Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:16 PM UTC

PDB ID	:	8J26 / pdb_00008j26
EMDB ID	:	EMD-35945
Title	:	CryoEM structure of SARS CoV-2 RBD and Aptamer complex
Authors	:	Rahman, M.S.; Jang, S.K.; Lee, J.O.
Deposited on	:	2023-04-14
Resolution	:	3.40 Å(reported)
Based on initial models	:	7KGJ, 6XDG

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:

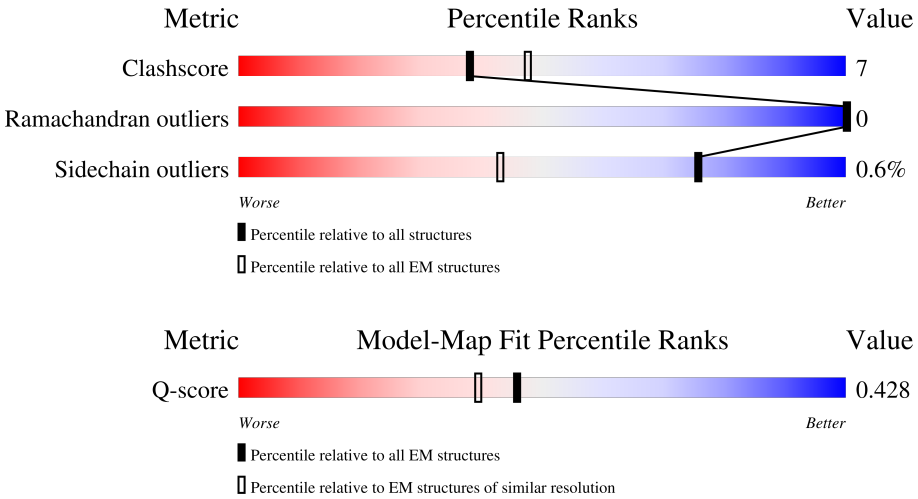
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.40 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.



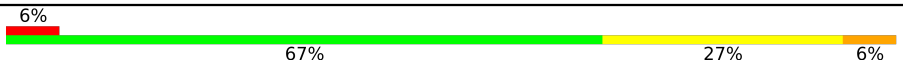
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	E	44	9% 55% 32% 9% 5%
2	A	224	40% 9% 51%
3	B	248	38% 12% 51%
4	C	253	69% 8% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	D	48	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5406 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 DNA chain called AM032-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	42	Total	C	N	O	P	0	0
			994	520	167	265	42		

- Molecule 2 is a protein called Fab light chain (REGN10987).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	109	Total	C	N	O	S	0	0
			797	495	133	166	3		

- Molecule 3 is a protein called Fab heavy chain (REGN10987).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	122	Total	C	N	O	S	0	0
			942	595	158	185	4		

- Molecule 4 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	196	Total	C	N	O	S	0	0
			1548	992	258	290	8		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	542	GLU	-	expression tag	UNP P0DTC2
C	543	ASN	-	expression tag	UNP P0DTC2
C	544	LEU	-	expression tag	UNP P0DTC2
C	545	TYR	-	expression tag	UNP P0DTC2
C	546	PHE	-	expression tag	UNP P0DTC2
C	547	GLN	-	expression tag	UNP P0DTC2
C	548	GLY	-	expression tag	UNP P0DTC2
C	549	ALA	-	expression tag	UNP P0DTC2
C	550	ALA	-	expression tag	UNP P0DTC2

Continued on next page...

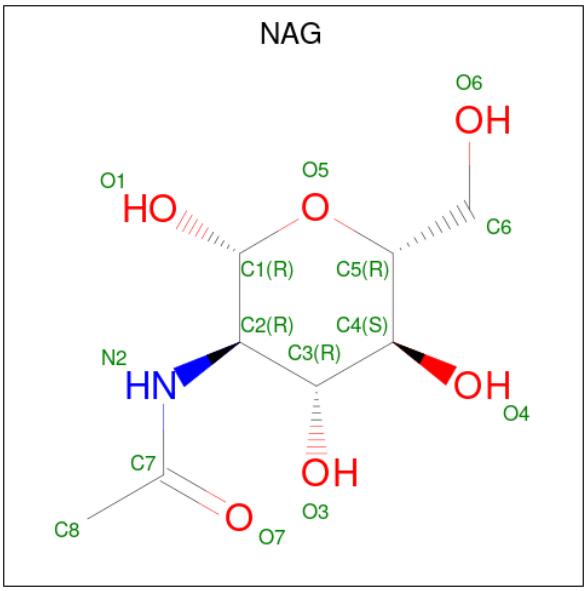
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	551	ALA	-	expression tag	UNP P0DTC2
C	552	GLY	-	expression tag	UNP P0DTC2
C	553	GLY	-	expression tag	UNP P0DTC2
C	554	SER	-	expression tag	UNP P0DTC2
C	555	HIS	-	expression tag	UNP P0DTC2
C	556	HIS	-	expression tag	UNP P0DTC2
C	557	HIS	-	expression tag	UNP P0DTC2
C	558	HIS	-	expression tag	UNP P0DTC2
C	559	HIS	-	expression tag	UNP P0DTC2
C	560	HIS	-	expression tag	UNP P0DTC2
C	561	GLY	-	expression tag	UNP P0DTC2
C	562	GLY	-	expression tag	UNP P0DTC2
C	563	SER	-	expression tag	UNP P0DTC2
C	564	ASP	-	expression tag	UNP P0DTC2
C	565	TYR	-	expression tag	UNP P0DTC2
C	566	LYS	-	expression tag	UNP P0DTC2
C	567	ASP	-	expression tag	UNP P0DTC2
C	568	ASP	-	expression tag	UNP P0DTC2
C	569	ASP	-	expression tag	UNP P0DTC2
C	570	ASP	-	expression tag	UNP P0DTC2
C	571	LYS	-	expression tag	UNP P0DTC2

- Molecule 5 is a DNA chain called AM047-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	D	48	1111	567	198	298	48	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



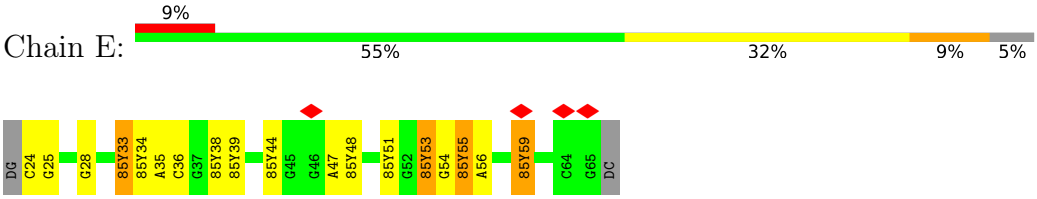
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	C	1	14	8	1	5	0

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.

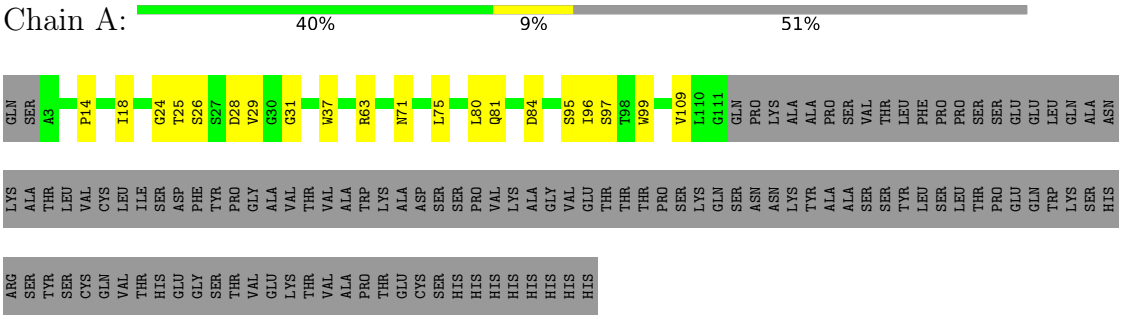
• Molecule 1: AM032-4

Chain E:



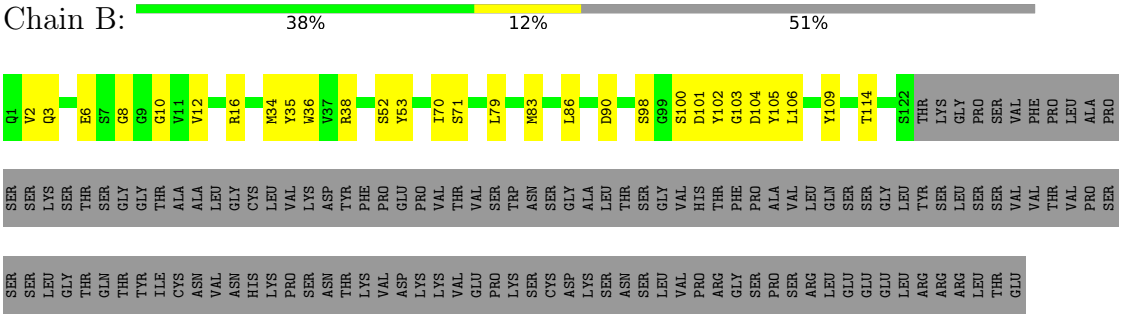
• Molecule 2: Fab light chain (REGN10987)

Chain A:



• Molecule 3: Fab heavy chain (REGN10987)

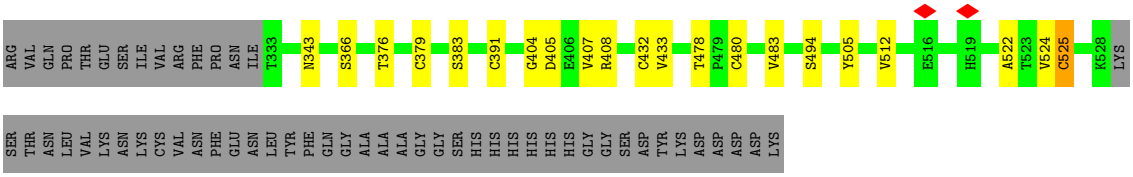
Chain B:



• Molecule 4: Spike protein S1

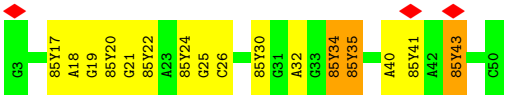
Chain C:





• Molecule 5: AM047-6





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	212000	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	314.496, 314.496, 314.496	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.819, 0.819, 0.819	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 85Y

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	E	0.17	0/740	0.37	0/1121
2	A	0.11	0/814	0.29	0/1106
3	B	0.13	0/963	0.29	0/1307
4	C	0.13	0/1592	0.28	0/2168
5	D	0.20	0/910	0.38	0/1385
All	All	0.15	0/5019	0.32	0/7087

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	E	994	0	354	13	0
2	A	797	0	765	13	0
3	B	942	0	901	18	0
4	C	1548	0	1461	16	0
5	D	1111	0	430	8	0
6	C	14	0	13	4	0
All	All	5406	0	3924	65	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 7.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:DA:N6	4:C:494:SER:O	2.07	0.88
4:C:343:ASN:OD1	6:C:701:NAG:N2	2.17	0.77
1:E:28:DG:N2	1:E:59:85Y:O21	2.20	0.74
3:B:35:TYR:OH	3:B:104:ASP:O	2.07	0.73
1:E:36:DC:O2	4:C:505:TYR:OH	2.07	0.72
2:A:25:THR:N	2:A:28:ASP:OD2	2.26	0.69
3:B:6:GLU:N	3:B:6:GLU:OE1	2.26	0.68
5:D:43:85Y:OP2	5:D:43:85Y:O3'	2.12	0.67
2:A:81:GLN:N	2:A:81:GLN:OE1	2.28	0.66
3:B:38:ARG:NH2	3:B:90:ASP:OD2	2.30	0.64
3:B:101:ASP:OD1	3:B:102:TYR:N	2.32	0.62
3:B:83:MET:HB3	3:B:86:LEU:HD21	1.81	0.62
4:C:405:ASP:O	4:C:408:ARG:NH1	2.34	0.61
4:C:379:CYS:HA	4:C:432:CYS:HB3	1.83	0.60
2:A:63:ARG:NH2	2:A:84:ASP:OD2	2.36	0.59
4:C:379:CYS:HA	4:C:432:CYS:CB	2.34	0.58
4:C:376:THR:N	5:D:35:85Y:O21	2.39	0.55
4:C:433:VAL:HG12	4:C:512:VAL:HG22	1.89	0.54
3:B:16:ARG:O	3:B:86:LEU:HD23	2.08	0.54
5:D:21:DG:H22	5:D:25:DG:H21	1.55	0.54
1:E:47:DA:N6	1:E:54:DG:C6	2.77	0.53
1:E:47:DA:H2'	1:E:47:DA:N3	2.24	0.53
1:E:47:DA:C6	1:E:54:DG:C6	2.98	0.51
3:B:100:SER:OG	3:B:101:ASP:N	2.44	0.51
1:E:47:DA:C5	1:E:54:DG:N1	2.80	0.50
1:E:24:DC:O2	1:E:25:DG:N1	2.44	0.50
3:B:2:VAL:HG11	3:B:109:TYR:CD2	2.47	0.50
1:E:33:85Y:O2	1:E:55:85Y:N3	2.45	0.50
4:C:524:VAL:O	4:C:524:VAL:HG13	2.12	0.49
3:B:106:LEU:HD12	3:B:106:LEU:O	2.13	0.49
4:C:478:THR:O	4:C:478:THR:OG1	2.31	0.48
3:B:71:SER:O	3:B:79:LEU:HD12	2.14	0.48
5:D:21:DG:H22	5:D:25:DG:N2	2.10	0.48
3:B:103:GLY:HA3	3:B:106:LEU:HD11	1.95	0.48
2:A:24:GLY:O	2:A:71:ASN:ND2	2.46	0.48
4:C:480:CYS:O	4:C:483:VAL:HG12	2.14	0.47
1:E:53:85Y:N3	1:E:54:DG:O6	2.48	0.46
3:B:36:TRP:HD1	3:B:70:ILE:HD12	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:37:TRP:CE3	2:A:75:LEU:HD12	2.51	0.46
3:B:8:GLY:HA2	3:B:114:THR:HG21	1.98	0.46
4:C:391:CYS:SG	4:C:522:ALA:HB1	2.56	0.46
3:B:3:GLN:HA	3:B:3:GLN:OE1	2.17	0.45
2:A:26:SER:O	2:A:31:GLY:N	2.49	0.45
1:E:55:85Y:O21	1:E:56:DA:N1	2.50	0.45
2:A:99:TRP:NE1	3:B:105:TYR:O	2.40	0.44
1:E:47:DA:C5	1:E:54:DG:C2	3.06	0.44
5:D:18:DA:C2'	5:D:19:DG:H21	2.31	0.43
4:C:404:GLY:O	4:C:407:VAL:HG12	2.19	0.43
3:B:34:MET:SD	3:B:98:SER:HA	2.59	0.43
4:C:391:CYS:HB3	4:C:525:CYS:HB3	1.76	0.43
2:A:28:ASP:OD1	2:A:29:VAL:HG22	2.19	0.42
4:C:366:SER:HB2	5:D:19:DG:H22	1.84	0.42
2:A:96:ILE:O	2:A:97:SER:OG	2.33	0.42
3:B:52:SER:OG	3:B:53:TYR:N	2.52	0.42
4:C:343:ASN:OD1	6:C:701:NAG:C2	2.67	0.42
5:D:32:DA:N1	5:D:34:85Y:N3	2.66	0.42
2:A:14:PRO:HD3	2:A:109:VAL:HG13	2.00	0.42
3:B:10:GLY:O	3:B:12:VAL:HG13	2.20	0.42
5:D:26:DC:H42	5:D:40:DA:N6	2.18	0.41
6:C:701:NAG:HO3	6:C:701:NAG:C7	2.31	0.41
2:A:95:SER:O	2:A:96:ILE:C	2.63	0.41
1:E:47:DA:C4	1:E:54:DG:C2	3.09	0.41
2:A:18:ILE:HG13	2:A:80:LEU:HD13	2.03	0.41
6:C:701:NAG:O7	6:C:701:NAG:O3	2.33	0.41
2:A:37:TRP:CD1	2:A:37:TRP:N	2.89	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	
2	A	107/224 (48%)	94 (88%)	13 (12%)	0	100	100
3	B	120/248 (48%)	108 (90%)	12 (10%)	0	100	100
4	C	194/253 (77%)	186 (96%)	8 (4%)	0	100	100
All	All	421/725 (58%)	388 (92%)	33 (8%)	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	
2	A	90/191 (47%)	90 (100%)	0	100	100
3	B	100/212 (47%)	100 (100%)	0	100	100
4	C	168/218 (77%)	166 (99%)	2 (1%)	63	72
All	All	358/621 (58%)	356 (99%)	2 (1%)	76	80

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	383	SER
4	C	525	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	39	GLN
4	C	409	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

19 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	$\#\|Z\| > 2$
1	85Y	E	48	1	33,36,37	4.63	16 (48%)	46,51,54	3.59	9 (19%)
5	85Y	D	20	5	33,36,37	4.67	16 (48%)	46,51,54	3.18	14 (30%)
1	85Y	E	51	1	33,36,37	4.67	16 (48%)	46,51,54	3.58	8 (17%)
1	85Y	E	53	1	33,36,37	4.63	17 (51%)	46,51,54	3.67	14 (30%)
5	85Y	D	30	5	33,36,37	4.63	16 (48%)	46,51,54	3.78	11 (23%)
5	85Y	D	41	5	33,36,37	4.62	16 (48%)	46,51,54	3.74	12 (26%)
5	85Y	D	22	5	33,36,37	4.66	16 (48%)	46,51,54	3.45	13 (28%)
5	85Y	D	34	5	33,36,37	4.64	16 (48%)	46,51,54	3.76	9 (19%)
5	85Y	D	17	5	33,36,37	4.60	16 (48%)	46,51,54	3.73	16 (34%)
1	85Y	E	59	1	33,36,37	4.69	16 (48%)	46,51,54	3.64	9 (19%)
1	85Y	E	44	1	33,36,37	4.66	16 (48%)	46,51,54	3.68	13 (28%)
1	85Y	E	39	1	33,36,37	4.64	16 (48%)	46,51,54	3.65	10 (21%)
5	85Y	D	24	5	33,36,37	4.66	16 (48%)	46,51,54	3.59	9 (19%)
5	85Y	D	43	5	33,36,37	4.66	16 (48%)	46,51,54	3.64	11 (23%)
1	85Y	E	34	1	33,36,37	4.64	16 (48%)	46,51,54	3.64	14 (30%)
5	85Y	D	35	5	33,36,37	4.59	16 (48%)	46,51,54	3.69	16 (34%)
1	85Y	E	55	1	33,36,37	4.63	16 (48%)	46,51,54	3.57	14 (30%)
1	85Y	E	38	1	33,36,37	4.61	16 (48%)	46,51,54	3.69	15 (32%)
1	85Y	E	33	1	33,36,37	4.67	16 (48%)	46,51,54	3.63	14 (30%)

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
1	85Y	E	48	1	-	10/16/30/31	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	85Y	D	20	5	-	1/16/30/31	0/4/4/4
1	85Y	E	51	1	-	8/16/30/31	0/4/4/4
1	85Y	E	53	1	-	9/16/30/31	0/4/4/4
5	85Y	D	30	5	-	8/16/30/31	0/4/4/4
5	85Y	D	41	5	-	8/16/30/31	0/4/4/4
5	85Y	D	22	5	-	11/16/30/31	0/4/4/4
5	85Y	D	34	5	-	8/16/30/31	0/4/4/4
5	85Y	D	17	5	-	8/16/30/31	0/4/4/4
1	85Y	E	59	1	-	8/16/30/31	0/4/4/4
1	85Y	E	44	1	-	0/16/30/31	0/4/4/4
1	85Y	E	39	1	-	4/16/30/31	0/4/4/4
5	85Y	D	24	5	-	9/16/30/31	0/4/4/4
5	85Y	D	43	5	-	11/16/30/31	0/4/4/4
1	85Y	E	34	1	-	10/16/30/31	0/4/4/4
5	85Y	D	35	5	-	8/16/30/31	0/4/4/4
1	85Y	E	55	1	-	9/16/30/31	0/4/4/4
1	85Y	E	38	1	-	8/16/30/31	0/4/4/4
1	85Y	E	33	1	-	7/16/30/31	0/4/4/4

All (305) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	30	85Y	C5-C4	12.30	1.68	1.45
1	E	33	85Y	C5-C4	12.20	1.67	1.45
5	D	20	85Y	C5-C4	12.19	1.67	1.45
5	D	22	85Y	C5-C4	12.17	1.67	1.45
1	E	59	85Y	C5-C4	12.14	1.67	1.45
1	E	34	85Y	C5-C4	12.11	1.67	1.45
5	D	43	85Y	C5-C4	12.11	1.67	1.45
5	D	41	85Y	C5-C4	12.10	1.67	1.45
1	E	51	85Y	C5-C4	12.07	1.67	1.45
5	D	24	85Y	C5-C4	12.07	1.67	1.45
1	E	39	85Y	C5-C4	12.06	1.67	1.45
5	D	34	85Y	C5-C4	12.05	1.67	1.45
1	E	38	85Y	C5-C4	12.01	1.67	1.45
5	D	35	85Y	C5-C4	12.01	1.67	1.45
1	E	55	85Y	C5-C4	12.00	1.67	1.45
1	E	53	85Y	C5-C4	12.00	1.67	1.45
1	E	48	85Y	C5-C4	11.98	1.67	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	17	85Y	C5-C4	11.95	1.67	1.45
1	E	44	85Y	C5-C4	11.93	1.67	1.45
5	D	43	85Y	C2-N1	10.89	1.55	1.38
1	E	51	85Y	C2-N1	10.88	1.55	1.38
5	D	41	85Y	C2-N1	10.79	1.55	1.38
1	E	44	85Y	C2-N1	10.78	1.55	1.38
1	E	59	85Y	C2-N1	10.76	1.55	1.38
5	D	30	85Y	C2-N1	10.75	1.55	1.38
5	D	34	85Y	C2-N1	10.74	1.55	1.38
5	D	24	85Y	C2-N1	10.72	1.55	1.38
1	E	55	85Y	C2-N1	10.70	1.55	1.38
5	D	20	85Y	C2-N1	10.63	1.55	1.38
1	E	39	85Y	C2-N1	10.63	1.55	1.38
1	E	33	85Y	C2-N1	10.59	1.55	1.38
1	E	34	85Y	C2-N1	10.59	1.55	1.38
5	D	22	85Y	C2-N1	10.58	1.55	1.38
1	E	38	85Y	C2-N1	10.57	1.55	1.38
1	E	48	85Y	C2-N1	10.56	1.55	1.38
1	E	53	85Y	C2-N1	10.52	1.54	1.38
5	D	17	85Y	C2-N1	10.48	1.54	1.38
5	D	35	85Y	C2-N1	10.37	1.54	1.38
5	D	43	85Y	C2'-C3'	-8.97	1.30	1.52
1	E	59	85Y	C6-N1	8.88	1.53	1.38
1	E	39	85Y	C2'-C3'	-8.86	1.30	1.52
1	E	44	85Y	C6-N1	8.86	1.53	1.38
1	E	33	85Y	C6-N1	8.86	1.53	1.38
5	D	30	85Y	C2'-C3'	-8.80	1.30	1.52
1	E	51	85Y	C2'-C3'	-8.80	1.30	1.52
1	E	48	85Y	C2'-C3'	-8.79	1.30	1.52
1	E	38	85Y	C2'-C3'	-8.79	1.30	1.52
5	D	24	85Y	C2'-C3'	-8.74	1.30	1.52
5	D	24	85Y	C6-N1	8.73	1.52	1.38
5	D	20	85Y	C2'-C3'	-8.72	1.30	1.52
5	D	41	85Y	C6-N1	8.67	1.52	1.38
1	E	53	85Y	C2'-C3'	-8.66	1.30	1.52
5	D	34	85Y	C6-N1	8.63	1.52	1.38
1	E	44	85Y	C2'-C3'	-8.63	1.30	1.52
5	D	22	85Y	C2'-C3'	-8.62	1.31	1.52
5	D	41	85Y	C2'-C3'	-8.61	1.31	1.52
1	E	59	85Y	C2'-C3'	-8.61	1.31	1.52
1	E	55	85Y	C2'-C3'	-8.60	1.31	1.52
5	D	34	85Y	C2'-C3'	-8.56	1.31	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	17	85Y	C2'-C3'	-8.55	1.31	1.52
1	E	34	85Y	C2'-C3'	-8.55	1.31	1.52
1	E	33	85Y	C2'-C3'	-8.55	1.31	1.52
1	E	55	85Y	C6-N1	8.49	1.52	1.38
1	E	39	85Y	C6-N1	8.45	1.52	1.38
1	E	51	85Y	C6-N1	8.43	1.52	1.38
1	E	34	85Y	C6-N1	8.42	1.52	1.38
5	D	22	85Y	C6-N1	8.42	1.52	1.38
5	D	20	85Y	C6-N1	8.41	1.52	1.38
5	D	43	85Y	C6-N1	8.41	1.52	1.38
1	E	48	85Y	C6-N1	8.40	1.52	1.38
5	D	30	85Y	C6-N1	8.36	1.52	1.38
5	D	35	85Y	C2'-C3'	-8.33	1.31	1.52
1	E	53	85Y	C6-N1	8.32	1.52	1.38
5	D	35	85Y	C6-N1	8.30	1.52	1.38
5	D	17	85Y	C6-N1	8.23	1.52	1.38
1	E	38	85Y	C6-N1	8.18	1.51	1.38
1	E	44	85Y	C4-N3	-7.83	1.24	1.38
1	E	33	85Y	C4-N3	-7.80	1.24	1.38
5	D	35	85Y	C4-N3	-7.73	1.24	1.38
5	D	30	85Y	C4-N3	-7.72	1.24	1.38
1	E	48	85Y	C4-N3	-7.66	1.24	1.38
5	D	41	85Y	C4-N3	-7.65	1.24	1.38
5	D	24	85Y	C4-N3	-7.65	1.24	1.38
1	E	55	85Y	C4-N3	-7.64	1.24	1.38
1	E	51	85Y	C4-N3	-7.64	1.24	1.38
1	E	34	85Y	C4-N3	-7.64	1.24	1.38
5	D	22	85Y	C4-N3	-7.63	1.24	1.38
5	D	20	85Y	C4-N3	-7.63	1.24	1.38
1	E	59	85Y	C4-N3	-7.63	1.24	1.38
5	D	17	85Y	C4-N3	-7.63	1.24	1.38
5	D	34	85Y	C4-N3	-7.57	1.24	1.38
1	E	38	85Y	C4-N3	-7.56	1.24	1.38
1	E	39	85Y	C4-N3	-7.55	1.24	1.38
1	E	53	85Y	C4-N3	-7.54	1.24	1.38
5	D	43	85Y	C4-N3	-7.43	1.24	1.38
5	D	43	85Y	O4'-C1'	6.32	1.56	1.42
5	D	22	85Y	O4'-C4'	-6.22	1.31	1.45
1	E	59	85Y	O4'-C1'	6.20	1.56	1.42
5	D	34	85Y	O4'-C4'	-6.19	1.31	1.45
5	D	35	85Y	O4'-C4'	-6.15	1.31	1.45
1	E	51	85Y	O4'-C1'	6.15	1.56	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	55	85Y	O4'-C4'	-6.08	1.31	1.45
5	D	24	85Y	O4'-C4'	-6.06	1.31	1.45
1	E	34	85Y	O4'-C4'	-6.05	1.31	1.45
5	D	24	85Y	O4'-C1'	6.05	1.55	1.42
5	D	20	85Y	O4'-C1'	6.01	1.55	1.42
1	E	48	85Y	O4'-C1'	6.00	1.55	1.42
1	E	39	85Y	O4'-C1'	5.97	1.55	1.42
1	E	33	85Y	C20-N22	5.97	1.43	1.33
1	E	44	85Y	O4'-C4'	-5.96	1.31	1.45
1	E	53	85Y	O4'-C4'	-5.95	1.31	1.45
1	E	55	85Y	O4'-C1'	5.94	1.55	1.42
5	D	30	85Y	O4'-C1'	5.93	1.55	1.42
1	E	44	85Y	O4'-C1'	5.93	1.55	1.42
5	D	17	85Y	O4'-C4'	-5.92	1.31	1.45
5	D	41	85Y	O4'-C4'	-5.91	1.31	1.45
1	E	38	85Y	O4'-C4'	-5.89	1.31	1.45
5	D	22	85Y	O4'-C1'	5.86	1.55	1.42
5	D	30	85Y	O4'-C4'	-5.86	1.32	1.45
5	D	41	85Y	O4'-C1'	5.85	1.55	1.42
1	E	33	85Y	O4'-C1'	5.84	1.55	1.42
1	E	48	85Y	O4'-C4'	-5.83	1.32	1.45
1	E	51	85Y	O4'-C4'	-5.83	1.32	1.45
1	E	59	85Y	O4'-C4'	-5.83	1.32	1.45
5	D	20	85Y	C20-N22	5.82	1.43	1.33
1	E	39	85Y	O4'-C4'	-5.82	1.32	1.45
1	E	53	85Y	C20-N22	5.81	1.43	1.33
5	D	34	85Y	O4'-C1'	5.80	1.55	1.42
1	E	33	85Y	O4'-C4'	-5.79	1.32	1.45
1	E	34	85Y	C20-N22	5.79	1.43	1.33
5	D	43	85Y	O4'-C4'	-5.79	1.32	1.45
5	D	22	85Y	C20-N22	5.77	1.43	1.33
1	E	59	85Y	C20-N22	5.77	1.43	1.33
5	D	20	85Y	O4'-C4'	-5.76	1.32	1.45
1	E	38	85Y	O4'-C1'	5.74	1.55	1.42
1	E	53	85Y	O4'-C1'	5.74	1.55	1.42
5	D	17	85Y	O4'-C1'	5.71	1.55	1.42
1	E	51	85Y	C20-N22	5.71	1.43	1.33
5	D	43	85Y	C20-N22	5.70	1.43	1.33
1	E	34	85Y	O4'-C1'	5.68	1.55	1.42
1	E	38	85Y	C20-N22	5.61	1.43	1.33
1	E	44	85Y	C20-N22	5.60	1.43	1.33
5	D	35	85Y	C20-N22	5.60	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	34	85Y	C20-N22	5.60	1.43	1.33
5	D	17	85Y	C20-N22	5.58	1.43	1.33
5	D	24	85Y	C20-N22	5.57	1.43	1.33
5	D	35	85Y	O4'-C1'	5.55	1.54	1.42
1	E	39	85Y	C20-N22	5.50	1.43	1.33
1	E	38	85Y	C1'-N1	-5.46	1.34	1.48
5	D	17	85Y	C1'-N1	-5.43	1.34	1.48
5	D	41	85Y	C20-N22	5.42	1.42	1.33
1	E	55	85Y	C20-N22	5.41	1.42	1.33
1	E	48	85Y	C1'-N1	-5.34	1.34	1.48
1	E	48	85Y	C20-N22	5.34	1.42	1.33
5	D	30	85Y	C20-N22	5.32	1.42	1.33
1	E	39	85Y	C1'-N1	-5.30	1.34	1.48
5	D	35	85Y	C1'-N1	-5.30	1.34	1.48
1	E	53	85Y	C1'-N1	-5.29	1.34	1.48
5	D	22	85Y	C1'-N1	-5.25	1.34	1.48
1	E	34	85Y	C1'-N1	-5.23	1.34	1.48
5	D	20	85Y	C1'-N1	-5.22	1.35	1.48
1	E	51	85Y	C1'-N1	-5.21	1.35	1.48
5	D	20	85Y	C23-N22	5.17	1.56	1.46
5	D	34	85Y	C1'-N1	-5.14	1.35	1.48
1	E	44	85Y	C23-N22	5.13	1.56	1.46
1	E	53	85Y	C23-N22	5.09	1.56	1.46
1	E	44	85Y	C1'-N1	-5.06	1.35	1.48
5	D	30	85Y	C1'-N1	-5.05	1.35	1.48
5	D	24	85Y	C23-N22	5.03	1.56	1.46
1	E	51	85Y	C23-N22	5.02	1.56	1.46
1	E	34	85Y	C23-N22	5.00	1.56	1.46
1	E	59	85Y	C23-N22	4.98	1.56	1.46
1	E	55	85Y	C1'-N1	-4.98	1.35	1.48
1	E	33	85Y	C1'-N1	-4.97	1.35	1.48
1	E	39	85Y	C23-N22	4.97	1.55	1.46
5	D	22	85Y	C23-N22	4.94	1.55	1.46
1	E	48	85Y	C23-N22	4.94	1.55	1.46
5	D	41	85Y	C1'-N1	-4.92	1.35	1.48
5	D	43	85Y	C1'-N1	-4.87	1.35	1.48
5	D	34	85Y	C23-N22	4.87	1.55	1.46
5	D	24	85Y	C1'-N1	-4.86	1.35	1.48
1	E	33	85Y	C23-N22	4.85	1.55	1.46
5	D	43	85Y	C23-N22	4.82	1.55	1.46
1	E	59	85Y	C1'-N1	-4.81	1.36	1.48
1	E	53	85Y	C3'-C4'	4.78	1.65	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	17	85Y	C3'-C4'	4.78	1.65	1.53
5	D	17	85Y	C23-N22	4.76	1.55	1.46
1	E	38	85Y	C3'-C4'	4.69	1.65	1.53
1	E	55	85Y	C23-N22	4.66	1.55	1.46
5	D	35	85Y	C23-N22	4.64	1.55	1.46
1	E	34	85Y	C3'-C4'	4.63	1.65	1.53
1	E	59	85Y	C3'-C4'	4.63	1.65	1.53
1	E	38	85Y	C23-N22	4.61	1.55	1.46
5	D	20	85Y	C3'-C4'	4.59	1.65	1.53
5	D	41	85Y	C3'-C4'	4.59	1.65	1.53
5	D	41	85Y	C23-N22	4.58	1.55	1.46
5	D	35	85Y	C3'-C4'	4.58	1.65	1.53
5	D	30	85Y	C23-N22	4.55	1.55	1.46
1	E	39	85Y	C3'-C4'	4.55	1.64	1.53
1	E	44	85Y	C3'-C4'	4.50	1.64	1.53
1	E	33	85Y	C3'-C4'	4.47	1.64	1.53
1	E	48	85Y	C3'-C4'	4.47	1.64	1.53
1	E	51	85Y	C3'-C4'	4.46	1.64	1.53
1	E	33	85Y	C5-C20	4.45	1.62	1.49
5	D	24	85Y	C3'-C4'	4.44	1.64	1.53
5	D	22	85Y	C3'-C4'	4.42	1.64	1.53
5	D	34	85Y	C3'-C4'	4.38	1.64	1.53
1	E	55	85Y	C3'-C4'	4.36	1.64	1.53
5	D	30	85Y	C3'-C4'	4.27	1.64	1.53
5	D	43	85Y	C3'-C4'	4.23	1.64	1.53
1	E	59	85Y	C5-C20	4.15	1.61	1.49
1	E	34	85Y	C5-C20	4.13	1.61	1.49
5	D	35	85Y	C5-C20	4.13	1.61	1.49
5	D	22	85Y	C5-C20	4.12	1.61	1.49
5	D	20	85Y	C5-C20	4.10	1.61	1.49
5	D	34	85Y	C5-C20	4.09	1.61	1.49
1	E	48	85Y	C5-C20	4.07	1.61	1.49
5	D	43	85Y	C5-C20	4.07	1.61	1.49
5	D	24	85Y	C5-C20	4.05	1.61	1.49
1	E	39	85Y	C5-C20	4.02	1.61	1.49
1	E	44	85Y	C5-C20	4.01	1.61	1.49
1	E	53	85Y	C5-C20	4.00	1.61	1.49
1	E	51	85Y	C5-C20	3.98	1.61	1.49
5	D	41	85Y	C5-C20	3.96	1.61	1.49
1	E	55	85Y	C5-C20	3.94	1.61	1.49
5	D	30	85Y	C5-C20	3.93	1.61	1.49
1	E	38	85Y	C5-C20	3.85	1.60	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	17	85Y	C5-C20	3.80	1.60	1.49
5	D	20	85Y	C29-C24	3.65	1.46	1.38
1	E	48	85Y	C29-C24	3.54	1.45	1.38
5	D	22	85Y	C29-C24	3.52	1.45	1.38
1	E	55	85Y	C29-C24	3.52	1.45	1.38
5	D	30	85Y	O2-C2	-3.44	1.17	1.23
5	D	17	85Y	O2-C2	-3.41	1.17	1.23
1	E	33	85Y	O2-C2	-3.40	1.17	1.23
1	E	59	85Y	C29-C24	3.39	1.45	1.38
1	E	55	85Y	O2-C2	-3.39	1.17	1.23
1	E	34	85Y	O2-C2	-3.39	1.17	1.23
5	D	35	85Y	O2-C2	-3.37	1.17	1.23
1	E	48	85Y	O2-C2	-3.37	1.17	1.23
1	E	33	85Y	C29-C24	3.36	1.45	1.38
5	D	20	85Y	O2-C2	-3.35	1.17	1.23
5	D	34	85Y	O2-C2	-3.35	1.17	1.23
1	E	53	85Y	O2-C2	-3.34	1.17	1.23
1	E	51	85Y	O2-C2	-3.31	1.17	1.23
1	E	38	85Y	O2-C2	-3.30	1.17	1.23
1	E	39	85Y	O2-C2	-3.30	1.17	1.23
5	D	22	85Y	O2-C2	-3.30	1.17	1.23
5	D	43	85Y	O2-C2	-3.30	1.17	1.23
5	D	43	85Y	C29-C24	3.30	1.45	1.38
5	D	41	85Y	O2-C2	-3.28	1.17	1.23
1	E	44	85Y	O2-C2	-3.27	1.17	1.23
5	D	24	85Y	O2-C2	-3.27	1.17	1.23
5	D	35	85Y	C29-C24	3.26	1.45	1.38
1	E	51	85Y	C29-C24	3.26	1.45	1.38
5	D	24	85Y	C29-C24	3.25	1.45	1.38
1	E	44	85Y	C29-C24	3.25	1.45	1.38
1	E	59	85Y	O2-C2	-3.24	1.17	1.23
1	E	39	85Y	C29-C24	3.20	1.45	1.38
1	E	34	85Y	C29-C24	3.16	1.45	1.38
5	D	34	85Y	C29-C24	3.14	1.45	1.38
5	D	17	85Y	C29-C24	3.12	1.45	1.38
1	E	53	85Y	C29-C24	3.10	1.45	1.38
1	E	38	85Y	C29-C24	3.09	1.45	1.38
5	D	41	85Y	C29-C24	3.02	1.44	1.38
5	D	30	85Y	C29-C24	3.01	1.44	1.38
5	D	35	85Y	O4-C4	-2.85	1.18	1.23
1	E	48	85Y	O4-C4	-2.78	1.18	1.23
5	D	24	85Y	O4-C4	-2.74	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	33	85Y	O4-C4	-2.71	1.18	1.23
1	E	38	85Y	O4-C4	-2.70	1.18	1.23
1	E	39	85Y	O4-C4	-2.70	1.18	1.23
1	E	51	85Y	O4-C4	-2.69	1.18	1.23
5	D	34	85Y	O4-C4	-2.65	1.18	1.23
1	E	34	85Y	O4-C4	-2.64	1.18	1.23
5	D	22	85Y	O4-C4	-2.63	1.18	1.23
1	E	44	85Y	O4-C4	-2.62	1.18	1.23
1	E	55	85Y	O4-C4	-2.62	1.18	1.23
1	E	53	85Y	O4-C4	-2.61	1.18	1.23
1	E	59	85Y	O4-C4	-2.61	1.18	1.23
5	D	17	85Y	O4-C4	-2.61	1.18	1.23
5	D	43	85Y	C2-N3	2.60	1.42	1.38
5	D	20	85Y	O4-C4	-2.60	1.18	1.23
5	D	41	85Y	O4-C4	-2.59	1.18	1.23
5	D	43	85Y	O4-C4	-2.59	1.18	1.23
5	D	30	85Y	O4-C4	-2.51	1.18	1.23
1	E	38	85Y	C2-N3	2.40	1.42	1.38
1	E	53	85Y	C2-N3	2.38	1.42	1.38
5	D	30	85Y	C2-N3	2.36	1.42	1.38
1	E	59	85Y	C2-N3	2.36	1.42	1.38
5	D	20	85Y	C2-N3	2.34	1.42	1.38
5	D	17	85Y	C2-N3	2.34	1.42	1.38
1	E	55	85Y	C2-N3	2.32	1.42	1.38
5	D	41	85Y	C2-N3	2.31	1.42	1.38
5	D	34	85Y	C2-N3	2.31	1.42	1.38
5	D	22	85Y	C2-N3	2.30	1.42	1.38
1	E	34	85Y	C2-N3	2.27	1.41	1.38
1	E	39	85Y	C2-N3	2.23	1.41	1.38
5	D	24	85Y	C2-N3	2.22	1.41	1.38
1	E	51	85Y	C2-N3	2.22	1.41	1.38
5	D	35	85Y	C2-N3	2.16	1.41	1.38
1	E	48	85Y	C2-N3	2.14	1.41	1.38
1	E	44	85Y	C2-N3	2.11	1.41	1.38
1	E	33	85Y	C2-N3	2.04	1.41	1.38
1	E	53	85Y	O5'-C5'	-2.02	1.38	1.44

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	34	85Y	C23-C24-C25	16.14	150.13	121.46
5	D	30	85Y	C23-C24-C25	15.85	149.62	121.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	48	85Y	C23-C24-C25	15.42	148.87	121.46
5	D	43	85Y	C23-C24-C25	15.37	148.78	121.46
5	D	41	85Y	C23-C24-C25	15.36	148.75	121.46
1	E	59	85Y	C23-C24-C25	15.35	148.73	121.46
1	E	53	85Y	C23-C24-C25	15.28	148.61	121.46
1	E	39	85Y	C23-C24-C25	15.23	148.53	121.46
5	D	24	85Y	C23-C24-C25	15.12	148.34	121.46
5	D	17	85Y	C23-C24-C25	15.10	148.29	121.46
1	E	44	85Y	C23-C24-C25	15.06	148.22	121.46
5	D	34	85Y	C23-C24-C29	-15.03	90.27	120.94
1	E	34	85Y	C23-C24-C25	14.97	148.07	121.46
1	E	51	85Y	C23-C24-C25	14.94	148.01	121.46
5	D	30	85Y	C23-C24-C29	-14.87	90.59	120.94
1	E	38	85Y	C23-C24-C25	14.74	147.66	121.46
1	E	33	85Y	C23-C24-C25	14.63	147.45	121.46
5	D	41	85Y	C23-C24-C29	-14.62	91.10	120.94
1	E	55	85Y	C23-C24-C25	14.37	146.99	121.46
5	D	17	85Y	C23-C24-C29	-14.33	91.69	120.94
5	D	35	85Y	C23-C24-C25	14.31	146.90	121.46
1	E	53	85Y	C23-C24-C29	-14.28	91.79	120.94
5	D	43	85Y	C23-C24-C29	-14.26	91.83	120.94
1	E	59	85Y	C23-C24-C29	-14.25	91.86	120.94
1	E	39	85Y	C23-C24-C29	-14.23	91.90	120.94
5	D	24	85Y	C23-C24-C29	-14.18	92.00	120.94
1	E	38	85Y	C23-C24-C29	-14.09	92.18	120.94
5	D	22	85Y	C23-C24-C25	14.08	146.48	121.46
1	E	34	85Y	C23-C24-C29	-14.03	92.31	120.94
1	E	44	85Y	C23-C24-C29	-13.86	92.65	120.94
1	E	51	85Y	C23-C24-C29	-13.78	92.81	120.94
1	E	48	85Y	C23-C24-C29	-13.74	92.91	120.94
5	D	35	85Y	C23-C24-C29	-13.53	93.33	120.94
1	E	33	85Y	C23-C24-C29	-13.45	93.49	120.94
1	E	55	85Y	C23-C24-C29	-13.19	94.03	120.94
5	D	22	85Y	C23-C24-C29	-12.85	94.72	120.94
5	D	20	85Y	C23-C24-C25	12.17	143.08	121.46
5	D	20	85Y	C23-C24-C29	-10.81	98.88	120.94
1	E	44	85Y	C4-N3-C2	-6.40	118.95	127.34
5	D	30	85Y	C4-N3-C2	-6.39	118.96	127.34
1	E	51	85Y	C4-N3-C2	-6.34	119.02	127.34
1	E	48	85Y	C4-N3-C2	-6.33	119.05	127.34
5	D	24	85Y	C4-N3-C2	-6.31	119.06	127.34
1	E	39	85Y	C4-N3-C2	-6.31	119.07	127.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	17	85Y	C4-N3-C2	-6.29	119.09	127.34
1	E	38	85Y	C4-N3-C2	-6.27	119.12	127.34
5	D	41	85Y	C4-N3-C2	-6.26	119.14	127.34
1	E	55	85Y	C4-N3-C2	-6.25	119.14	127.34
1	E	33	85Y	C4-N3-C2	-6.25	119.14	127.34
5	D	22	85Y	C4-N3-C2	-6.25	119.14	127.34
1	E	34	85Y	C4-N3-C2	-6.24	119.16	127.34
1	E	59	85Y	C4-N3-C2	-6.20	119.21	127.34
5	D	20	85Y	C4-N3-C2	-6.16	119.27	127.34
5	D	34	85Y	C4-N3-C2	-6.15	119.28	127.34
1	E	48	85Y	C5-C4-N3	6.08	125.09	114.45
1	E	53	85Y	C4-N3-C2	-6.08	119.37	127.34
1	E	33	85Y	C5-C4-N3	6.08	125.08	114.45
5	D	35	85Y	C4-N3-C2	-6.05	119.41	127.34
1	E	39	85Y	C5-C4-N3	5.93	124.82	114.45
1	E	44	85Y	C5-C4-N3	5.91	124.79	114.45
1	E	51	85Y	C5-C4-N3	5.89	124.75	114.45
1	E	34	85Y	C5-C4-N3	5.86	124.70	114.45
5	D	24	85Y	C5-C4-N3	5.86	124.69	114.45
5	D	35	85Y	C5-C4-N3	5.84	124.67	114.45
5	D	34	85Y	C5-C4-N3	5.84	124.67	114.45
1	E	44	85Y	C5-C6-N1	-5.83	114.58	123.06
5	D	22	85Y	C5-C4-N3	5.82	124.62	114.45
1	E	59	85Y	C5-C4-N3	5.77	124.55	114.45
5	D	20	85Y	C5-C4-N3	5.77	124.53	114.45
5	D	43	85Y	C4-N3-C2	-5.76	119.78	127.34
5	D	17	85Y	C5-C4-N3	5.75	124.51	114.45
1	E	53	85Y	C5-C4-N3	5.72	124.46	114.45
1	E	38	85Y	C5-C4-N3	5.70	124.42	114.45
5	D	41	85Y	C5-C4-N3	5.67	124.37	114.45
1	E	55	85Y	C5-C4-N3	5.64	124.31	114.45
5	D	17	85Y	C5-C6-N1	-5.52	115.03	123.06
1	E	38	85Y	C5-C6-N1	-5.50	115.06	123.06
5	D	30	85Y	C5-C4-N3	5.50	124.07	114.45
1	E	39	85Y	C5-C6-N1	-5.50	115.06	123.06
1	E	51	85Y	C5-C6-N1	-5.43	115.16	123.06
5	D	43	85Y	C5-C4-N3	5.42	123.93	114.45
5	D	22	85Y	C5-C6-N1	-5.38	115.23	123.06
1	E	48	85Y	C5-C6-N1	-5.36	115.26	123.06
5	D	30	85Y	C5-C6-N1	-5.32	115.32	123.06
1	E	34	85Y	C5-C6-N1	-5.28	115.37	123.06
5	D	34	85Y	C5-C6-N1	-5.27	115.40	123.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	55	85Y	C5-C6-N1	-5.18	115.52	123.06
1	E	33	85Y	C5-C6-N1	-5.16	115.56	123.06
5	D	20	85Y	C5-C6-N1	-5.13	115.59	123.06
1	E	53	85Y	C5-C6-N1	-5.11	115.62	123.06
5	D	41	85Y	C5-C6-N1	-5.08	115.66	123.06
5	D	24	85Y	C5-C6-N1	-5.01	115.77	123.06
5	D	35	85Y	C5-C6-N1	-5.00	115.78	123.06
5	D	30	85Y	N3-C2-N1	4.94	121.32	114.89
1	E	59	85Y	C5-C6-N1	-4.93	115.89	123.06
5	D	41	85Y	N3-C2-N1	4.74	121.06	114.89
1	E	59	85Y	N3-C2-N1	4.68	120.99	114.89
5	D	24	85Y	N3-C2-N1	4.65	120.94	114.89
1	E	55	85Y	N3-C2-N1	4.64	120.94	114.89
1	E	33	85Y	N3-C2-N1	4.63	120.91	114.89
1	E	44	85Y	N3-C2-N1	4.57	120.84	114.89
5	D	43	85Y	C20-C5-C4	4.57	126.30	122.64
5	D	43	85Y	N3-C2-N1	4.47	120.71	114.89
5	D	35	85Y	C5-C20-N22	4.38	126.02	116.67
5	D	20	85Y	N3-C2-N1	4.32	120.52	114.89
1	E	51	85Y	N3-C2-N1	4.27	120.45	114.89
5	D	22	85Y	N3-C2-N1	4.26	120.44	114.89
5	D	34	85Y	N3-C2-N1	4.26	120.43	114.89
1	E	34	85Y	N3-C2-N1	4.24	120.41	114.89
5	D	35	85Y	N3-C2-N1	4.21	120.38	114.89
5	D	35	85Y	C24-C23-N22	-4.21	104.20	113.07
5	D	35	85Y	C20-C5-C4	4.15	125.97	122.64
1	E	53	85Y	N3-C2-N1	4.13	120.27	114.89
1	E	39	85Y	N3-C2-N1	4.10	120.22	114.89
5	D	17	85Y	N3-C2-N1	4.08	120.21	114.89
5	D	43	85Y	C5-C6-N1	-4.08	117.13	123.06
1	E	38	85Y	N3-C2-N1	4.07	120.19	114.89
1	E	55	85Y	C5-C20-N22	4.07	125.34	116.67
1	E	48	85Y	N3-C2-N1	4.05	120.16	114.89
1	E	38	85Y	C24-C23-N22	-3.98	104.68	113.07
5	D	20	85Y	C24-C23-N22	3.91	121.31	113.07
5	D	35	85Y	O21-C20-N22	-3.60	116.85	123.35
1	E	44	85Y	C20-C5-C4	-3.50	119.84	122.64
1	E	33	85Y	O4'-C1'-N1	3.43	113.95	107.86
1	E	55	85Y	C24-C23-N22	-3.38	105.95	113.07
5	D	17	85Y	C23-N22-C20	-3.17	117.54	122.07
1	E	33	85Y	O21-C20-N22	-3.13	117.69	123.35
5	D	35	85Y	O4-C4-N3	-3.13	114.23	120.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	33	85Y	C5-C20-N22	3.12	123.33	116.67
5	D	41	85Y	C24-C23-N22	-3.10	106.55	113.07
1	E	44	85Y	O4-C4-C5	-3.06	119.23	125.98
1	E	55	85Y	O21-C20-N22	-3.00	117.93	123.35
1	E	33	85Y	C4'-O4'-C1'	-3.00	102.38	109.51
5	D	20	85Y	C23-N22-C20	-2.96	117.84	122.07
1	E	33	85Y	O4-C4-N3	-2.95	114.57	120.11
5	D	17	85Y	O4'-C1'-N1	2.95	113.09	107.86
1	E	39	85Y	O4-C4-C5	-2.85	119.71	125.98
1	E	48	85Y	O4-C4-C5	-2.83	119.73	125.98
5	D	34	85Y	O4-C4-C5	-2.82	119.78	125.98
1	E	44	85Y	C2'-C3'-C4'	2.81	108.51	102.80
5	D	17	85Y	O4-C4-C5	-2.81	119.79	125.98
1	E	38	85Y	O4-C4-C5	-2.78	119.86	125.98
1	E	33	85Y	O4'-C1'-C2'	-2.76	101.09	106.25
5	D	22	85Y	O4-C4-C5	-2.75	119.92	125.98
5	D	24	85Y	O4-C4-C5	-2.74	119.94	125.98
1	E	53	85Y	O4-C4-C5	-2.72	119.99	125.98
1	E	51	85Y	O4-C4-C5	-2.71	120.00	125.98
5	D	30	85Y	C24-C23-N22	-2.69	107.41	113.07
1	E	34	85Y	O4-C4-C5	-2.68	120.08	125.98
5	D	41	85Y	O4-C4-C5	-2.68	120.08	125.98
1	E	59	85Y	O4-C4-C5	-2.67	120.09	125.98
1	E	55	85Y	O4-C4-C5	-2.64	120.15	125.98
5	D	20	85Y	O4-C4-C5	-2.63	120.18	125.98
1	E	48	85Y	O4-C4-N3	-2.63	115.17	120.11
5	D	20	85Y	C5-C20-N22	2.61	122.24	116.67
5	D	22	85Y	C5-C20-N22	2.61	122.23	116.67
1	E	34	85Y	O4-C4-N3	-2.60	115.23	120.11
1	E	38	85Y	O4'-C1'-N1	2.60	112.47	107.86
1	E	53	85Y	C4'-O4'-C1'	-2.59	103.35	109.51
1	E	51	85Y	O4-C4-N3	-2.59	115.25	120.11
5	D	20	85Y	O4-C4-N3	-2.57	115.29	120.11
5	D	30	85Y	O2-C2-N1	-2.57	119.45	122.80
5	D	30	85Y	O4-C4-N3	-2.56	115.30	120.11
5	D	41	85Y	O2-C2-N1	-2.56	119.47	122.80
1	E	33	85Y	O4-C4-C5	-2.56	120.35	125.98
5	D	41	85Y	C23-N22-C20	-2.56	118.42	122.07
5	D	35	85Y	C4'-O4'-C1'	-2.54	103.47	109.51
1	E	38	85Y	C20-C5-C4	2.54	124.68	122.64
5	D	43	85Y	O4-C4-C5	-2.54	120.39	125.98
1	E	59	85Y	O4-C4-N3	-2.53	115.36	120.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	34	85Y	C4'-O4'-C1'	-2.53	103.50	109.51
5	D	24	85Y	O4-C4-N3	-2.53	115.36	120.11
1	E	38	85Y	C4'-O4'-C1'	-2.52	103.51	109.51
5	D	20	85Y	C20-C5-C4	2.48	124.63	122.64
5	D	22	85Y	O4-C4-N3	-2.48	115.45	120.11
1	E	55	85Y	O21-C20-C5	-2.47	116.73	121.04
1	E	39	85Y	O4-C4-N3	-2.47	115.47	120.11
1	E	53	85Y	O4'-C1'-N1	2.47	112.24	107.86
5	D	22	85Y	O21-C20-N22	-2.46	118.91	123.35
1	E	55	85Y	O4-C4-N3	-2.44	115.53	120.11
5	D	41	85Y	O4-C4-N3	-2.43	115.55	120.11
5	D	30	85Y	O4-C4-C5	-2.43	120.63	125.98
1	E	53	85Y	O4-C4-N3	-2.42	115.56	120.11
5	D	34	85Y	O4-C4-N3	-2.42	115.56	120.11
5	D	20	85Y	O2-C2-N1	-2.39	119.69	122.80
1	E	59	85Y	O2-C2-N1	-2.38	119.70	122.80
5	D	43	85Y	O2-C2-N1	-2.37	119.71	122.80
5	D	22	85Y	O2-C2-N1	-2.37	119.71	122.80
5	D	24	85Y	O2-C2-N1	-2.37	119.71	122.80
5	D	41	85Y	O4'-C1'-C2'	-2.37	101.82	106.25
1	E	38	85Y	C23-N22-C20	-2.36	118.69	122.07
1	E	55	85Y	O2-C2-N1	-2.36	119.73	122.80
5	D	43	85Y	O4-C4-N3	-2.36	115.68	120.11
1	E	55	85Y	C20-C5-C4	2.36	124.53	122.64
5	D	17	85Y	O4-C4-N3	-2.35	115.69	120.11
1	E	34	85Y	C24-C23-N22	-2.34	108.14	113.07
1	E	38	85Y	O4-C4-N3	-2.34	115.72	120.11
1	E	44	85Y	O2-C2-N1	-2.33	119.76	122.80
1	E	38	85Y	O2-C2-N1	-2.30	119.80	122.80
1	E	53	85Y	C20-C5-C4	2.27	124.46	122.64
5	D	17	85Y	O2-C2-N1	-2.27	119.84	122.80
1	E	44	85Y	C3'-C2'-C1'	2.26	108.13	102.60
1	E	53	85Y	O2-C2-N1	-2.26	119.86	122.80
5	D	30	85Y	O4'-C1'-C2'	-2.25	102.04	106.25
5	D	35	85Y	O21-C20-C5	-2.24	117.13	121.04
5	D	17	85Y	C5-C20-N22	2.24	121.45	116.67
5	D	35	85Y	O4-C4-C5	-2.22	121.10	125.98
1	E	34	85Y	O2-C2-N1	-2.21	119.92	122.80
1	E	44	85Y	O4-C4-N3	-2.20	115.98	120.11
1	E	39	85Y	O4'-C1'-N1	2.19	111.74	107.86
5	D	20	85Y	O21-C20-N22	-2.19	119.41	123.35
1	E	53	85Y	O4'-C1'-C2'	-2.14	102.24	106.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	35	85Y	O2-C2-N1	-2.13	120.02	122.80
5	D	17	85Y	C2'-C3'-C4'	2.13	107.12	102.80
5	D	22	85Y	C4'-O4'-C1'	-2.12	104.48	109.51
5	D	17	85Y	C1'-N1-C6	-2.11	117.19	120.74
1	E	39	85Y	O2-C2-N1	-2.11	120.05	122.80
5	D	34	85Y	O2-C2-N1	-2.10	120.06	122.80
1	E	34	85Y	C20-C5-C4	2.10	124.32	122.64
5	D	17	85Y	C4'-O4'-C1'	-2.08	104.56	109.51
1	E	34	85Y	O4'-C1'-C2'	-2.08	102.36	106.25
1	E	38	85Y	O4'-C1'-C2'	-2.07	102.38	106.25
1	E	33	85Y	O2-C2-N1	-2.07	120.11	122.80
5	D	43	85Y	C6-N1-C2	-2.06	119.25	121.30
5	D	17	85Y	C1'-N1-C2	2.06	121.69	117.66
5	D	22	85Y	C2'-C3'-C4'	2.06	106.98	102.80
1	E	53	85Y	C2'-C3'-C4'	2.06	106.98	102.80
1	E	48	85Y	O2-C2-N1	-2.05	120.12	122.80
1	E	34	85Y	C2'-C3'-C4'	2.04	106.94	102.80
1	E	44	85Y	O4'-C1'-N1	2.03	111.46	107.86
5	D	35	85Y	O4'-C1'-C2'	-2.02	102.46	106.25

There are no chirality outliers.

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	33	85Y	O21-C20-C5-C4
1	E	33	85Y	N22-C20-C5-C4
1	E	33	85Y	C5-C20-N22-C23
1	E	33	85Y	O21-C20-N22-C23
1	E	34	85Y	O21-C20-C5-C4
1	E	34	85Y	N22-C20-C5-C4
1	E	34	85Y	N22-C20-C5-C6
1	E	34	85Y	O4'-C1'-N1-C2
1	E	34	85Y	O4'-C1'-N1-C6
1	E	38	85Y	O21-C20-C5-C4
1	E	38	85Y	O21-C20-C5-C6
1	E	38	85Y	N22-C20-C5-C4
1	E	38	85Y	O4'-C1'-N1-C2
1	E	38	85Y	O4'-C1'-N1-C6
1	E	39	85Y	O21-C20-C5-C4
1	E	39	85Y	O4'-C1'-N1-C2
1	E	39	85Y	O4'-C1'-N1-C6
1	E	48	85Y	O21-C20-C5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	E	48	85Y	O21-C20-C5-C6
1	E	48	85Y	N22-C20-C5-C4
1	E	48	85Y	N22-C20-C5-C6
1	E	48	85Y	O4'-C1'-N1-C2
1	E	51	85Y	O21-C20-C5-C4
1	E	51	85Y	N22-C20-C5-C4
1	E	51	85Y	N22-C20-C5-C6
1	E	53	85Y	O21-C20-C5-C4
1	E	53	85Y	O21-C20-C5-C6
1	E	53	85Y	N22-C20-C5-C4
1	E	53	85Y	N22-C20-C5-C6
1	E	53	85Y	C24-C23-N22-C20
1	E	53	85Y	O4'-C1'-N1-C2
1	E	53	85Y	O4'-C1'-N1-C6
1	E	55	85Y	O21-C20-C5-C4
1	E	55	85Y	O21-C20-C5-C6
1	E	55	85Y	N22-C20-C5-C4
1	E	55	85Y	N22-C20-C5-C6
1	E	55	85Y	C5-C20-N22-C23
1	E	55	85Y	O21-C20-N22-C23
1	E	59	85Y	O21-C20-C5-C4
1	E	59	85Y	O21-C20-C5-C6
1	E	59	85Y	N22-C20-C5-C4
1	E	59	85Y	N22-C20-C5-C6
1	E	59	85Y	O4'-C1'-N1-C2
5	D	17	85Y	O21-C20-C5-C4
5	D	17	85Y	O21-C20-C5-C6
5	D	17	85Y	N22-C20-C5-C4
5	D	17	85Y	N22-C20-C5-C6
5	D	17	85Y	O4'-C1'-N1-C2
5	D	17	85Y	O4'-C1'-N1-C6
5	D	22	85Y	O21-C20-C5-C4
5	D	22	85Y	O21-C20-C5-C6
5	D	22	85Y	N22-C20-C5-C4
5	D	22	85Y	N22-C20-C5-C6
5	D	22	85Y	C5-C20-N22-C23
5	D	22	85Y	O21-C20-N22-C23
5	D	22	85Y	C4'-C5'-O5'-P
5	D	24	85Y	O21-C20-C5-C4
5	D	24	85Y	N22-C20-C5-C4
5	D	30	85Y	O21-C20-C5-C4
5	D	30	85Y	O21-C20-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	30	85Y	N22-C20-C5-C4
5	D	30	85Y	N22-C20-C5-C6
5	D	34	85Y	O21-C20-C5-C4
5	D	34	85Y	O21-C20-C5-C6
5	D	34	85Y	N22-C20-C5-C4
5	D	34	85Y	N22-C20-C5-C6
5	D	34	85Y	O4'-C4'-C5'-O5'
5	D	34	85Y	C3'-C4'-C5'-O5'
5	D	35	85Y	O21-C20-C5-C4
5	D	35	85Y	N22-C20-C5-C4
5	D	35	85Y	C5-C20-N22-C23
5	D	35	85Y	O21-C20-N22-C23
5	D	41	85Y	O21-C20-C5-C4
5	D	41	85Y	O21-C20-C5-C6
5	D	41	85Y	N22-C20-C5-C4
5	D	41	85Y	N22-C20-C5-C6
5	D	43	85Y	O21-C20-C5-C4
5	D	43	85Y	O21-C20-C5-C6
5	D	43	85Y	N22-C20-C5-C4
5	D	43	85Y	N22-C20-C5-C6
5	D	43	85Y	O4'-C1'-N1-C2
5	D	24	85Y	C24-C23-N22-C20
1	E	48	85Y	O4'-C1'-N1-C6
1	E	59	85Y	O4'-C1'-N1-C6
5	D	43	85Y	O4'-C1'-N1-C6
5	D	22	85Y	O4'-C1'-N1-C2
5	D	41	85Y	O4'-C1'-N1-C2
1	E	48	85Y	O4'-C4'-C5'-O5'
1	E	48	85Y	C3'-C4'-C5'-O5'
1	E	53	85Y	C3'-C4'-C5'-O5'
5	D	17	85Y	O4'-C4'-C5'-O5'
1	E	55	85Y	C4'-C5'-O5'-P
5	D	34	85Y	C24-C23-N22-C20
1	E	48	85Y	C24-C23-N22-C20
1	E	34	85Y	O4'-C4'-C5'-O5'
1	E	53	85Y	O4'-C4'-C5'-O5'
5	D	43	85Y	O4'-C4'-C5'-O5'
5	D	43	85Y	C3'-C4'-C5'-O5'
5	D	41	85Y	O4'-C1'-N1-C6
1	E	34	85Y	C24-C23-N22-C20
5	D	41	85Y	C2'-C1'-N1-C6
5	D	22	85Y	O4'-C1'-N1-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	30	85Y	O4'-C1'-N1-C6
1	E	34	85Y	C3'-C4'-C5'-O5'
5	D	22	85Y	C3'-C4'-C5'-O5'
1	E	59	85Y	C2'-C1'-N1-C6
5	D	30	85Y	C2'-C1'-N1-C6
5	D	30	85Y	C2'-C1'-N1-C2
1	E	51	85Y	C3'-C4'-C5'-O5'
5	D	30	85Y	O4'-C1'-N1-C2
1	E	51	85Y	O4'-C4'-C5'-O5'
5	D	20	85Y	O4'-C4'-C5'-O5'
5	D	35	85Y	O4'-C4'-C5'-O5'
5	D	35	85Y	C3'-C4'-C5'-O5'
5	D	41	85Y	C2'-C1'-N1-C2
1	E	55	85Y	C3'-C4'-C5'-O5'
5	D	22	85Y	O4'-C4'-C5'-O5'
1	E	51	85Y	C2'-C1'-N1-C2
5	D	17	85Y	C3'-C4'-C5'-O5'
5	D	24	85Y	C2'-C1'-N1-C6
5	D	43	85Y	C2'-C1'-N1-C6
1	E	33	85Y	O21-C20-C5-C6
1	E	34	85Y	O21-C20-C5-C6
1	E	51	85Y	O21-C20-C5-C6
5	D	24	85Y	O21-C20-C5-C6
5	D	35	85Y	O21-C20-C5-C6
1	E	33	85Y	N22-C20-C5-C6
1	E	38	85Y	N22-C20-C5-C6
5	D	35	85Y	N22-C20-C5-C6
1	E	59	85Y	C2'-C1'-N1-C2
5	D	34	85Y	C4'-C5'-O5'-P
5	D	43	85Y	C2'-C1'-N1-C2
5	D	24	85Y	C2'-C1'-N1-C2
1	E	38	85Y	C3'-C4'-C5'-O5'
5	D	24	85Y	O4'-C1'-N1-C6
1	E	51	85Y	C2'-C1'-N1-C6
5	D	43	85Y	C4'-C5'-O5'-P
1	E	39	85Y	O21-C20-C5-C6
5	D	24	85Y	O4'-C1'-N1-C2
1	E	48	85Y	C4'-C5'-O5'-P
1	E	55	85Y	O4'-C4'-C5'-O5'
5	D	24	85Y	N22-C20-C5-C6
1	E	34	85Y	C4'-C5'-O5'-P
1	E	38	85Y	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	E	33	85Y	C2'-C1'-N1-C2

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	53	85Y	1	0
5	D	34	85Y	1	0
1	E	59	85Y	1	0
5	D	43	85Y	1	0
5	D	35	85Y	1	0
1	E	55	85Y	2	0
1	E	33	85Y	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
6	NAG	C	701	4	14,14,15	0.78	0	17,19,21	0.94	1 (5%)

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
6	NAG	C	701	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	701	NAG	C1-O5-C5	2.13	115.04	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

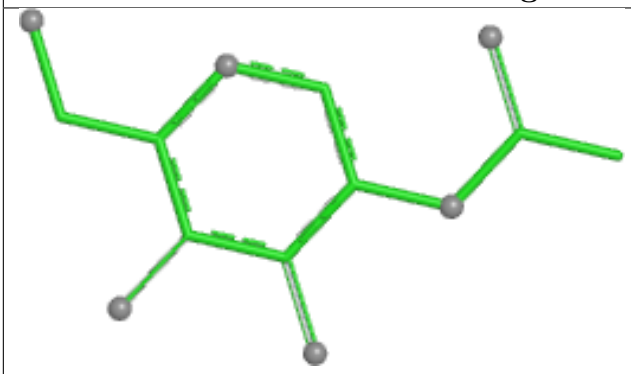
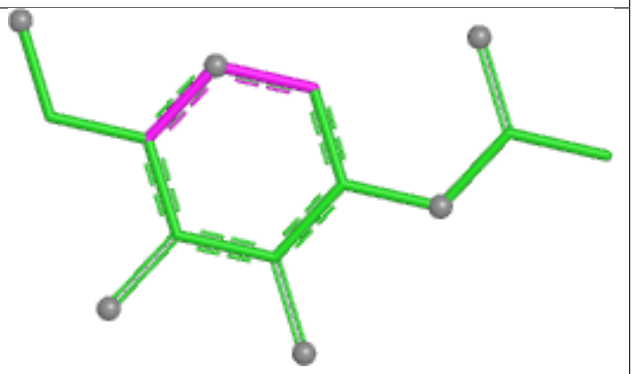
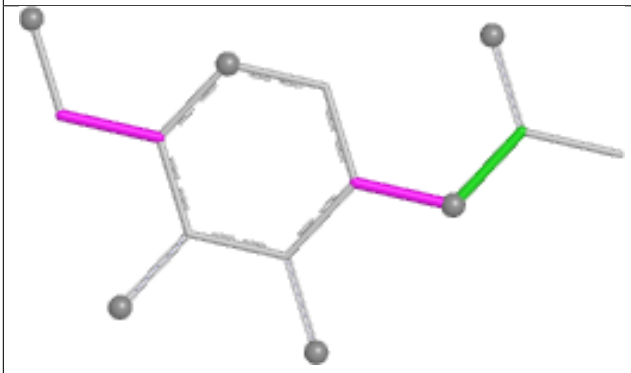
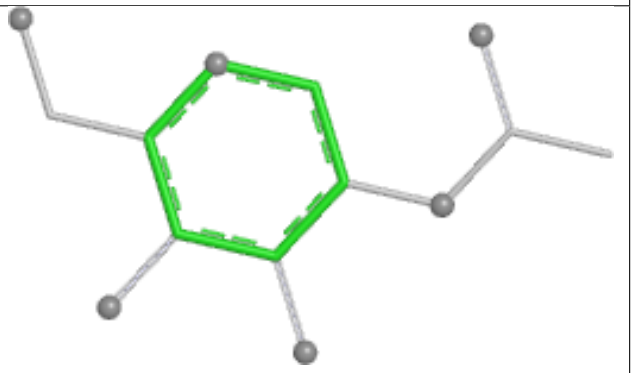
Mol	Chain	Res	Type	Atoms
6	C	701	NAG	C4-C5-C6-O6
6	C	701	NAG	O5-C5-C6-O6
6	C	701	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	701	NAG	4	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 NAG C 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35945. These allow visual inspection of the internal detail of the map and identification of artifacts.

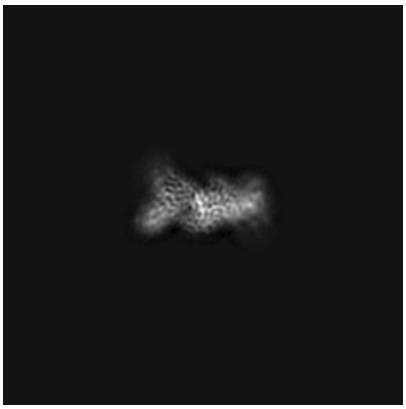
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

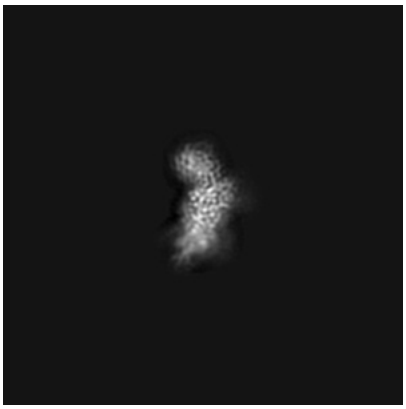
6.1.1 Primary map



X

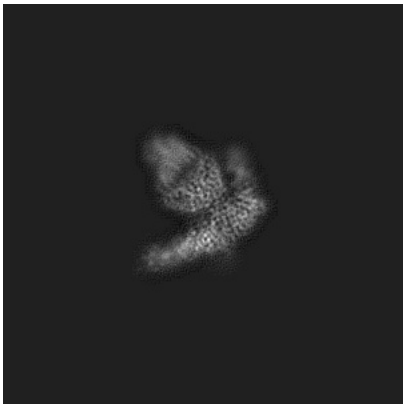


Y

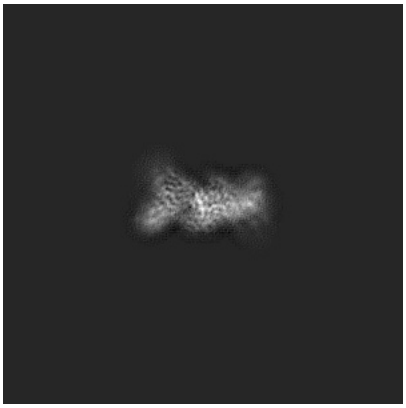


Z

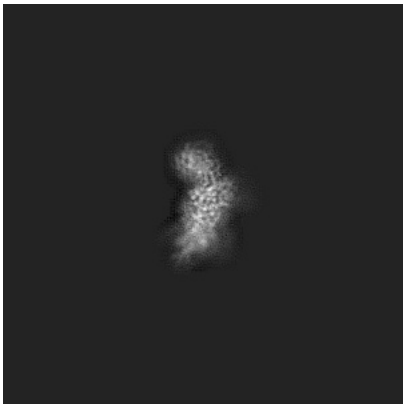
6.1.2 Raw map



X



Y

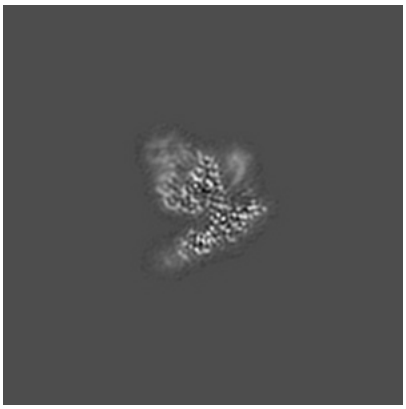


Z

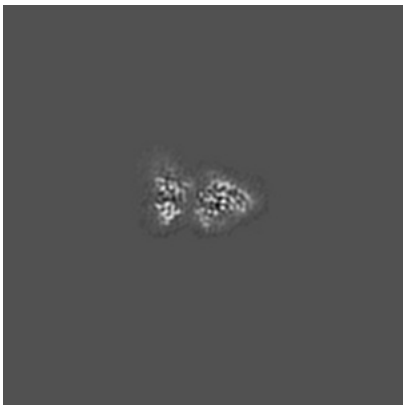
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 192

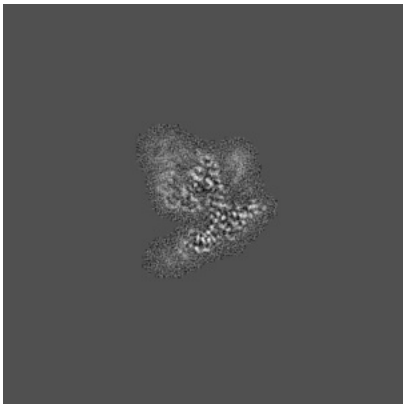


Y Index: 192

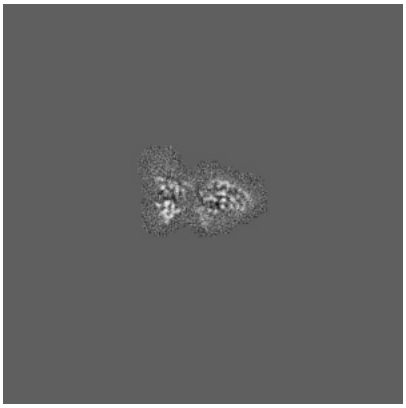


Z Index: 192

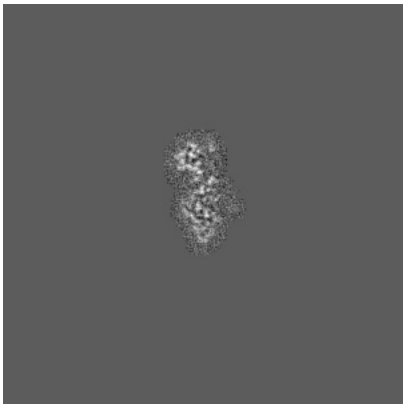
6.2.2 Raw map



X Index: 192



Y Index: 192

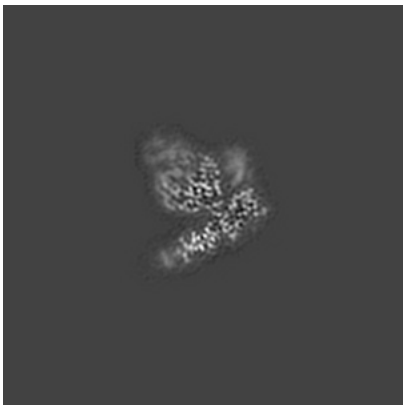


Z Index: 192

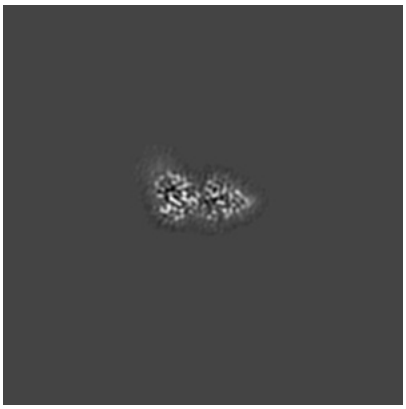
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 189

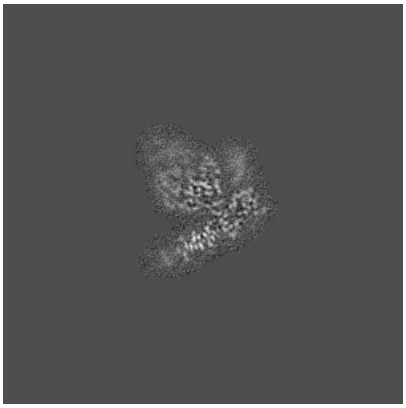


Y Index: 201

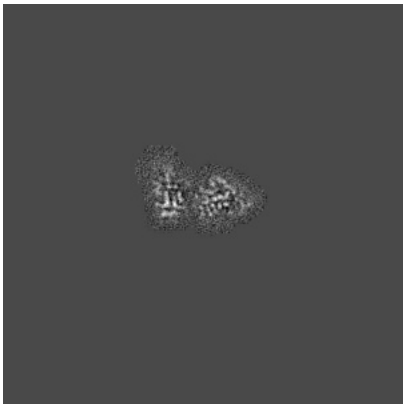


Z Index: 191

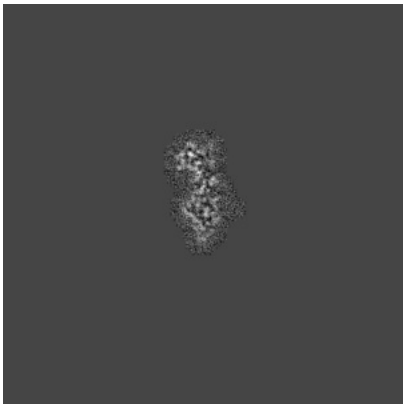
6.3.2 Raw map



X Index: 189



Y Index: 197

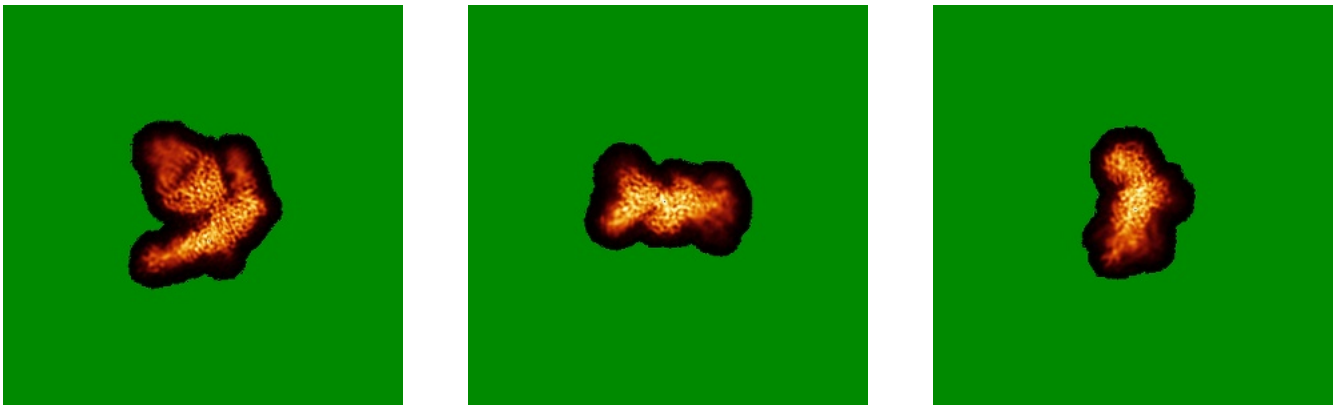


Z Index: 191

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

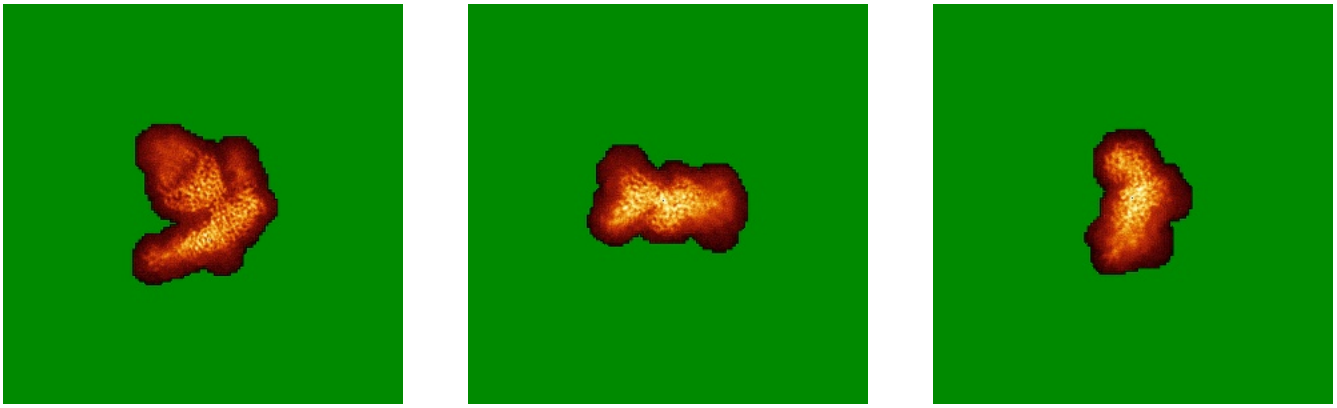
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

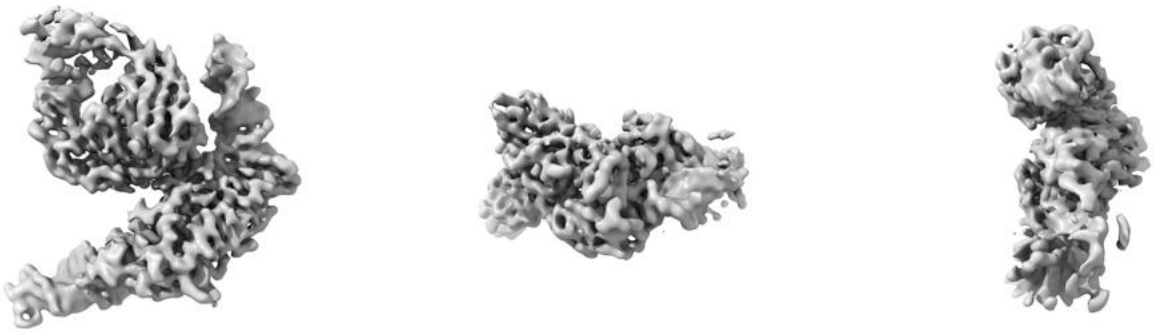


X Y Z

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)

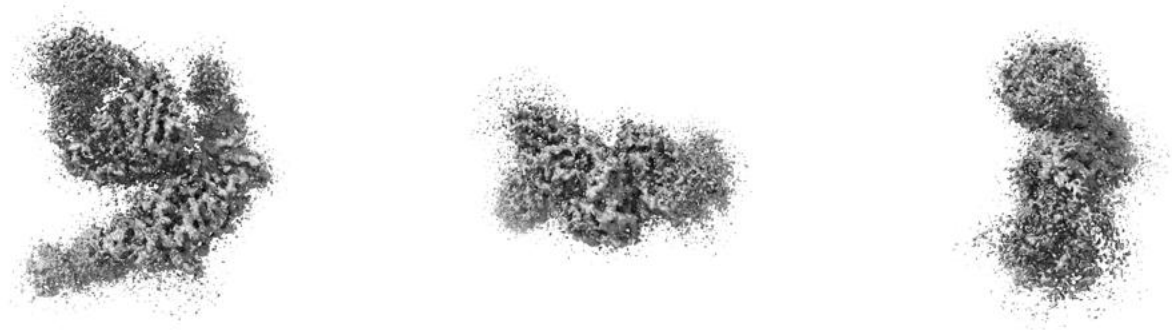
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. 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.

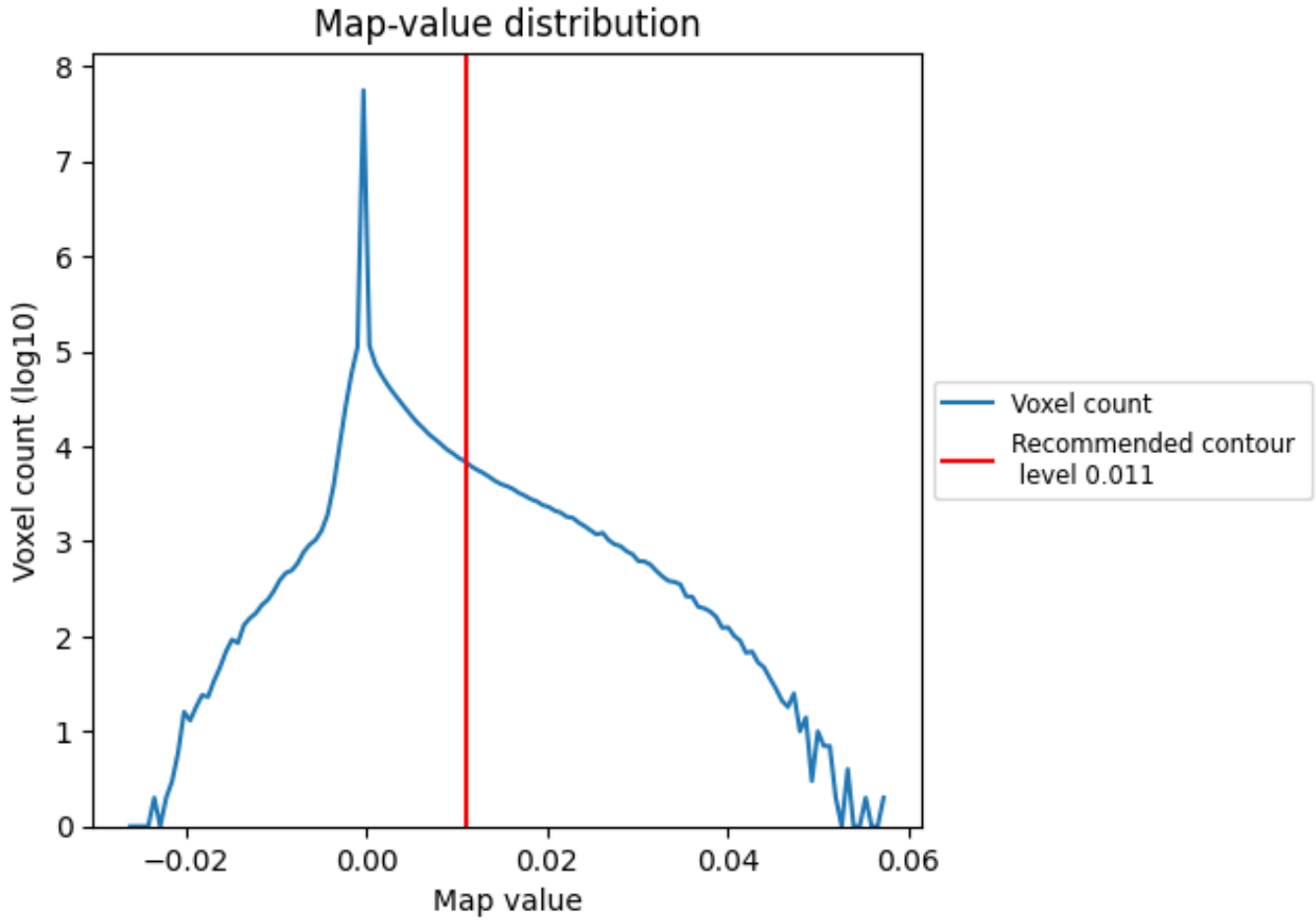
6.6 Mask visualisation (i)

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

7 Map analysis

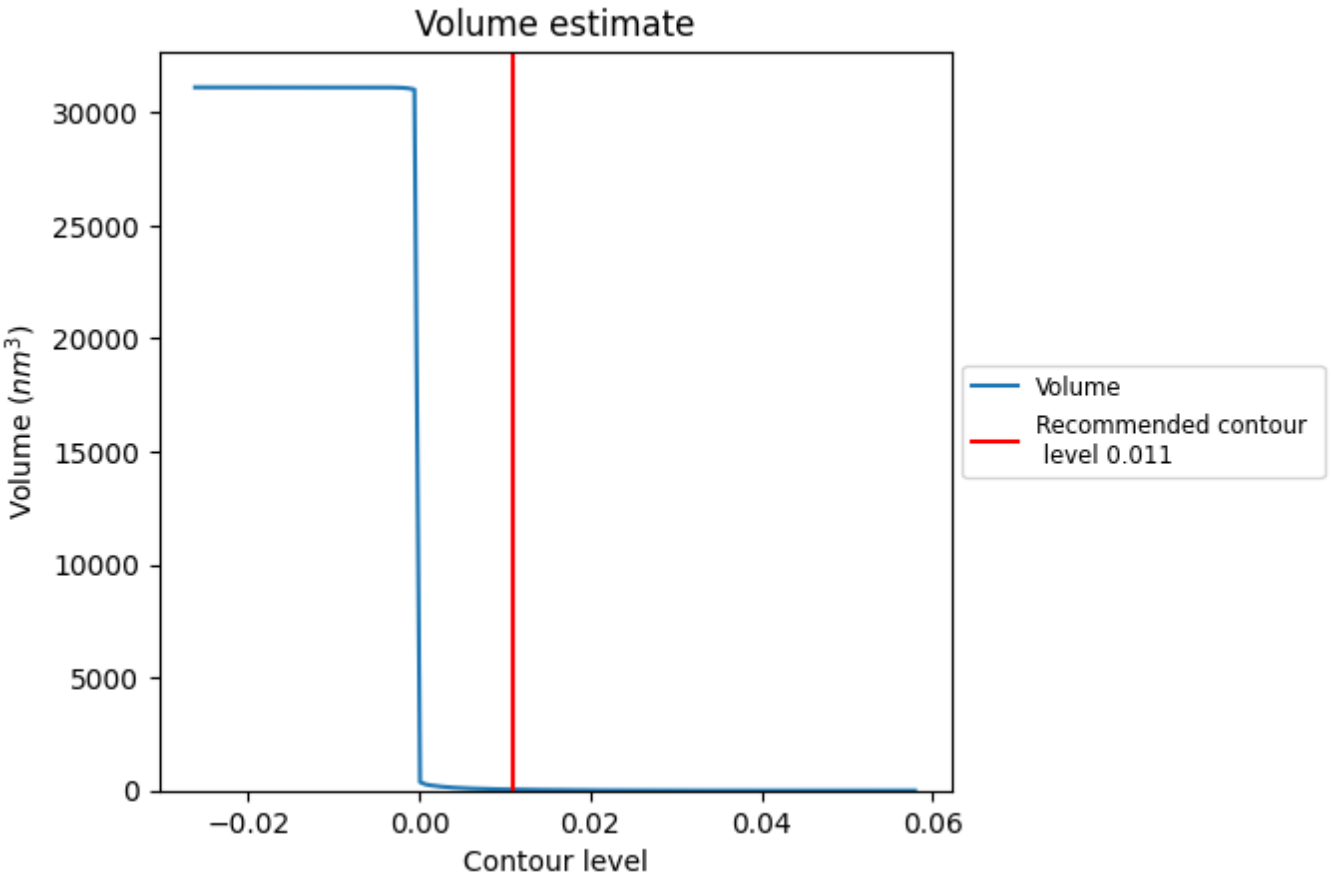
This section contains the results of statistical analysis of the map.

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.

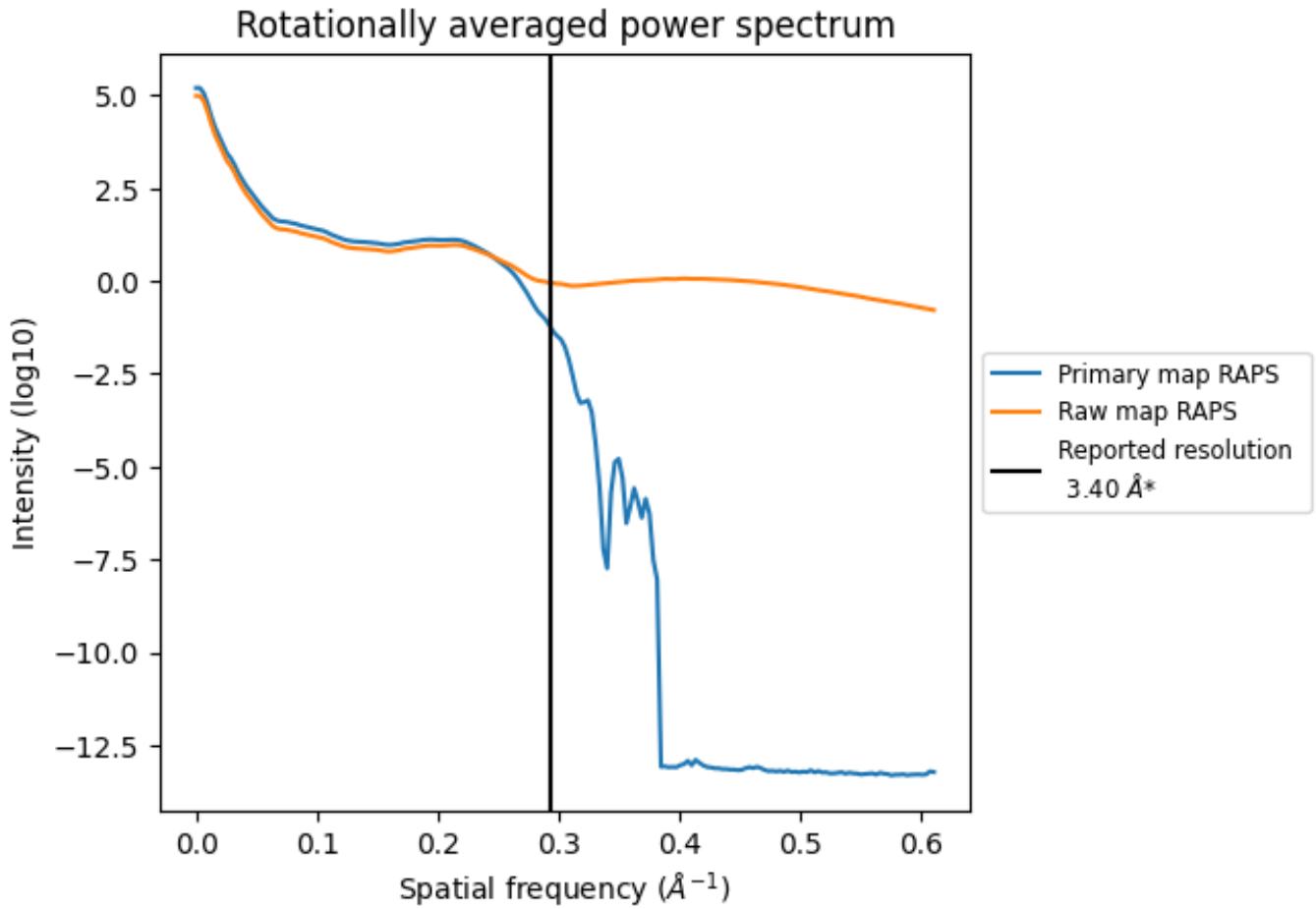
7.2 Volume estimate



The volume at the recommended contour level is 46 nm^3; this corresponds to an approximate mass of 42 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)

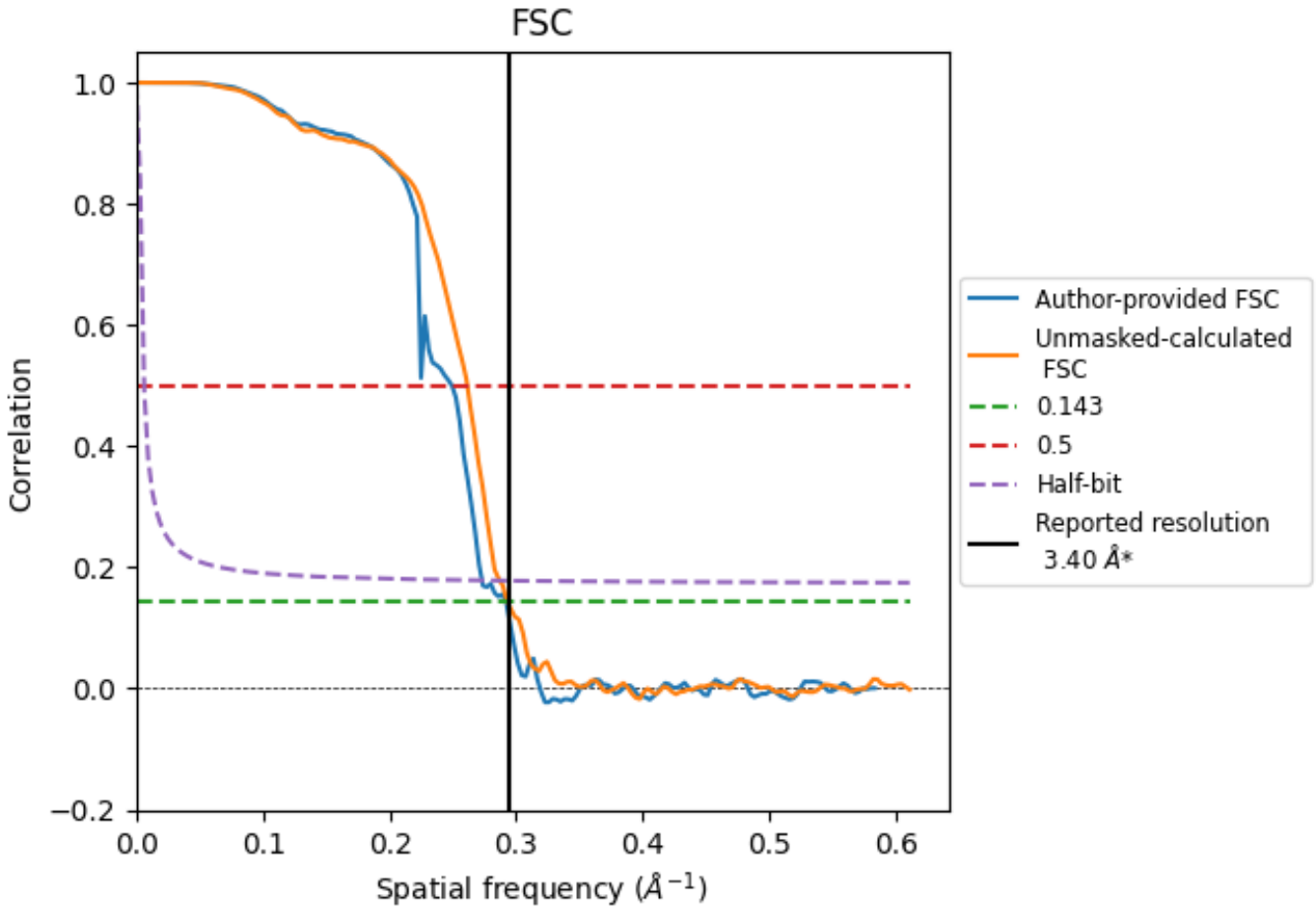


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

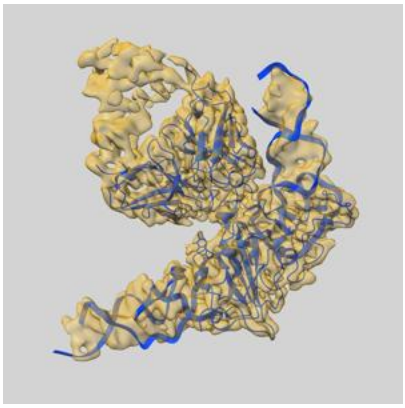
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	4.01	3.66
Unmasked-calculated*	3.41	3.83	3.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

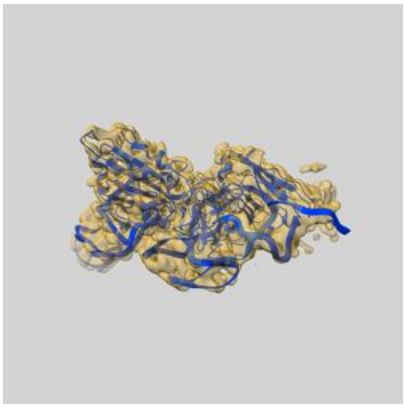
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35945 and PDB model 8J26. Per-residue inclusion information can be found in section 3 on page 7.

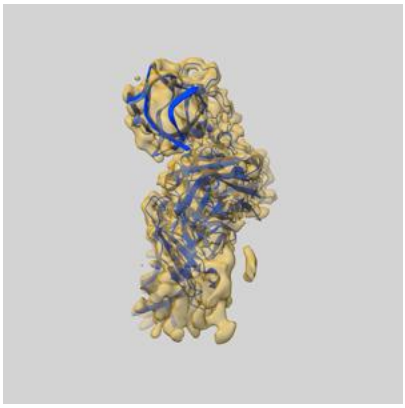
9.1 Map-model overlay



X



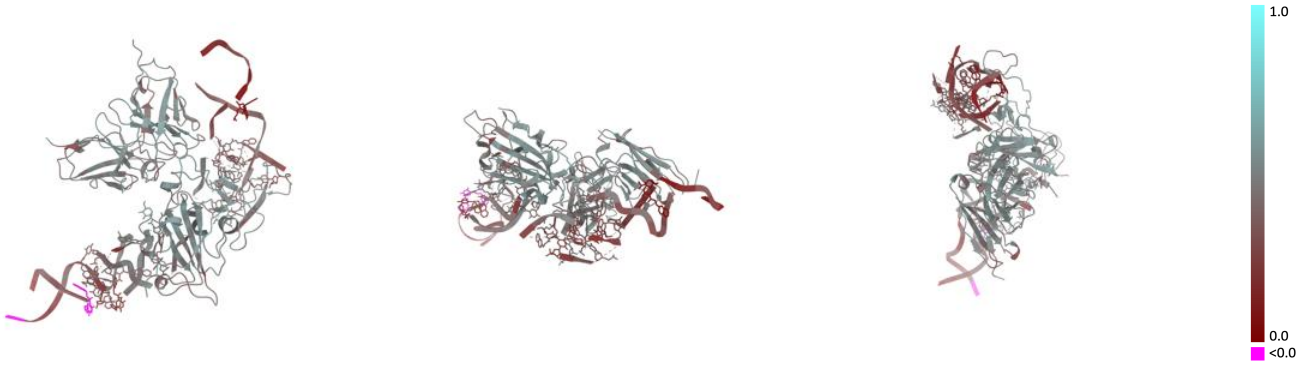
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 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.

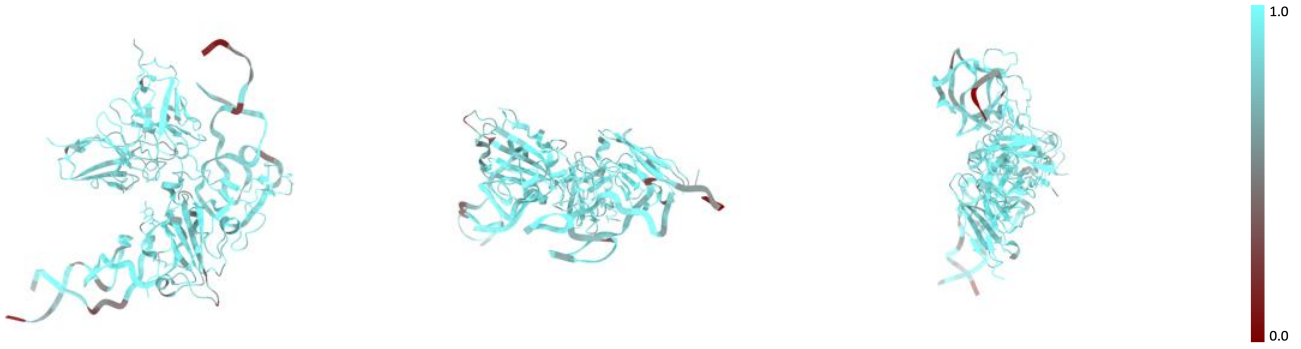
9.2 Q-score mapped to coordinate model



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.

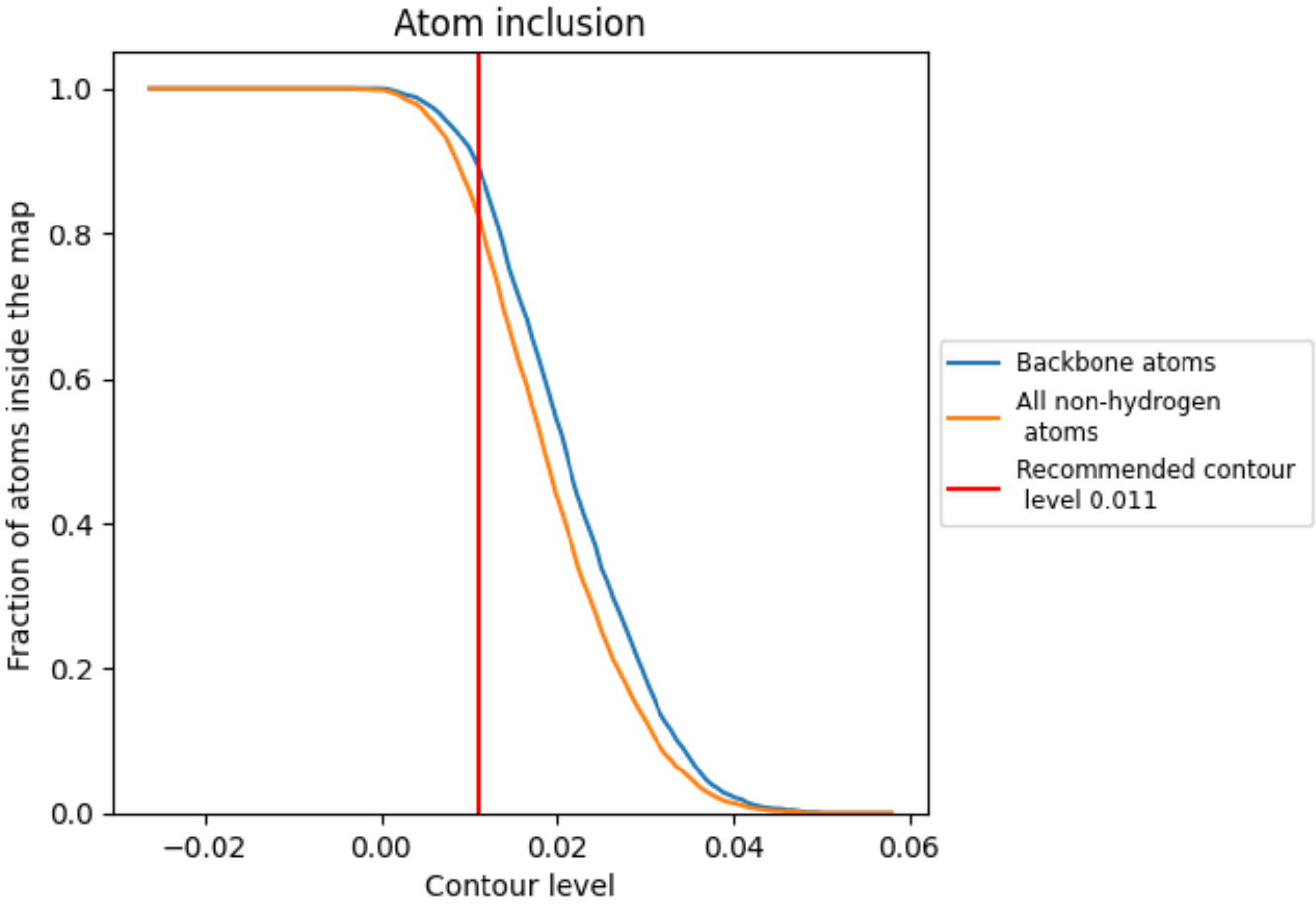
9.3 Atom inclusion mapped to coordinate model



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 (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8260	0.4280
A	0.8640	0.4840
B	0.8820	0.4960
C	0.8570	0.5080
D	0.7990	0.3250
E	0.7260	0.3090

