:ASN:O	4:D:379:ARG:NH2	2.49	0.44
1:A:817:SER:OG	1:A:820:GLN:OE1	2.35	0.44
9:A:2001:AGS:O3G	9:A:2001:AGS:O2B	2.35	0.44
1:A:459:ILE:HG22	1:A:492:VAL:HG11	1.99	0.44
2:B:563:CYS:HB2	2:B:568:ILE:HB	2.00	0.44
1:A:712:ARG:NE	1:A:784:GLU:OE2	2.50	0.44
2:B:322:LYS:NZ	2:B:457:ASP:OD1	2.39	0.43
3:C:598:LYS:HG3	3:C:611:CYS:SG	2.57	0.43
3:C:558:ARG:NH2	3:C:570:ALA:O	2.51	0.43
2:B:420:LEU:HB3	2:B:450:ILE:HG22	2.00	0.43
5:E:109:VAL:HG13	5:E:156:LEU:HD12	1.99	0.43
4:D:278:ILE:HG21	4:D:284:MET:HG3	2.00	0.43
4:D:327:ASN:ND2	4:D:337:LEU:HB2	2.34	0.43
2:B:315:LEU:HD11	2:B:456:THR:HG23	2.00	0.43
3:C:151:TYR:HB2	3:C:187:LEU:HD21	2.01	0.43
3:C:189:GLU:HB3	3:C:229:TYR:CZ	2.53	0.43
3:C:138:ASN:HD22	4:D:488:SER:HB2	1.84	0.42
1:A:822:LEU:HD13	1:A:892:VAL:HG21	2.00	0.42
4:D:235:PHE:HB3	4:D:267:ARG:HB3	2.01	0.42
5:E:31:SER:OG	5:E:153:ASN:ND2	2.51	0.42
3:C:261:ARG:NH2	5:E:260:ASP:OD1	2.41	0.42
6:F:342:ILE:HA	6:F:345:PHE:HB3	2.01	0.42
1:A:547:GLU:OE2	2:B:561:HIS:NE2	2.37	0.42
3:C:133:PRO:HG3	3:C:210:SER:HB2	2.01	0.42
3:C:280:ILE:HD12	3:C:314:LEU:HD22	2.01	0.42
5:E:332:LEU:HD11	5:E:432:LEU:HD13	2.02	0.42
5:E:469:ASN:ND2	5:E:472:ASP:OD2	2.53	0.42
1:A:489:VAL:HG11	1:A:564:LEU:HD13	2.02	0.42
3:C:557:ILE:HD11	3:C:566:LEU:HD11	2.00	0.42
4:D:55:ARG:HA	4:D:58:GLN:HG2	2.01	0.42
4:D:105:GLN:HG3	5:E:183:CYS:HB2	2.02	0.42
1:A:850:PHE:HE1	1:A:863:ILE:HG22	1.84	0.41
2:B:557:LYS:O	2:B:561:HIS:ND1	2.53	0.41
1:A:791:ILE:HD11	1:A:900:GLU:HB2	2.02	0.41
3:C:108:LEU:HD11	3:C:265:LYS:HE2	2.03	0.41
3:C:374:ALA:HB1	6:F:429:LEU:HD23	2.02	0.41
4:D:133:ASN:H	4:D:137:HIS:HD2	1.69	0.41
5:E:142:ASP:N	5:E:142:ASP:OD1	2.53	0.41
5:E:243:ILE:HD11	5:E:265:LYS:HD2	2.02	0.41
3:C:585:MET:HA	3:C:588:ILE:HG22	2.03	0.41
1:A:880:PHE:HB2	1:A:895:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:ARG:HH12	1:A:683:ARG:NE	2.15	0.41
1:A:803:LEU:HD11	1:A:832:LEU:HD22	2.02	0.41
2:B:317:TYR:HE1	2:B:477:PHE:HB3	1.85	0.41
2:B:435:ASN:OD1	2:B:469:LYS:NZ	2.46	0.41
3:C:306:MET:O	3:C:313:ASN:ND2	2.54	0.41
3:C:527:LEU:HD21	3:C:547:THR:HG21	2.02	0.40
5:E:243:ILE:HG21	5:E:262:ILE:HG12	2.03	0.40
5:E:327:ILE:HD11	5:E:423:ASN:HD22	1.86	0.40
3:C:214:ASN:HB2	4:D:495:THR:HG23	2.03	0.40
2:B:308:LEU:HD22	2:B:451:ALA:HB1	2.03	0.40
2:B:331:ILE:HG23	3:C:27:PRO:HB3	2.04	0.40
2:B:338:ILE:HG21	2:B:418:ILE:HB	2.02	0.40
3:C:67:HIS:HD2	3:C:287:THR:HG22	1.87	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	486/914 (53%)	469 (96%)	17 (4%)	0	100	100
2	B	370/620 (60%)	346 (94%)	24 (6%)	0	100	100
3	C	579/616 (94%)	555 (96%)	24 (4%)	0	100	100
4	D	430/529 (81%)	416 (97%)	14 (3%)	0	100	100
5	E	456/479 (95%)	435 (95%)	21 (5%)	0	100	100
6	F	158/435 (36%)	151 (96%)	7 (4%)	0	100	100
All	All	2479/3593 (69%)	2372 (96%)	107 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	438/813 (54%)	436 (100%)	2 (0%)	88 96
2	B	340/573 (59%)	339 (100%)	1 (0%)	92 97
3	C	544/576 (94%)	541 (99%)	3 (1%)	86 95
4	D	405/488 (83%)	405 (100%)	0	100 100
5	E	424/440 (96%)	420 (99%)	4 (1%)	78 92
6	F	153/406 (38%)	152 (99%)	1 (1%)	84 94
All	All	2304/3296 (70%)	2293 (100%)	11 (0%)	89 96

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	ARG
1	A	834	GLU
2	B	303	GLN
3	C	214	ASN
3	C	354	LEU
3	C	400	ASN
5	E	56	ASN
5	E	276	GLU
5	E	321	THR
5	E	370	GLU
6	F	283	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	836	ASN
1	A	895	ASN
1	A	906	ASN
2	B	310	GLN
2	B	364	ASN
2	B	425	HIS

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Mol	Chain	Res	Type
2	B	426	ASN
2	B	467	ASN
2	B	478	HIS
2	B	538	ASN
2	B	585	HIS
3	C	53	ASN
3	C	62	HIS
3	C	67	HIS
3	C	214	ASN
3	C	239	ASN
3	C	246	ASN
3	C	250	ASN
3	C	312	HIS
3	C	313	ASN
3	C	383	ASN
3	C	400	ASN
3	C	429	HIS
3	C	536	ASN
4	D	105	GLN
4	D	126	GLN
4	D	137	HIS
4	D	233	ASN
4	D	240	HIS
4	D	371	GLN
4	D	521	ASN
5	E	32	ASN
5	E	58	HIS
5	E	118	GLN
5	E	163	ASN
5	E	253	ASN
5	E	391	GLN
5	E	422	GLN
5	E	423	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
9	AGS	E	2001	10	26,33,33	0.83	0	26,52,52	0.94	2 (7%)
9	AGS	D	2001	10	26,33,33	0.73	0	26,52,52	1.12	2 (7%)
9	AGS	A	2001	10	26,33,33	0.78	0	26,52,52	1.05	2 (7%)

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
9	AGS	E	2001	10	-	4/17/38/38	0/3/3/3
9	AGS	D	2001	10	-	4/17/38/38	0/3/3/3
9	AGS	A	2001	10	-	7/17/38/38	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	2001	AGS	PA-O3A-PB	-4.17	118.50	132.83
9	A	2001	AGS	PA-O3A-PB	-3.55	120.64	132.83
9	E	2001	AGS	PA-O3A-PB	-2.79	123.24	132.83
9	E	2001	AGS	C5-C6-N6	2.30	123.84	120.35
9	A	2001	AGS	C5-C6-N6	2.27	123.81	120.35
9	D	2001	AGS	C5-C6-N6	2.27	123.81	120.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	2001	AGS	C5'-O5'-PA-O1A
9	A	2001	AGS	C5'-O5'-PA-O2A
9	D	2001	AGS	O4'-C4'-C5'-O5'
9	D	2001	AGS	C3'-C4'-C5'-O5'
9	E	2001	AGS	PB-O3B-PG-O2G
9	E	2001	AGS	PB-O3B-PG-O3G
9	A	2001	AGS	O4'-C4'-C5'-O5'
9	E	2001	AGS	O4'-C4'-C5'-O5'
9	E	2001	AGS	PG-O3B-PB-O1B
9	A	2001	AGS	C3'-C4'-C5'-O5'
9	A	2001	AGS	C5'-O5'-PA-O3A
9	D	2001	AGS	PA-O3A-PB-O2B
9	A	2001	AGS	PG-O3B-PB-O2B
9	A	2001	AGS	PA-O3A-PB-O2B
9	D	2001	AGS	PA-O3A-PB-O1B

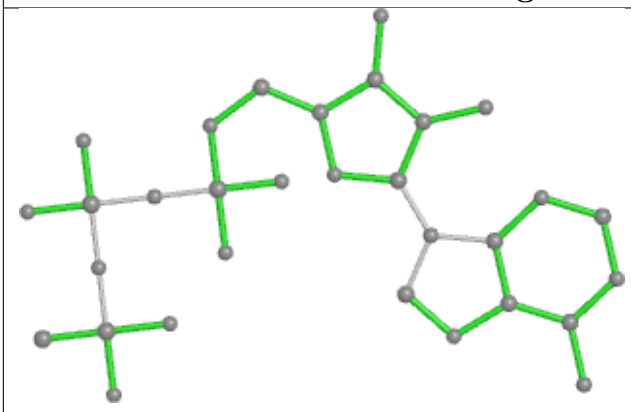
There are no ring outliers.

3 monomers are involved in 4 short contacts:

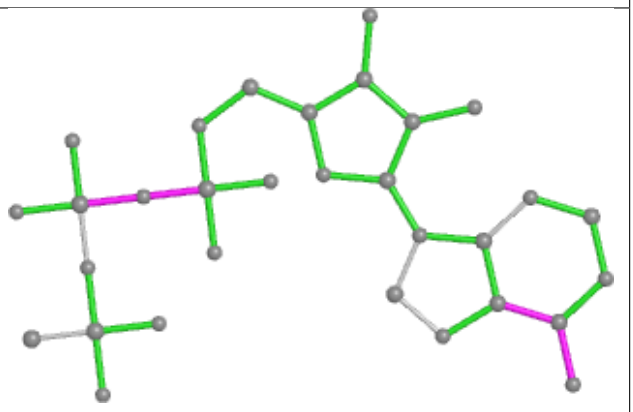
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	2001	AGS	1	0
9	D	2001	AGS	2	0
9	A	2001	AGS	1	0

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.

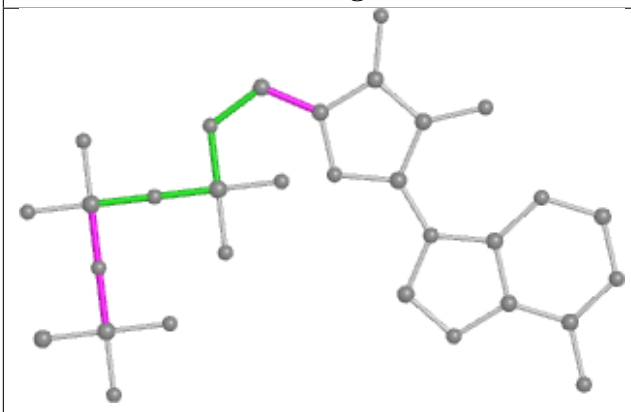
Ligand AGS E 2001



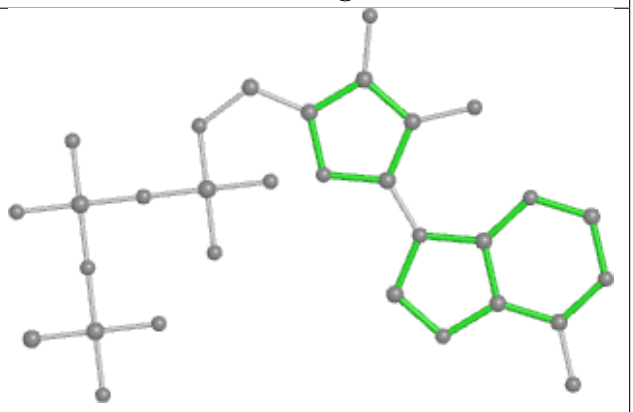
Bond lengths



Bond angles

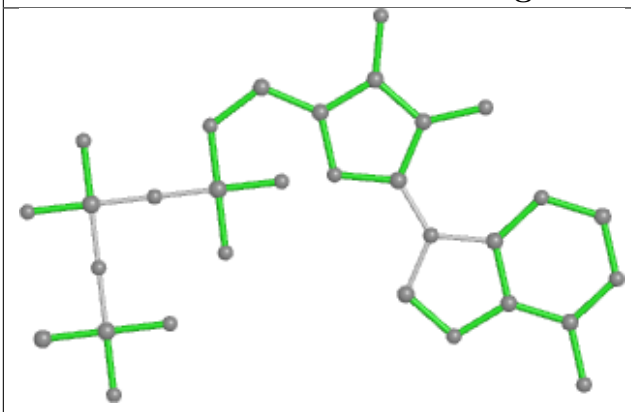


Torsions

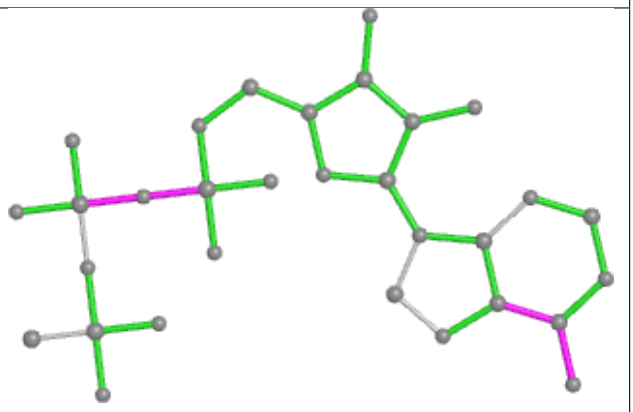


Rings

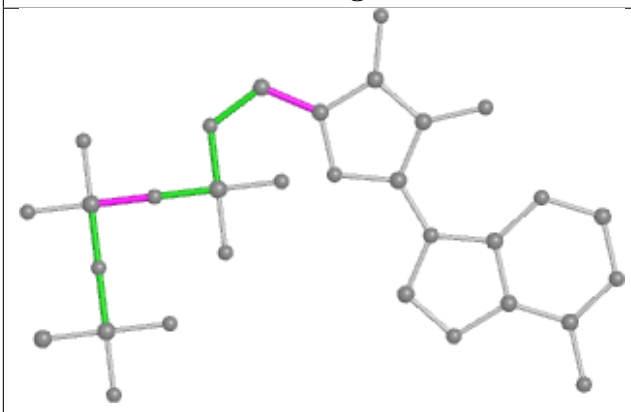
Ligand AGS D 2001



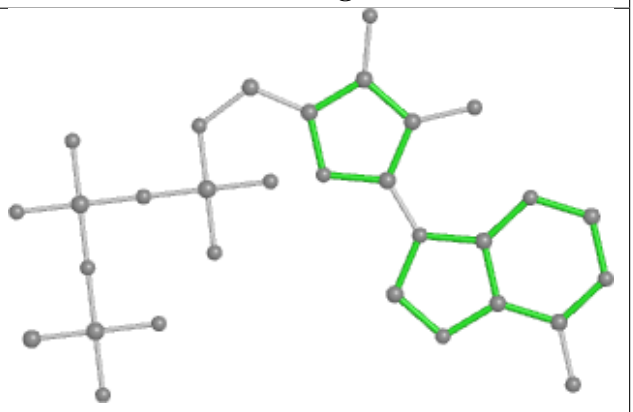
Bond lengths



Bond angles

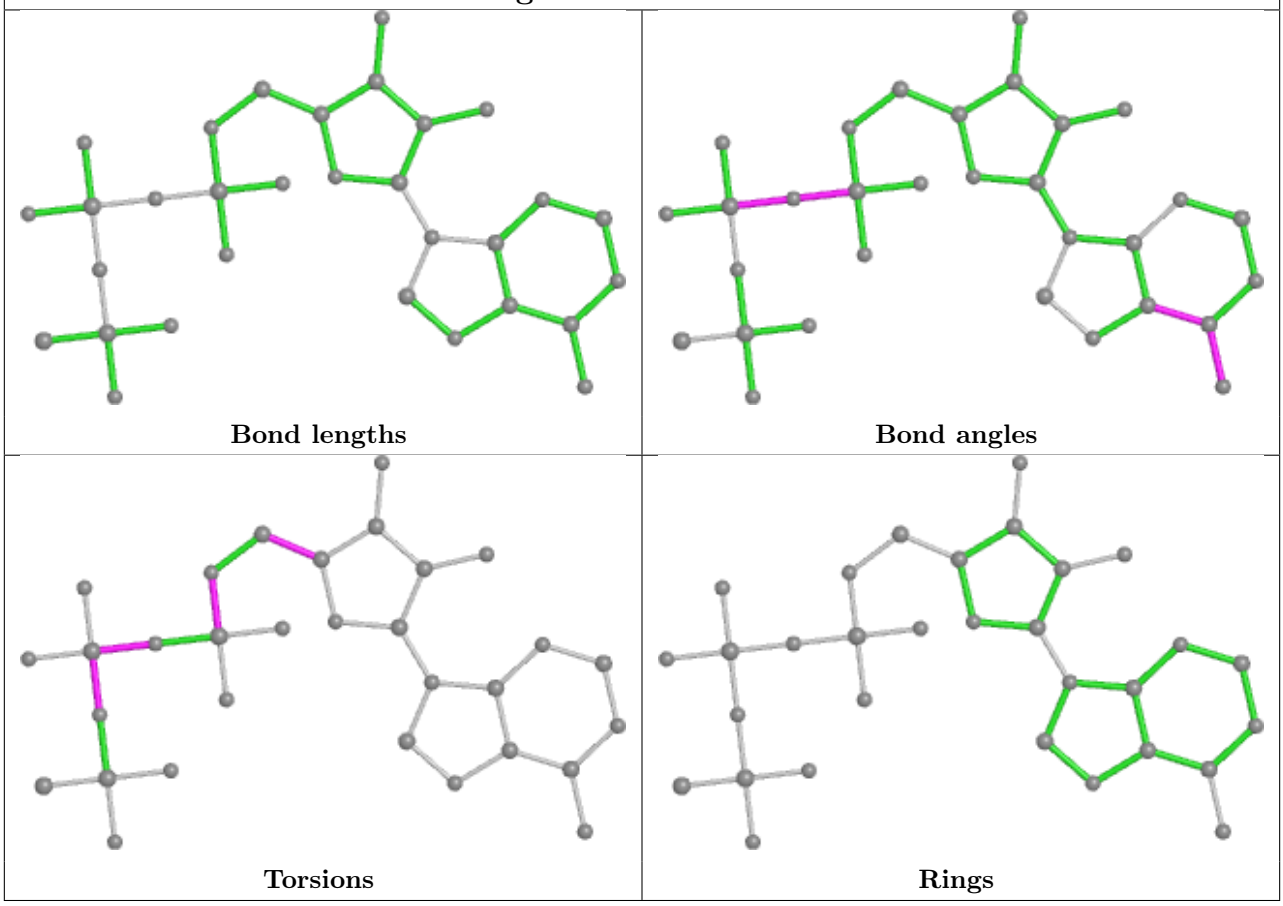


Torsions



Rings

Ligand AGS A 2001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

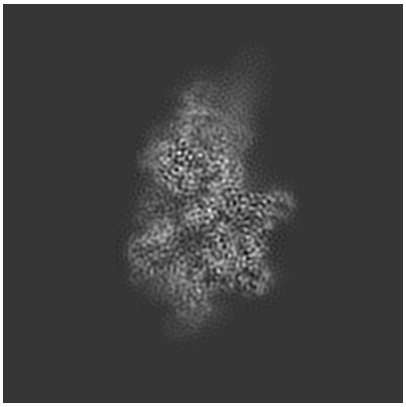
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6941. These allow visual inspection of the internal detail of the map and identification of artifacts.

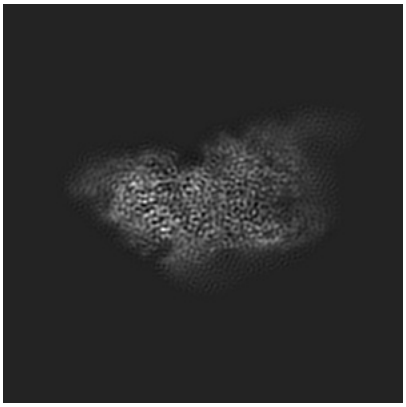
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

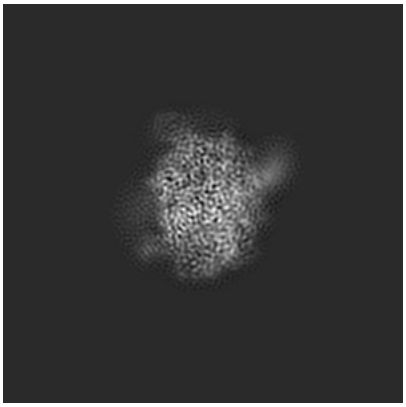
6.1.1 Primary map



X



Y

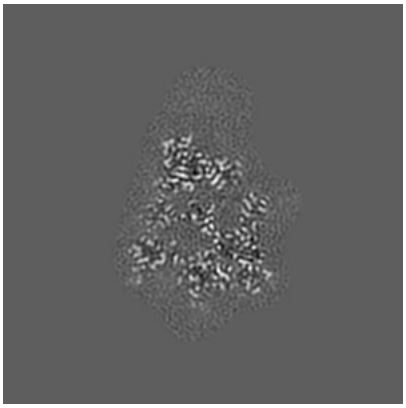


Z

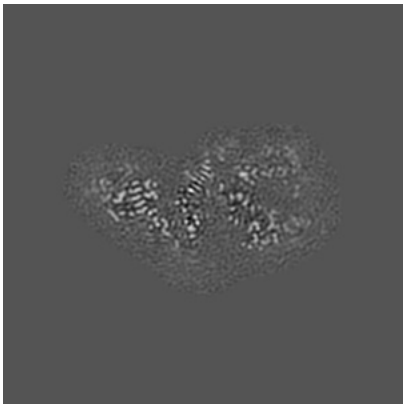
The images above show the map projected in three orthogonal directions.

6.2 Central slices

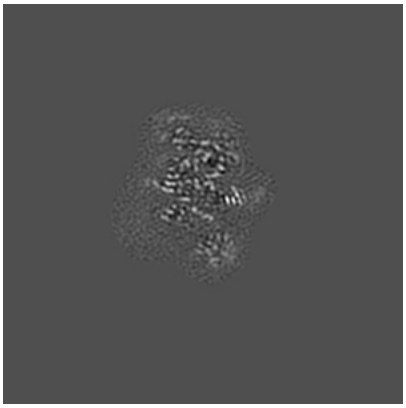
6.2.1 Primary map



X Index: 128



Y Index: 128

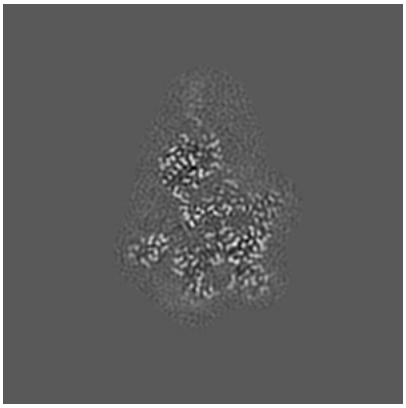


Z Index: 128

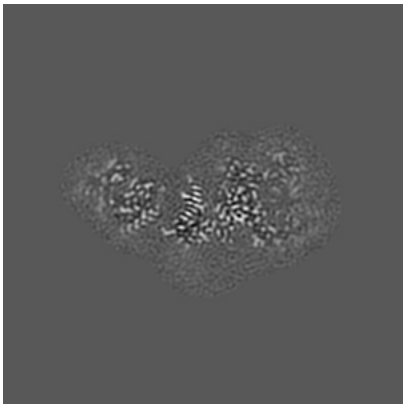
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 120



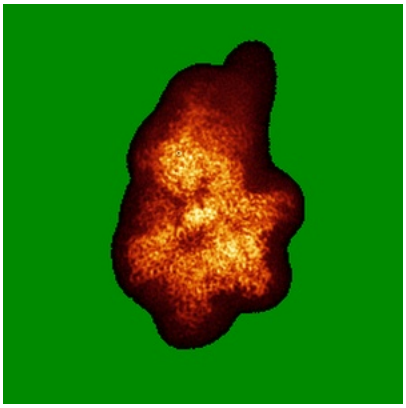
Y Index: 122

Z Index: 95

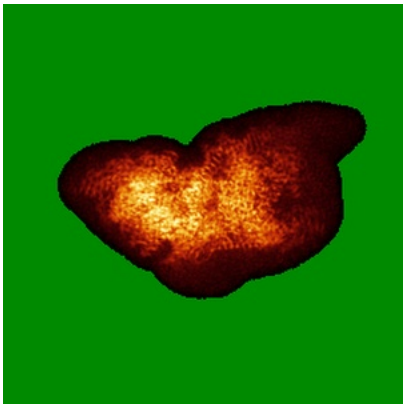
The images above show the largest variance slices of the map in three orthogonal directions.

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

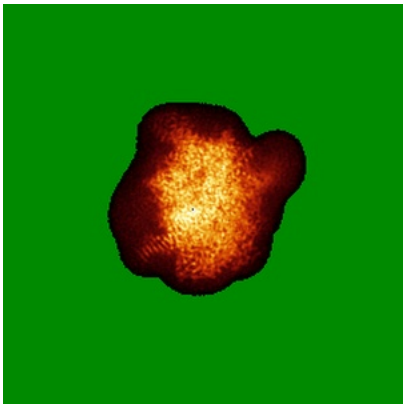
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

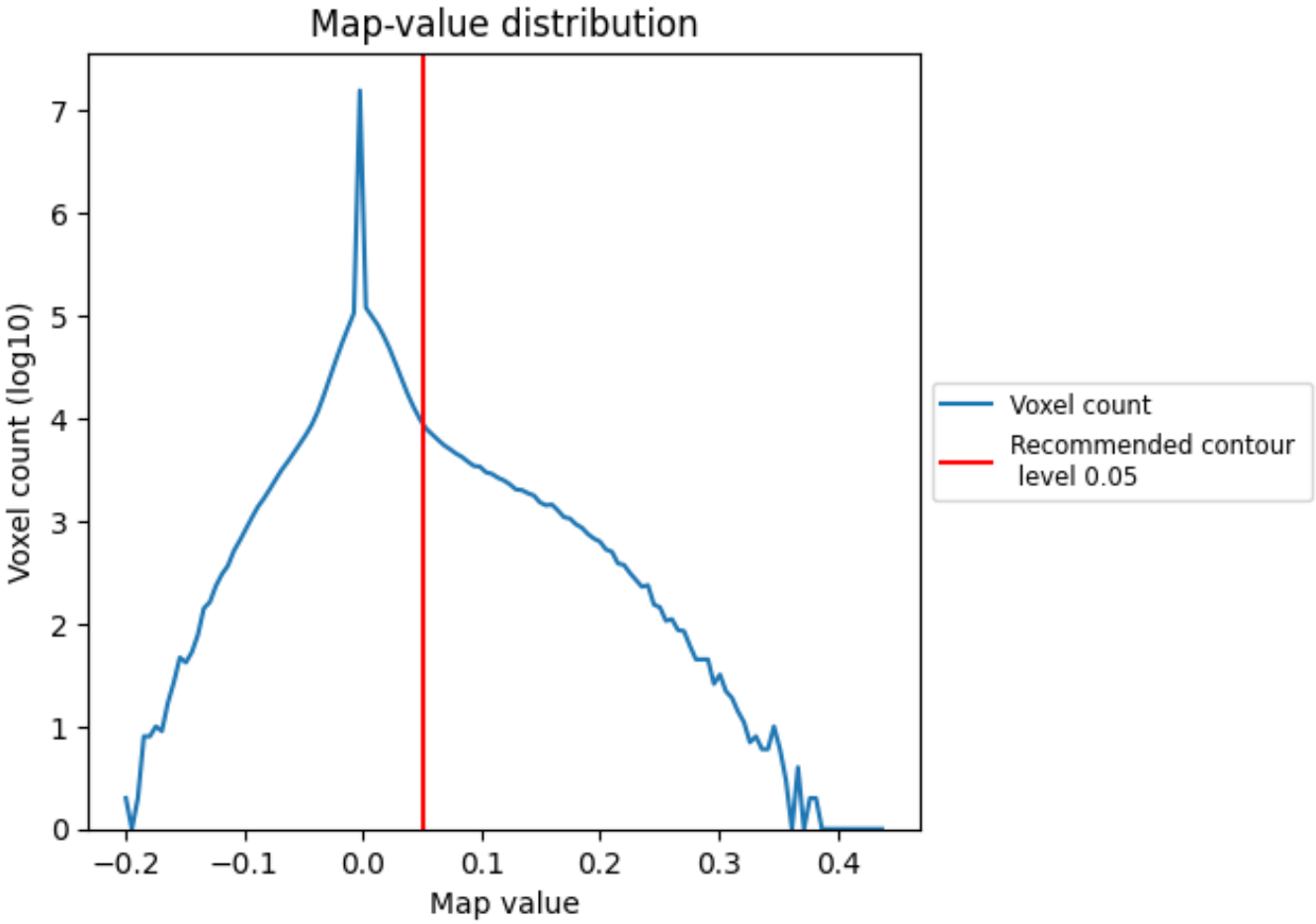
6.6 Mask visualisation (i)

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

7 Map analysis

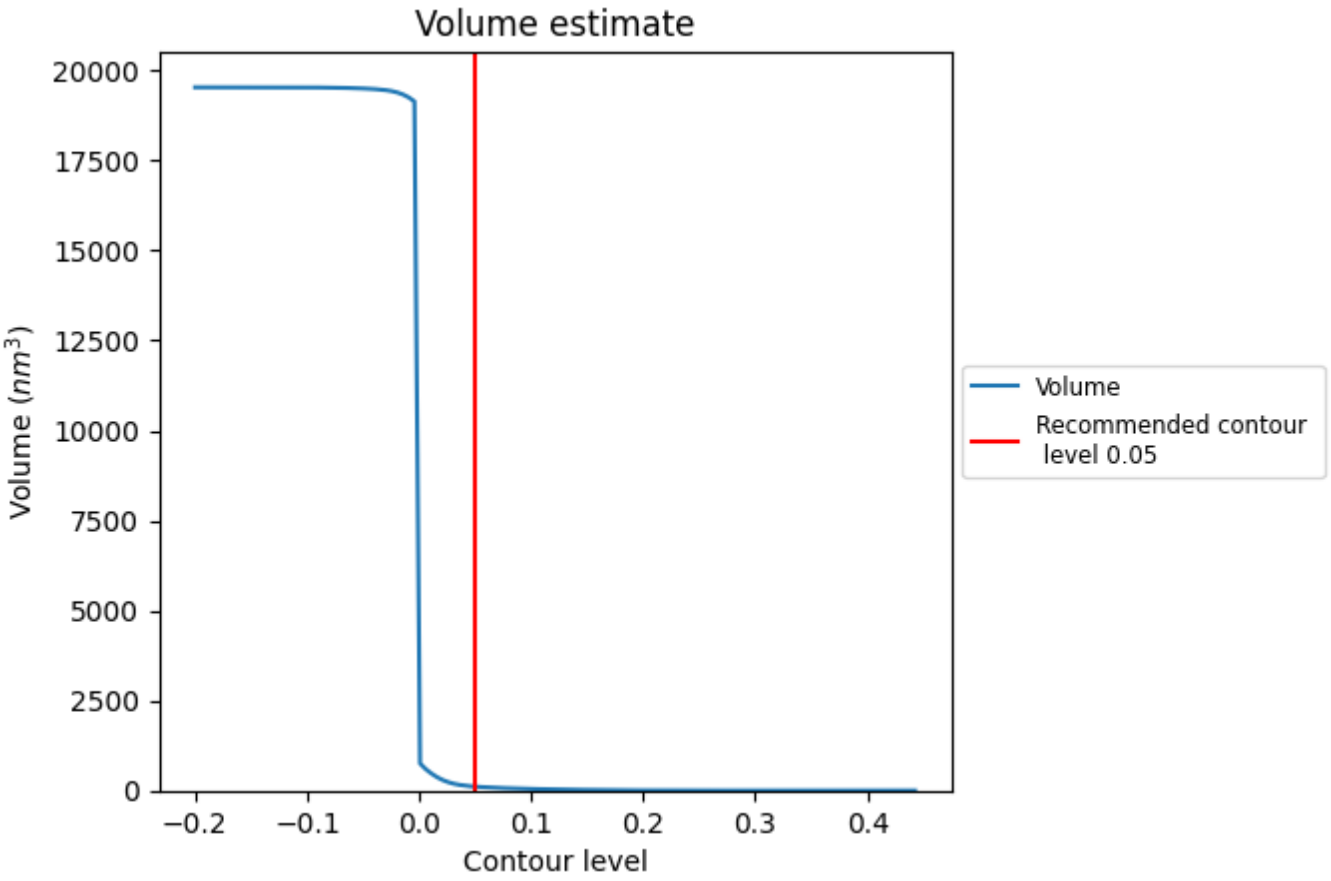
This section contains the results of statistical analysis of the map.

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.

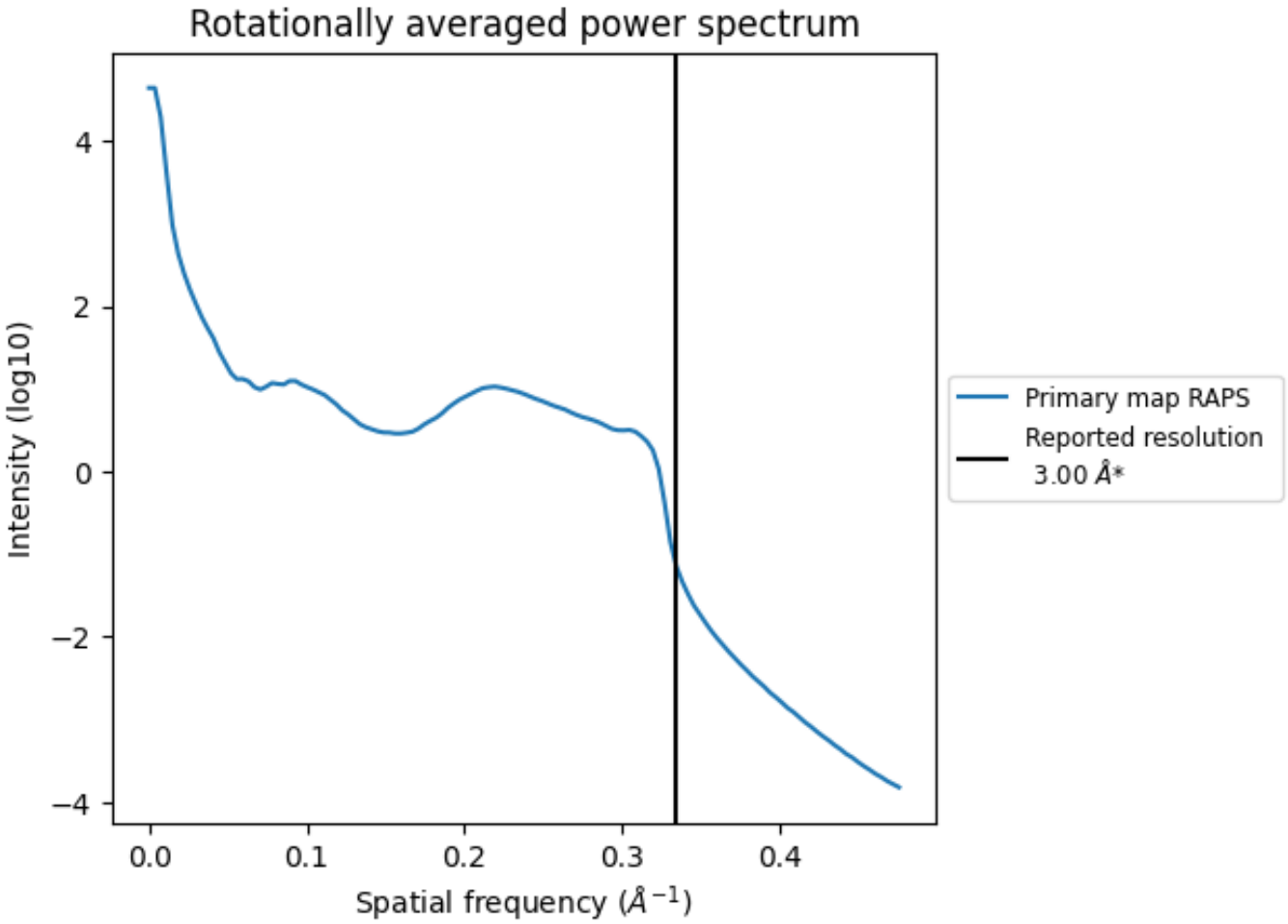
7.2 Volume estimate



The volume at the recommended contour level is 109 nm^3; this corresponds to an approximate mass of 99 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 0.333 Å^{-1}

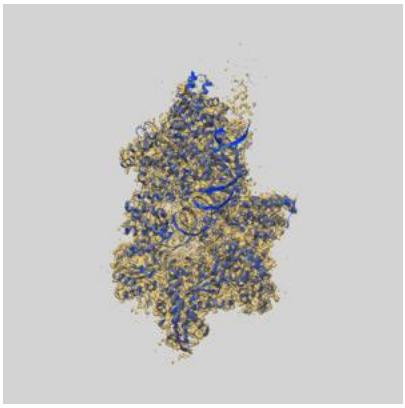
8 Fourier-Shell correlation (i)

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

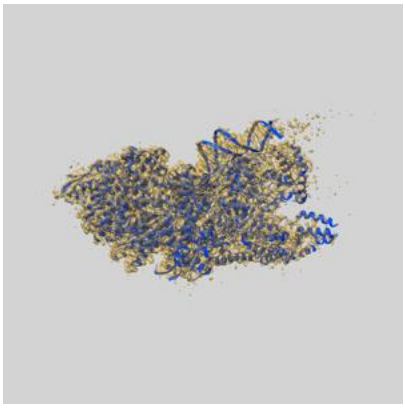
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6941 and PDB model 5ZR1. Per-residue inclusion information can be found in section 3 on page 6.

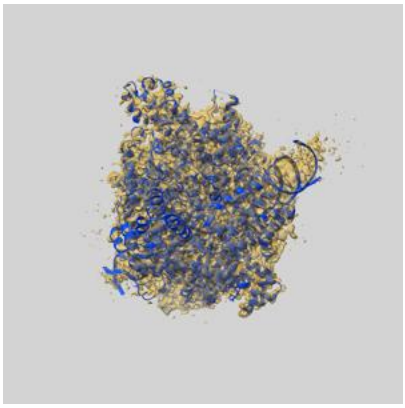
9.1 Map-model overlay



X



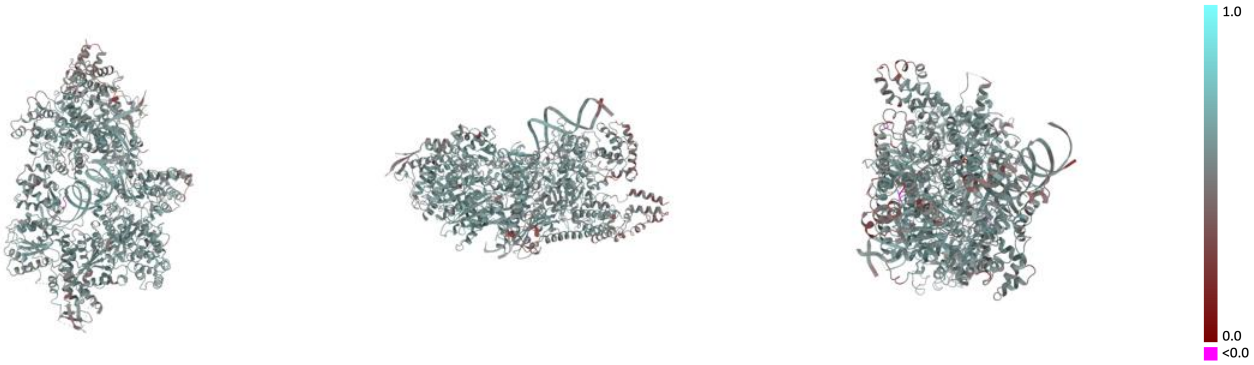
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

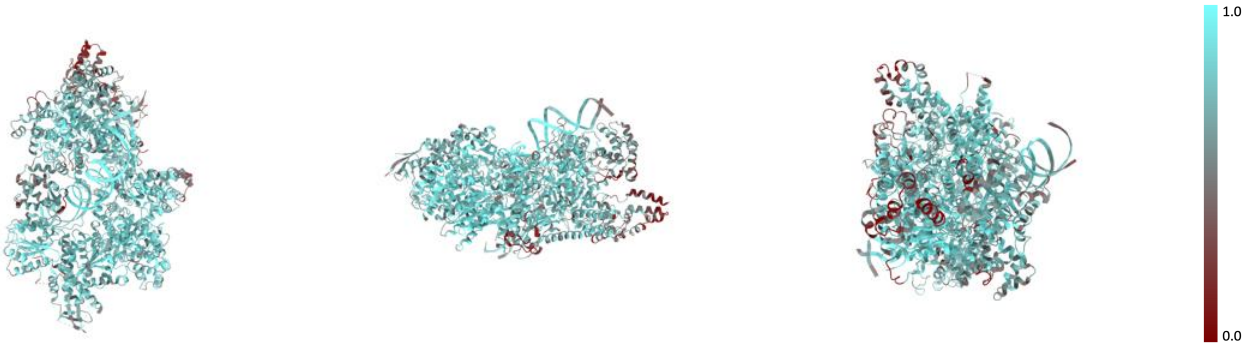
9.2 Q-score mapped to coordinate model



X Y Z

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

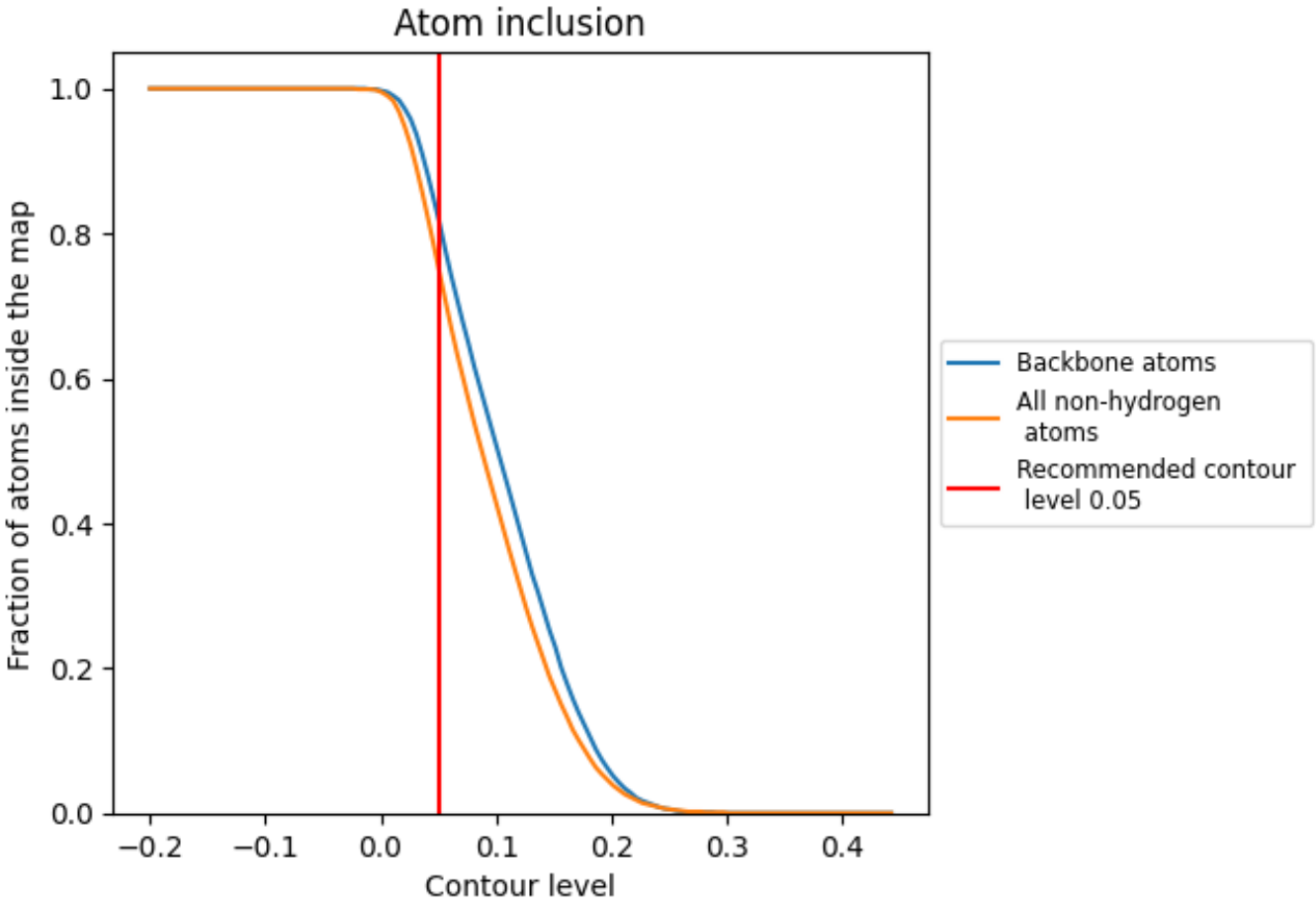
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7530	0.5470
A	0.7640	0.5440
B	0.7670	0.5630
C	0.6780	0.5230
D	0.8330	0.5730
E	0.7580	0.5490
F	0.5790	0.4870
G	0.8560	0.5690
H	0.8770	0.5960