Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 04:40 PM EDT

PDB ID	:	7RTM
EMDB ID	:	EMD-24683
Title	:	Cryo-EM Structure of the Sodium-driven Chloride/Bicarbonate Exchanger NDCBE (SLC4A8)
Authors	:	Wang, W.G.; Tsirulnikov, K.; Zhekova, H.; Kayik, G.; Muhammad-Khan, H.; Azimov, R.; Abuladze, N.; Kao, L.; Newman, D.; Noskov, S.Y.; Zhou, Z.H.; Pushkin, A.; Kurtz, I.
Deposited on	:	2021-08-13
Resolution	:	3.40 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:

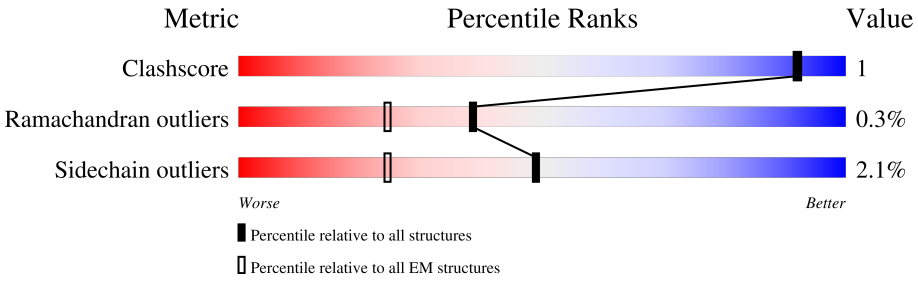
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	571	58% 83% 15%
1	B	571	59% 81% 17%
2	C	3	100% 67% 33%
2	D	3	100% 100%

2 Entry composition

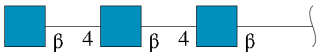
There are 5 unique types of molecules in this entry. The entry contains 9161 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Electroneutral sodium bicarbonate exchanger 1.

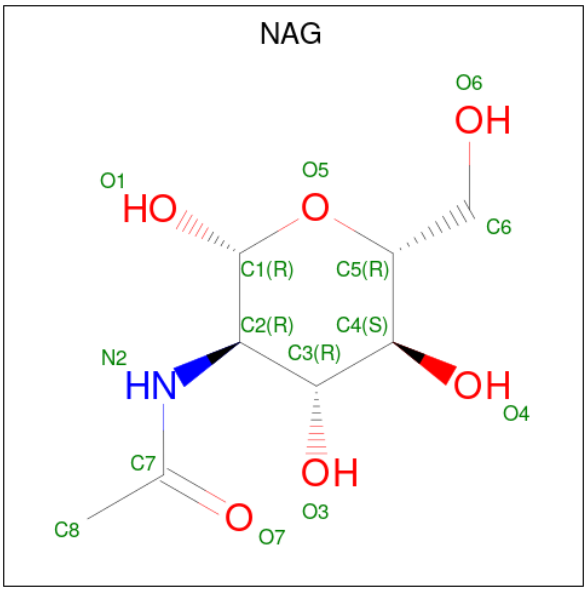
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	571	Total	C	N	O	S	0	0
			4520	2993	722	767	38		
1	B	571	Total	C	N	O	S	0	0
			4519	2993	722	766	38		

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	3	Total	C	N	O	0	0
			42	24	3	15		
2	D	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

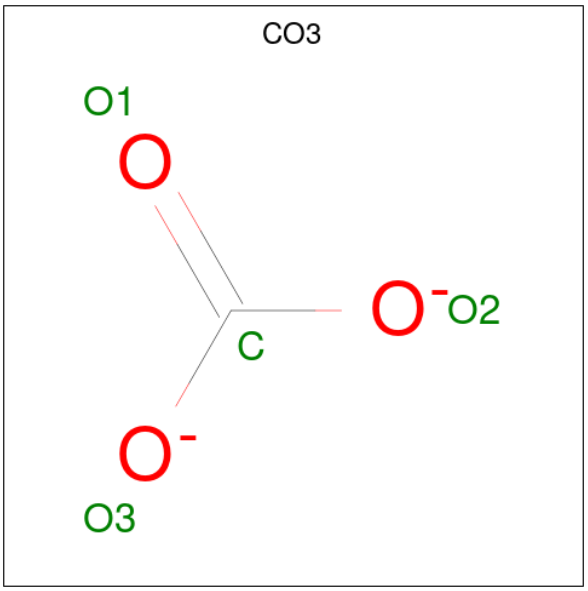


Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Na 1 1	0
4	B	1	Total Na 1 1	0

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO_3) (labeled as "Ligand of Interest" by depositor).



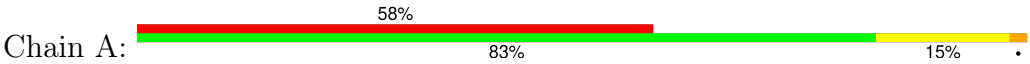
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			4	1	3	
5	B	1	Total	C	O	0
			4	1	3	

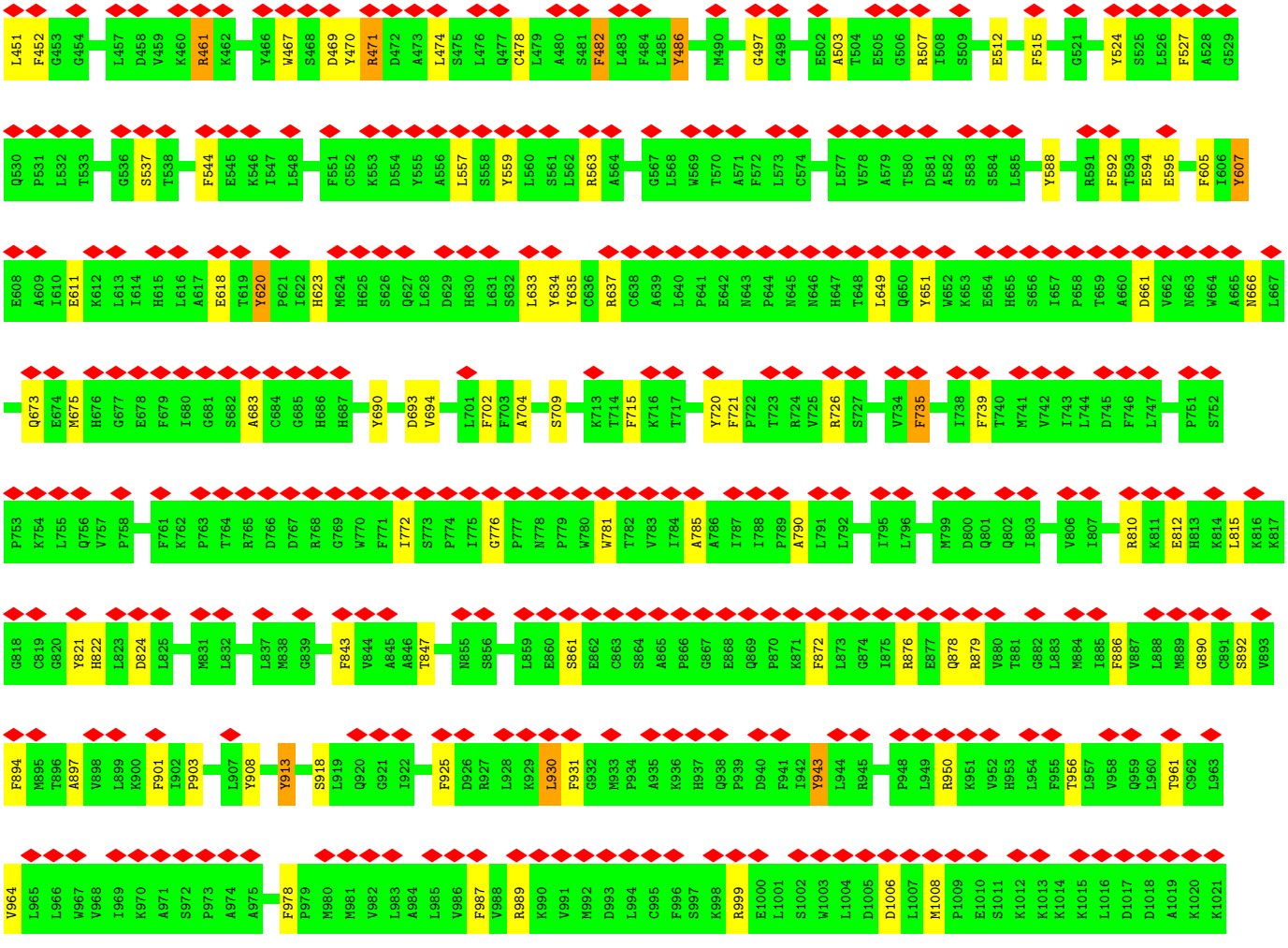
3 Residue-property plots (i)

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: Electroneutral sodium bicarbonate exchanger 1

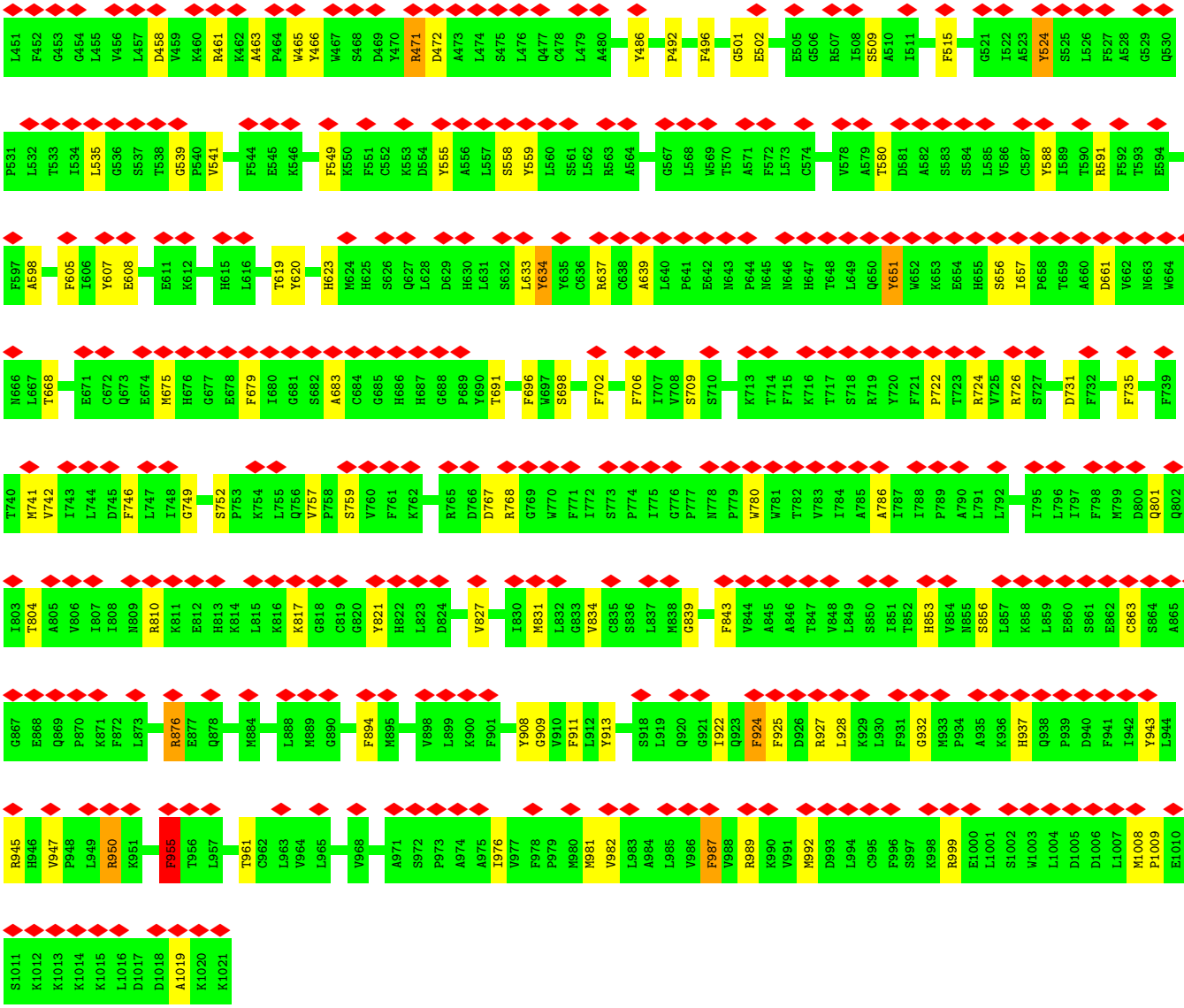
Chain A:





• Molecule 1: Electroneutral sodium bicarbonate exchanger 1

Chain B:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	380776	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	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0351	Depositor
Map size (Å)	265.36002, 265.36002, 265.36002	wwPDB
Map dimensions	248, 248, 248	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, NAG, NA

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	1.50	34/4647 (0.7%)	1.73	94/6319 (1.5%)
1	B	1.53	35/4646 (0.8%)	1.72	99/6318 (1.6%)
All	All	1.51	69/9293 (0.7%)	1.73	193/12637 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	11
All	All	0	20

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	ARG	NE-CZ	9.09	1.44	1.33
1	B	501	GLY	CA-C	-7.95	1.39	1.51
1	B	607	TYR	CG-CD1	7.32	1.48	1.39
1	B	863	CYS	CB-SG	7.11	1.94	1.82
1	A	607	TYR	CZ-OH	6.97	1.49	1.37
1	A	588	TYR	CE2-CZ	6.94	1.47	1.38
1	A	821	TYR	CZ-OH	6.83	1.49	1.37
1	B	726	ARG	NE-CZ	6.71	1.41	1.33
1	A	918	SER	CB-OG	6.44	1.50	1.42
1	B	696	PHE	CG-CD1	6.43	1.48	1.38
1	B	927	ARG	NE-CZ	6.41	1.41	1.33
1	B	620	TYR	CZ-OH	6.40	1.48	1.37
1	B	724	ARG	CZ-NH2	6.32	1.41	1.33
1	B	591	ARG	CZ-NH2	6.25	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	950	ARG	CZ-NH1	6.23	1.41	1.33
1	B	853	HIS	CB-CG	6.18	1.61	1.50
1	B	620	TYR	CE2-CZ	6.15	1.46	1.38
1	B	856	SER	CA-CB	6.11	1.62	1.52
1	A	810	ARG	CZ-NH2	6.05	1.41	1.33
1	B	810	ARG	CZ-NH1	6.00	1.40	1.33
1	A	461	ARG	CZ-NH1	5.98	1.40	1.33
1	A	524	TYR	CE2-CZ	5.96	1.46	1.38
1	A	925	PHE	CG-CD1	5.96	1.47	1.38
1	B	605	PHE	CG-CD1	5.95	1.47	1.38
1	B	749	GLY	CA-C	-5.94	1.42	1.51
1	A	470	TYR	CE2-CZ	5.86	1.46	1.38
1	A	821	TYR	CG-CD1	5.79	1.46	1.39
1	B	651	TYR	CZ-OH	5.76	1.47	1.37
1	B	843	PHE	CG-CD1	5.73	1.47	1.38
1	B	768	ARG	CZ-NH2	5.70	1.40	1.33
1	B	702	PHE	N-CA	-5.68	1.34	1.46
1	A	618	GLU	CB-CG	5.68	1.62	1.52
1	A	709	SER	CA-CB	5.68	1.61	1.52
1	B	722	PRO	N-CD	5.65	1.55	1.47
1	A	452	PHE	CE2-CZ	5.64	1.48	1.37
1	A	595	GLU	CD-OE2	5.56	1.31	1.25
1	A	702	PHE	CG-CD2	5.54	1.47	1.38
1	A	897	ALA	C-N	5.53	1.46	1.34
1	A	524	TYR	CZ-OH	5.52	1.47	1.37
1	B	637	ARG	NE-CZ	5.52	1.40	1.33
1	A	607	TYR	CG-CD2	5.51	1.46	1.39
1	B	801	GLN	N-CA	-5.50	1.35	1.46
1	A	872	PHE	CB-CG	5.49	1.60	1.51
1	B	465	TRP	NE1-CE2	-5.48	1.30	1.37
1	A	843	PHE	CG-CD1	5.45	1.47	1.38
1	A	537	SER	CB-OG	5.44	1.49	1.42
1	B	607	TYR	CE1-CZ	-5.44	1.31	1.38
1	B	1009	PRO	N-CD	-5.43	1.40	1.47
1	A	989	ARG	NE-CZ	5.42	1.40	1.33
1	B	937	HIS	CB-CG	5.39	1.59	1.50
1	A	894	PHE	CG-CD1	5.36	1.46	1.38
1	A	478	CYS	N-CA	-5.36	1.35	1.46
1	A	739	PHE	CB-CG	5.34	1.60	1.51
1	A	594	GLU	CG-CD	5.29	1.59	1.51
1	A	890	GLY	N-CA	-5.27	1.38	1.46
1	B	932	GLY	CA-C	-5.20	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	591	ARG	CD-NE	5.20	1.55	1.46
1	B	757	VAL	C-N	5.19	1.44	1.34
1	B	555	TYR	CG-CD2	5.14	1.45	1.39
1	A	872	PHE	CG-CD1	5.13	1.46	1.38
1	A	563	ARG	CZ-NH2	5.12	1.39	1.33
1	A	861	SER	CA-CB	5.11	1.60	1.52
1	B	502	GLU	CD-OE2	5.10	1.31	1.25
1	A	901	PHE	CE2-CZ	5.09	1.47	1.37
1	B	492	PRO	CA-C	-5.08	1.42	1.52
1	B	839	GLY	N-CA	5.05	1.53	1.46
1	A	497	GLY	N-CA	5.05	1.53	1.46
1	B	913	TYR	CD2-CE2	5.04	1.47	1.39
1	B	651	TYR	CE2-CZ	5.02	1.45	1.38

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	690	TYR	CB-CG-CD1	15.35	130.21	121.00
1	B	588	TYR	CB-CG-CD1	14.62	129.77	121.00
1	B	588	TYR	CB-CG-CD2	-14.59	112.25	121.00
1	B	950	ARG	NE-CZ-NH2	-14.52	113.04	120.30
1	A	507	ARG	NE-CZ-NH2	13.71	127.15	120.30
1	B	724	ARG	NE-CZ-NH1	13.67	127.13	120.30
1	A	507	ARG	NE-CZ-NH1	-11.99	114.31	120.30
1	A	690	TYR	CB-CG-CD2	-11.80	113.92	121.00
1	A	987	PHE	CB-CG-CD1	11.09	128.56	120.80
1	A	563	ARG	NE-CZ-NH1	-10.60	115.00	120.30
1	A	461	ARG	NE-CZ-NH1	-10.54	115.03	120.30
1	A	515	PHE	CB-CG-CD2	10.48	128.13	120.80
1	B	989	ARG	NE-CZ-NH2	-10.47	115.06	120.30
1	B	950	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	B	486	TYR	CB-CG-CD1	10.06	127.04	121.00
1	A	637	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	B	724	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	620	TYR	CB-CG-CD1	-9.91	115.05	121.00
1	B	651	TYR	CB-CG-CD2	9.82	126.89	121.00
1	A	950	ARG	NE-CZ-NH1	-9.78	115.41	120.30
1	A	715	PHE	CB-CG-CD1	-9.71	114.01	120.80
1	B	471	ARG	NE-CZ-NH2	9.46	125.03	120.30
1	A	913	TYR	CB-CG-CD2	-9.40	115.36	121.00
1	A	720	TYR	CB-CG-CD2	-9.37	115.38	121.00
1	A	876	ARG	NE-CZ-NH1	-9.28	115.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	886	PHE	CB-CG-CD2	9.18	127.22	120.80
1	A	721	PHE	CB-CG-CD1	9.17	127.22	120.80
1	A	987	PHE	CB-CG-CD2	-9.02	114.49	120.80
1	B	706	PHE	CB-CG-CD1	8.87	127.01	120.80
1	B	466	TYR	CB-CG-CD2	-8.82	115.71	121.00
1	A	605	PHE	CB-CG-CD1	-8.73	114.69	120.80
1	B	661	ASP	CB-CG-OD2	8.65	126.08	118.30
1	A	821	TYR	CB-CG-CD1	-8.59	115.84	121.00
1	A	634	TYR	CG-CD2-CE2	8.56	128.15	121.30
1	A	702	PHE	CB-CG-CD1	-8.54	114.82	120.80
1	B	831	MET	CG-SD-CE	8.39	113.63	100.20
1	B	472	ASP	CB-CG-OD1	-8.37	110.77	118.30
1	B	927	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	B	945	ARG	NE-CZ-NH2	8.19	124.39	120.30
1	B	821	TYR	CB-CG-CD2	-8.19	116.09	121.00
1	B	768	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	B	726	ARG	NE-CZ-NH2	8.07	124.33	120.30
1	A	693	ASP	CB-CG-OD2	7.98	125.48	118.30
1	A	824	ASP	CB-CG-OD1	7.92	125.43	118.30
1	B	746	PHE	CB-CG-CD1	-7.92	115.26	120.80
1	B	924	PHE	CB-CG-CD2	-7.76	115.37	120.80
1	B	731	ASP	CB-CG-OD1	7.75	125.27	118.30
1	A	661	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	A	876	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	A	634	TYR	CB-CG-CD1	7.55	125.53	121.00
1	A	620	TYR	CB-CG-CD2	7.54	125.53	121.00
1	A	702	PHE	CB-CG-CD2	7.34	125.94	120.80
1	A	607	TYR	CB-CG-CD2	7.30	125.38	121.00
1	A	715	PHE	CB-CG-CD2	7.24	125.87	120.80
1	B	741	MET	CG-SD-CE	-7.22	88.65	100.20
1	B	486	TYR	CB-CG-CD2	-7.19	116.69	121.00
1	B	928	LEU	CB-CG-CD1	7.14	123.13	111.00
1	A	607	TYR	CB-CG-CD1	-7.11	116.74	121.00
1	A	894	PHE	CB-CG-CD1	-7.09	115.84	120.80
1	A	1006	ASP	CB-CG-OD1	7.08	124.67	118.30
1	B	924	PHE	CG-CD2-CE2	-7.07	113.03	120.80
1	A	726	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	A	482	PHE	CB-CG-CD1	7.02	125.71	120.80
1	A	781	TRP	CD1-CG-CD2	6.94	111.85	106.30
1	B	742	VAL	CA-CB-CG2	-6.88	100.57	110.90
1	A	735	PHE	CB-CG-CD1	-6.85	116.00	120.80
1	B	651	TYR	CB-CG-CD1	-6.84	116.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1019	ALA	CB-CA-C	-6.79	99.92	110.10
1	A	739	PHE	CB-CG-CD2	-6.76	116.07	120.80
1	A	790	ALA	N-CA-CB	6.70	119.48	110.10
1	B	810	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	A	524	TYR	CG-CD2-CE2	-6.64	115.99	121.30
1	A	467	TRP	O-C-N	-6.62	112.11	122.70
1	A	989	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	A	649	LEU	CB-CG-CD2	6.58	122.19	111.00
1	B	668	THR	N-CA-CB	6.56	122.77	110.30
1	B	607	TYR	CG-CD1-CE1	-6.56	116.05	121.30
1	A	908	TYR	CB-CG-CD2	-6.56	117.07	121.00
1	B	496	PHE	CB-CG-CD2	-6.55	116.21	120.80
1	B	834	VAL	CG1-CB-CG2	6.54	121.37	110.90
1	A	847	THR	CA-CB-CG2	-6.54	103.25	112.40
1	B	735	PHE	CB-CG-CD1	6.53	125.37	120.80
1	B	696	PHE	CB-CG-CD1	6.49	125.34	120.80
1	A	704	ALA	N-CA-CB	6.45	119.12	110.10
1	B	981	MET	N-CA-CB	6.44	122.19	110.60
1	A	503	ALA	CB-CA-C	-6.32	100.62	110.10
1	A	588	TYR	CB-CG-CD1	-6.30	117.22	121.00
1	A	892	SER	N-CA-CB	6.29	119.94	110.50
1	B	591	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	461	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	B	607	TYR	CB-CG-CD1	-6.26	117.25	121.00
1	B	515	PHE	CB-CG-CD1	-6.21	116.45	120.80
1	B	466	TYR	CB-CG-CD1	6.18	124.71	121.00
1	B	894	PHE	CZ-CE2-CD2	6.15	127.48	120.10
1	A	781	TRP	CE2-CD2-CG	-6.09	102.43	107.30
1	A	634	TYR	CD1-CG-CD2	-6.06	111.23	117.90
1	A	524	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	B	961	THR	N-CA-CB	6.02	121.73	110.30
1	A	821	TYR	CG-CD1-CE1	-5.98	116.52	121.30
1	A	469	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	472	ASP	CB-CG-OD2	5.97	123.68	118.30
1	B	922	ILE	N-CA-C	-5.97	94.87	111.00
1	B	1008	MET	CG-SD-CE	-5.95	90.68	100.20
1	A	785	ALA	O-C-N	-5.93	113.20	122.70
1	B	639	ALA	N-CA-CB	5.93	118.41	110.10
1	B	982	VAL	CA-CB-CG1	5.93	119.80	110.90
1	B	989	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A	999	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	B	458	ASP	CB-CG-OD2	-5.88	113.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	482	PHE	CB-CG-CD2	-5.86	116.70	120.80
1	B	876	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	A	694	VAL	CA-CB-CG2	-5.82	102.17	110.90
1	B	843	PHE	CB-CG-CD1	5.78	124.85	120.80
1	B	987	PHE	CG-CD1-CE1	-5.78	114.44	120.80
1	A	588	TYR	CB-CG-CD2	5.78	124.47	121.00
1	A	930	LEU	O-C-N	-5.76	113.49	122.70
1	B	894	PHE	CG-CD2-CE2	-5.75	114.47	120.80
1	A	544	PHE	CD1-CE1-CZ	-5.75	113.20	120.10
1	B	634	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	A	503	ALA	N-CA-CB	5.73	118.12	110.10
1	B	992	MET	CG-SD-CE	-5.71	91.06	100.20
1	B	524	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	A	931	PHE	CB-CG-CD2	-5.69	116.82	120.80
1	B	767	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	B	827	VAL	CG1-CB-CG2	-5.68	101.81	110.90
1	A	735	PHE	CB-CG-CD2	5.68	124.78	120.80
1	A	903	PRO	N-CD-CG	5.67	111.71	103.20
1	B	759	SER	CB-CA-C	-5.67	99.33	110.10
1	A	961	THR	CA-CB-CG2	-5.64	104.51	112.40
1	A	611	GLU	N-CA-CB	5.63	120.74	110.60
1	A	527	PHE	CZ-CE2-CD2	5.63	126.85	120.10
1	A	451	LEU	CB-CG-CD2	5.60	120.52	111.00
1	A	486	TYR	CB-CG-CD1	5.59	124.36	121.00
1	A	964	VAL	CA-CB-CG2	-5.59	102.52	110.90
1	B	619	THR	CA-CB-CG2	-5.59	104.58	112.40
1	A	978	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	B	925	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	A	588	TYR	CD1-CE1-CZ	5.57	124.81	119.80
1	B	535	LEU	CB-CG-CD2	5.57	120.47	111.00
1	A	620	TYR	CG-CD1-CE1	-5.55	116.86	121.30
1	B	605	PHE	CB-CG-CD2	-5.55	116.91	120.80
1	B	876	ARG	CD-NE-CZ	-5.55	115.83	123.60
1	A	683	ALA	N-CA-CB	-5.55	102.33	110.10
1	A	474	LEU	CB-CG-CD2	5.54	120.42	111.00
1	B	731	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	635	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	B	675	MET	CG-SD-CE	-5.52	91.36	100.20
1	B	780	TRP	CD1-CG-CD2	-5.50	101.90	106.30
1	B	608	GLU	OE1-CD-OE2	5.48	129.87	123.30
1	B	810	ARG	N-CA-CB	5.47	120.45	110.60
1	A	781	TRP	CG-CD2-CE3	5.45	138.81	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	956	THR	N-CA-CB	5.43	120.63	110.30
1	B	698	SER	N-CA-CB	5.42	118.64	110.50
1	B	463	ALA	CA-C-N	5.41	132.26	117.10
1	B	541	VAL	CA-CB-CG2	-5.40	102.80	110.90
1	B	679	PHE	N-CA-C	-5.39	96.44	111.00
1	B	786	ALA	CB-CA-C	5.38	118.17	110.10
1	B	633	LEU	CB-CG-CD1	5.38	120.14	111.00
1	B	558	SER	N-CA-CB	5.37	118.56	110.50
1	B	683	ALA	CB-CA-C	5.35	118.13	110.10
1	B	463	ALA	CA-C-O	-5.33	108.90	120.10
1	B	913	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	B	955	PHE	CB-CG-CD1	-5.32	117.08	120.80
1	A	559	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	A	467	TRP	CH2-CZ2-CE2	5.31	122.71	117.40
1	A	908	TYR	CB-CG-CD1	5.31	124.19	121.00
1	A	524	TYR	CD1-CG-CD2	5.30	123.73	117.90
1	A	592	PHE	CB-CG-CD1	5.29	124.51	120.80
1	A	1008	MET	N-CA-C	-5.28	96.74	111.00
1	B	461	ARG	O-C-N	-5.27	114.27	122.70
1	B	947	VAL	CA-CB-CG1	5.25	118.77	110.90
1	B	987	PHE	CB-CG-CD2	-5.25	117.13	120.80
1	A	726	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	605	PHE	CB-CG-CD1	5.24	124.47	120.80
1	A	588	TYR	CA-CB-CG	-5.22	103.49	113.40
1	A	527	PHE	CG-CD2-CE2	-5.21	115.06	120.80
1	B	549	PHE	CB-CG-CD1	5.21	124.45	120.80
1	B	924	PHE	CZ-CE2-CD2	5.21	126.35	120.10
1	B	539	GLY	CA-C-O	-5.20	111.25	120.60
1	B	559	TYR	O-C-N	5.19	131.00	122.70
1	B	709	SER	N-CA-CB	5.18	118.27	110.50
1	B	817	LYS	N-CA-CB	5.16	119.89	110.60
1	A	471	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	999	ARG	CD-NE-CZ	5.15	130.81	123.60
1	A	633	LEU	CB-CG-CD1	5.14	119.74	111.00
1	A	908	TYR	O-C-N	-5.14	114.47	123.20
1	B	804	THR	CA-CB-CG2	-5.12	105.23	112.40
1	B	909	GLY	O-C-N	5.06	130.79	122.70
1	B	863	CYS	N-CA-CB	5.05	119.69	110.60
1	B	913	TYR	CG-CD2-CE2	-5.04	117.27	121.30
1	A	515	PHE	CB-CG-CD1	-5.04	117.28	120.80
1	B	656	SER	N-CA-C	5.03	124.58	111.00
1	B	598	ALA	N-CA-CB	5.01	117.12	110.10

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	461	ARG	Sidechain
1	A	471	ARG	Sidechain
1	A	486	TYR	Sidechain
1	A	607	TYR	Sidechain
1	A	620	TYR	Sidechain
1	A	651	TYR	Sidechain
1	A	735	PHE	Sidechain
1	A	822	HIS	Sidechain
1	A	913	TYR	Sidechain
1	B	471	ARG	Sidechain
1	B	524	TYR	Sidechain
1	B	634	TYR	Sidechain
1	B	651	TYR	Sidechain
1	B	876	ARG	Sidechain
1	B	908	TYR	Sidechain
1	B	911	PHE	Sidechain
1	B	924	PHE	Sidechain
1	B	950	ARG	Sidechain
1	B	955	PHE	Sidechain
1	B	987	PHE	Sidechain

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	4520	0	4635	1	0
1	B	4519	0	4633	0	0
2	C	42	0	37	1	0
2	D	42	0	37	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	9161	0	9368	2	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 1.

All (2) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:NAG:O4	2:C:2:NAG:N2	2.43	0.49
1:A:943:TYR:CD1	1:A:943:TYR:N	2.80	0.47

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	569/571 (100%)	528 (93%)	39 (7%)	2 (0%)	30	60
1	B	569/571 (100%)	530 (93%)	38 (7%)	1 (0%)	44	72
All	All	1138/1142 (100%)	1058 (93%)	77 (7%)	3 (0%)	38	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	943	TYR
1	A	772	ILE
1	A	776	GLY

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	501/501 (100%)	488 (97%)	13 (3%)	41 64
1	B	500/501 (100%)	492 (98%)	8 (2%)	58 75
All	All	1001/1002 (100%)	980 (98%)	21 (2%)	49 69

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

Mol	Chain	Res	Type
1	A	482	PHE
1	A	512	GLU
1	A	557	LEU
1	A	623	HIS
1	A	666	ASN
1	A	673	GLN
1	A	675	MET
1	A	812	GLU
1	A	815	LEU
1	A	878	GLN
1	A	879	ARG
1	A	930	LEU
1	A	943	TYR
1	B	509	SER
1	B	580	THR
1	B	623	HIS
1	B	657	ILE
1	B	691	THR
1	B	752	SER
1	B	955	PHE
1	B	976	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

6 monosaccharides 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	$\#\|Z\| > 2$
2	NAG	C	1	2	14,14,15	0.29	0	17,19,21	0.60	0
2	NAG	C	2	2	14,14,15	0.97	1 (7%)	17,19,21	2.79	1 (5%)
2	NAG	C	3	2	14,14,15	0.28	0	17,19,21	0.46	0
2	NAG	D	1	2	14,14,15	0.36	0	17,19,21	0.93	1 (5%)
2	NAG	D	2	2	14,14,15	0.39	0	17,19,21	1.06	1 (5%)
2	NAG	D	3	2	14,14,15	0.48	0	17,19,21	1.38	2 (11%)

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
2	NAG	C	1	2	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	3	2	-	4/6/23/26	0/1/1/1
2	NAG	D	1	2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	3	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O5-C1	3.40	1.49	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	C1-O5-C5	11.12	127.09	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	NAG	C1-O5-C5	3.48	116.86	112.19
2	D	2	NAG	C1-O5-C5	3.38	116.71	112.19
2	D	3	NAG	O5-C1-C2	2.64	115.38	111.29
2	D	1	NAG	C2-N2-C7	2.35	126.05	122.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	D	3	NAG	C1-C2-N2-C7
2	D	3	NAG	C8-C7-N2-C2
2	D	3	NAG	O7-C7-N2-C2
2	C	3	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	3	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	3	NAG	C8-C7-N2-C2
2	C	3	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7

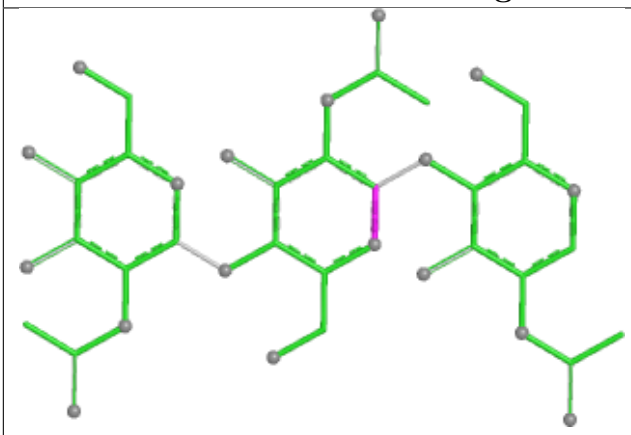
There are no ring outliers.

1 monomer is involved in 1 short contact:

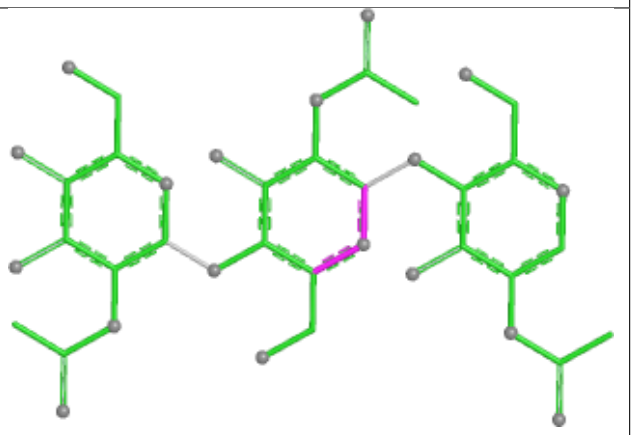
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

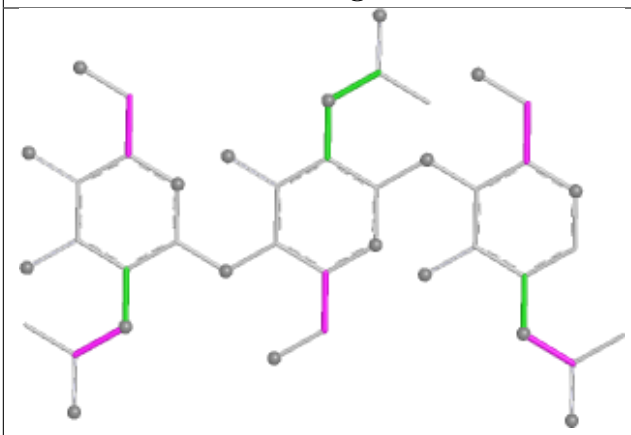
Oligosaccharide Chain C



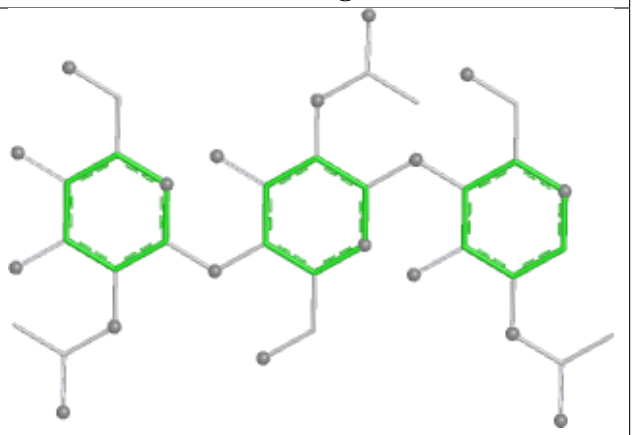
Bond lengths



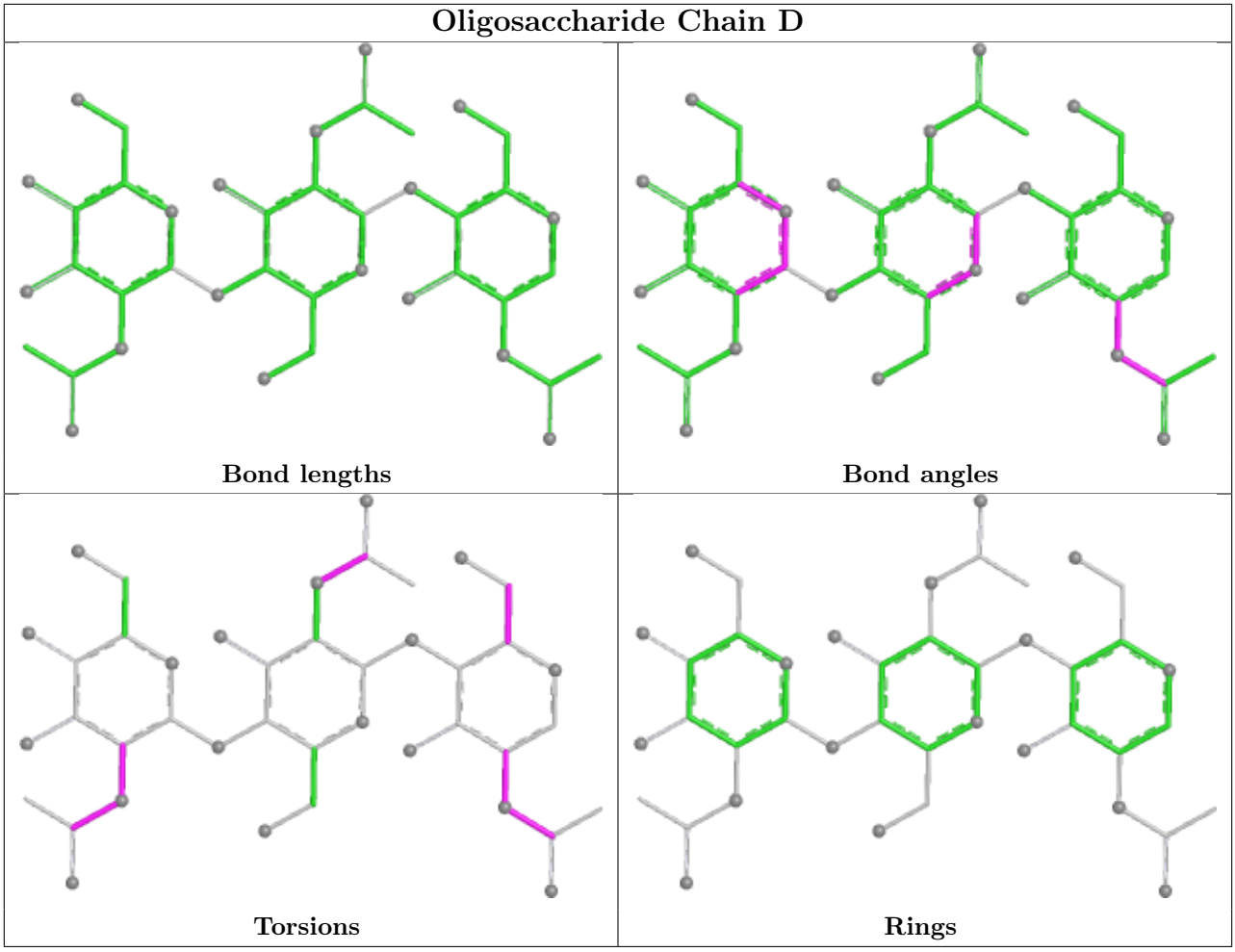
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	NAG	B	1101	-	14,14,15	0.22	0	17,19,21	0.37	0
5	CO3	B	1103	4	3,3,3	0.80	0	2,3,3	0.06	0
3	NAG	A	1101	-	14,14,15	0.24	0	17,19,21	0.35	0
5	CO3	A	1103	4	3,3,3	0.79	0	2,3,3	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1101	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1101	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

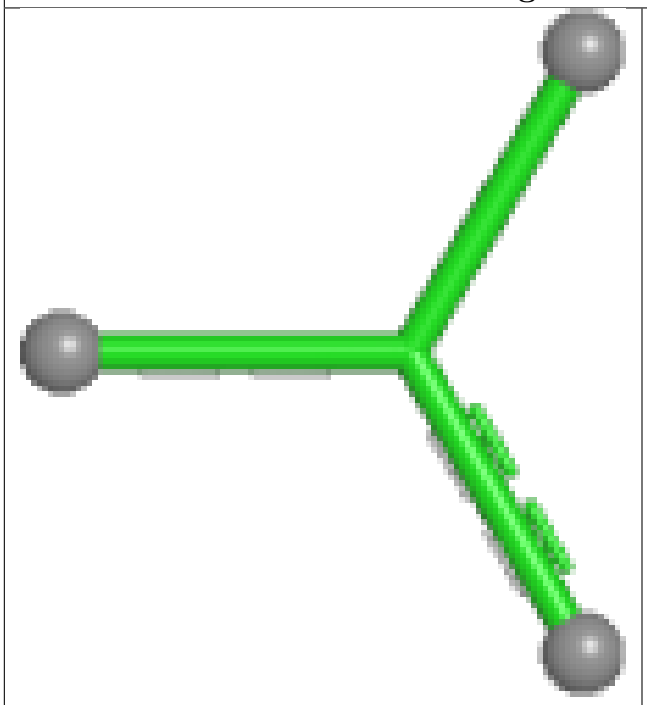
Mol	Chain	Res	Type	Atoms
3	B	1101	NAG	C4-C5-C6-O6
3	B	1101	NAG	O5-C5-C6-O6
3	A	1101	NAG	O5-C5-C6-O6
3	A	1101	NAG	C4-C5-C6-O6
3	A	1101	NAG	C8-C7-N2-C2
3	A	1101	NAG	O7-C7-N2-C2

There are no ring outliers.

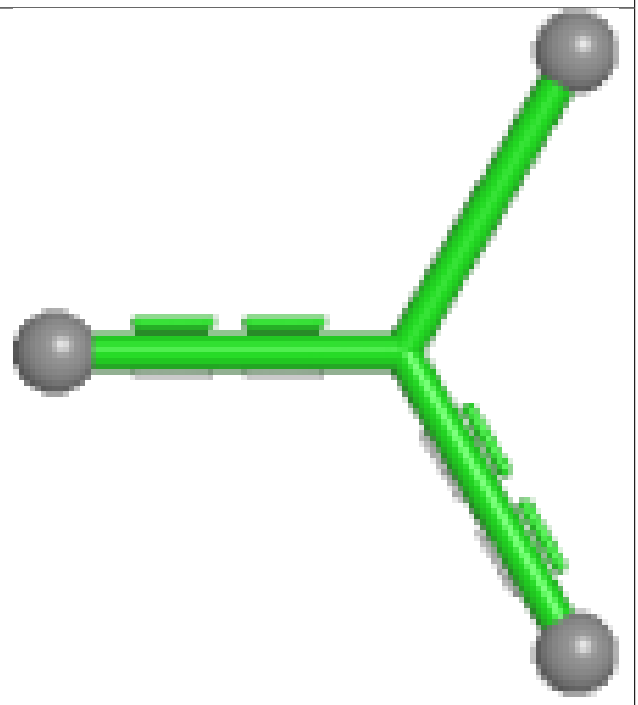
No monomer is involved in short contacts.

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.

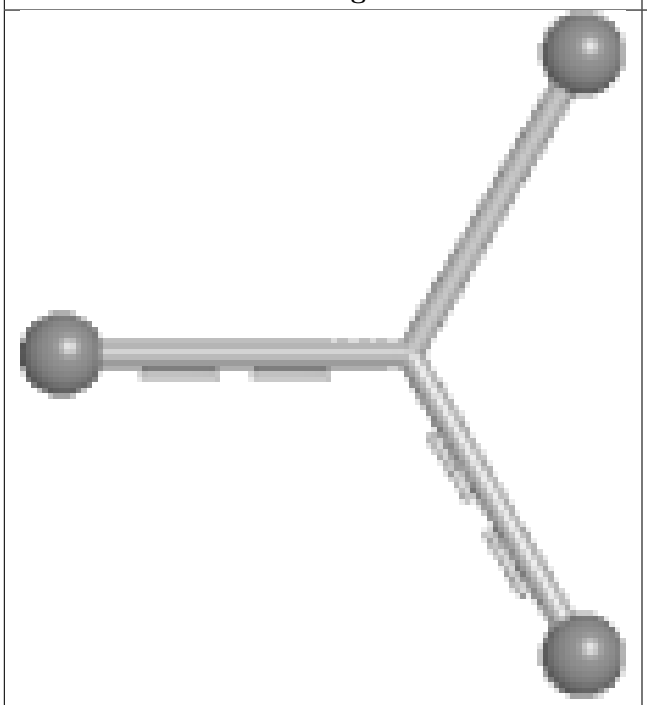
Ligand CO3 B 1103



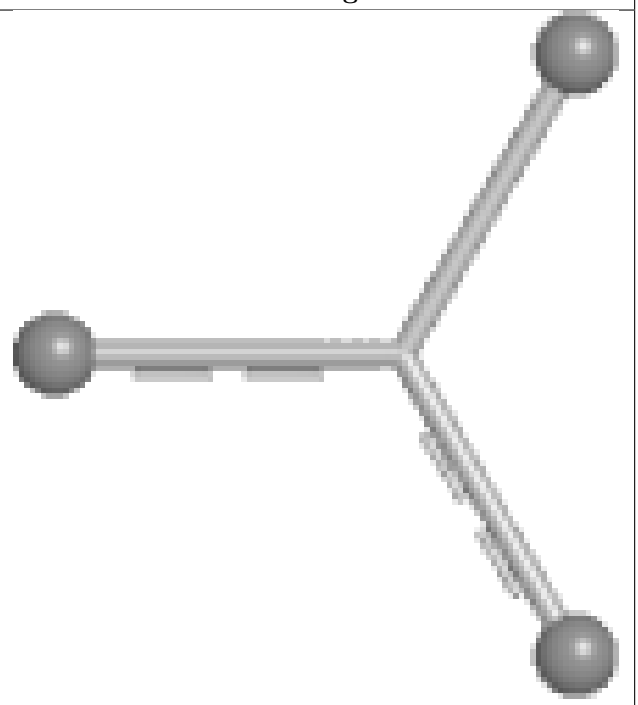
Bond lengths



Bond angles

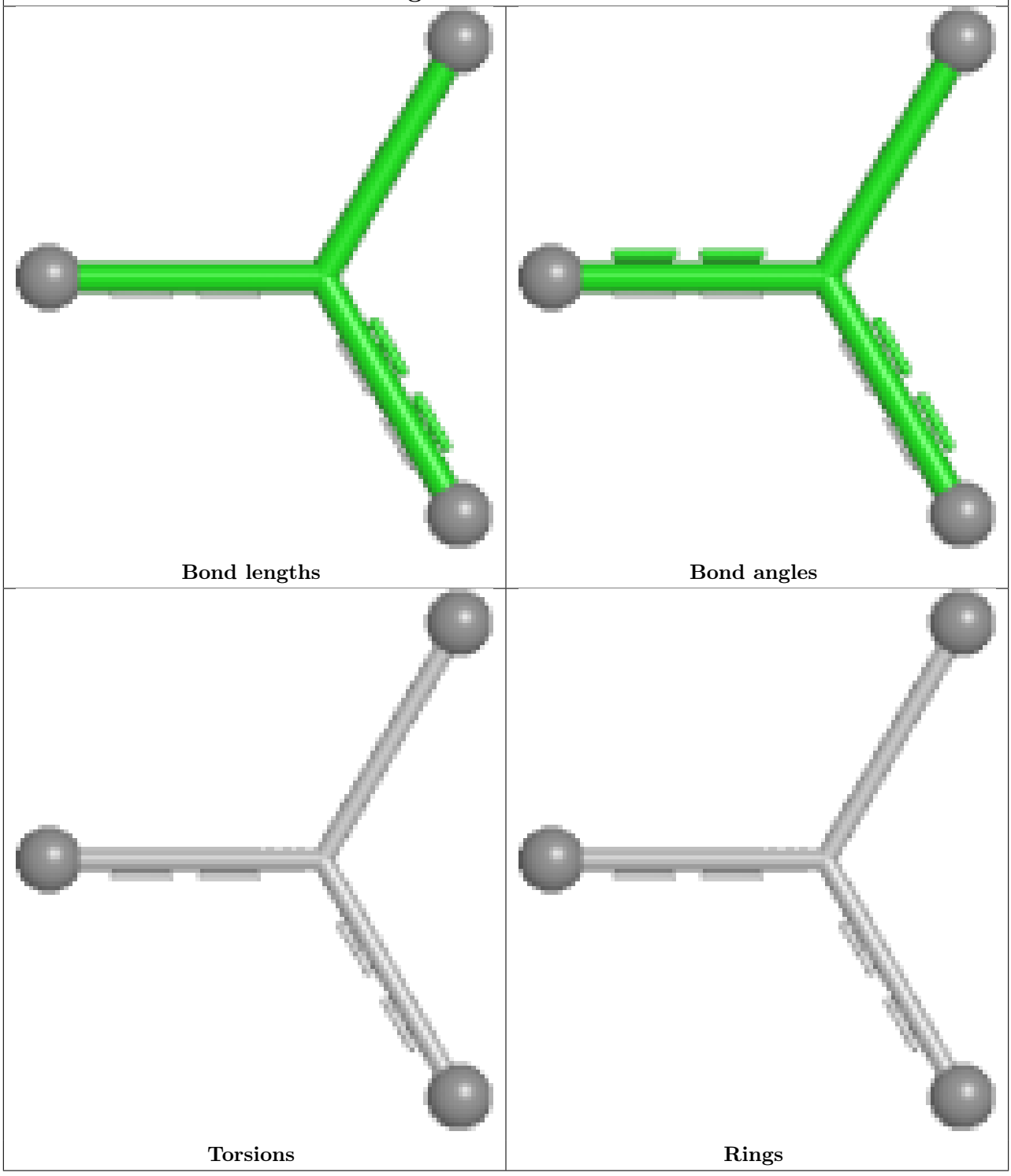


Torsions



Rings

Ligand CO3 A 1103



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.

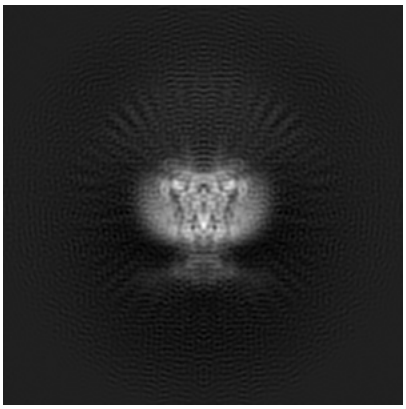
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24683. These allow visual inspection of the internal detail of the map and identification of artifacts.

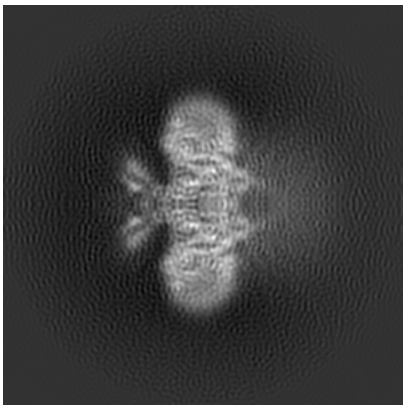
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

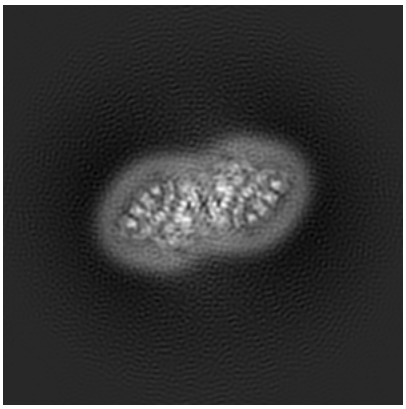
6.1.1 Primary map



X

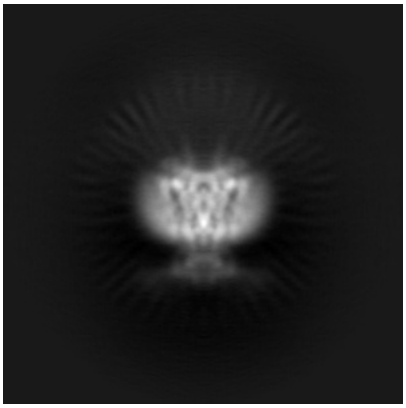


Y

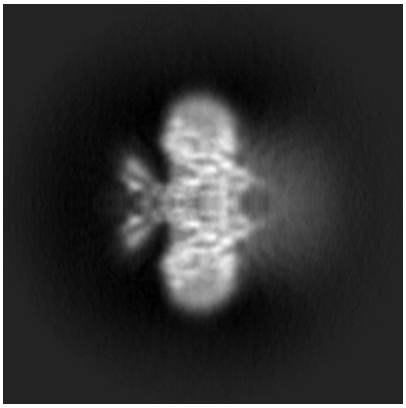


Z

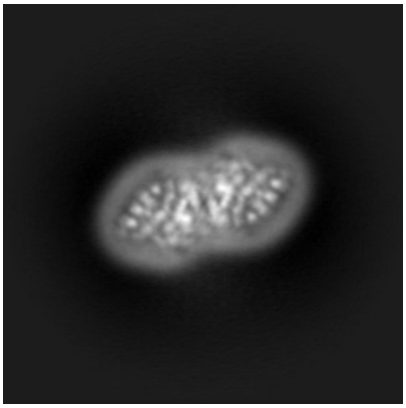
6.1.2 Raw map



X



Y

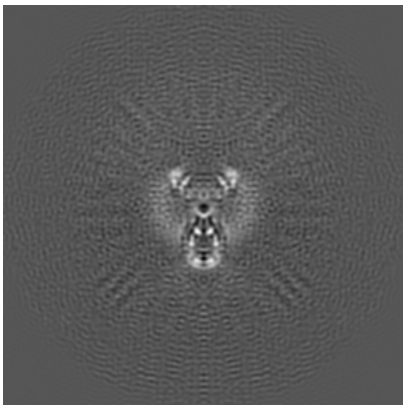


Z

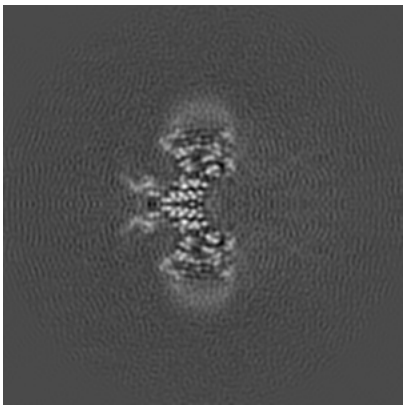
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

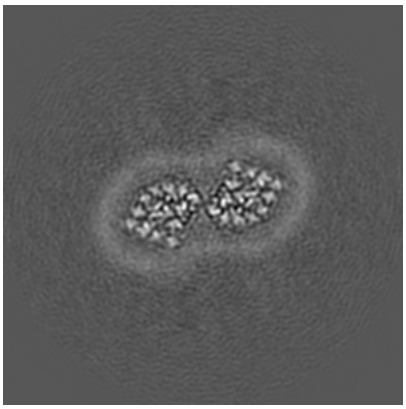
6.2.1 Primary map



X Index: 124

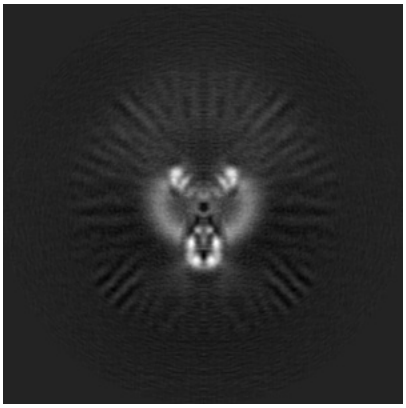


Y Index: 124

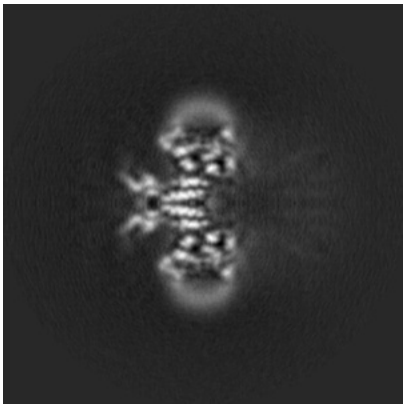


Z Index: 124

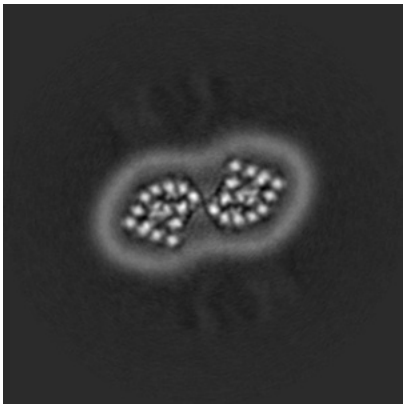
6.2.2 Raw map



X Index: 124



Y Index: 124

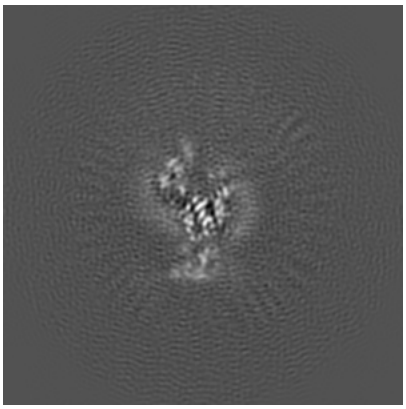


Z Index: 124

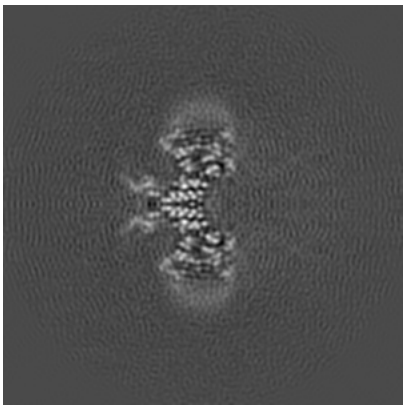
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

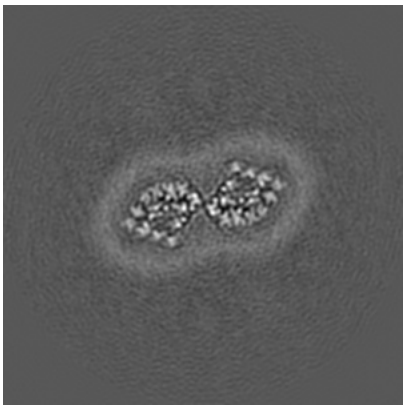
6.3.1 Primary map



X Index: 112

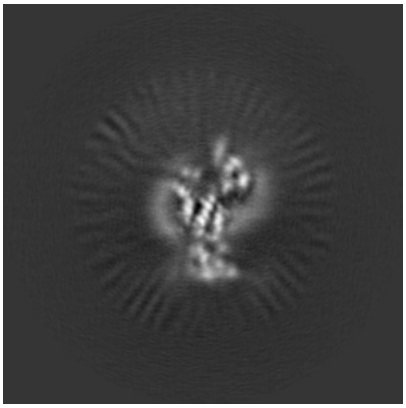


Y Index: 124

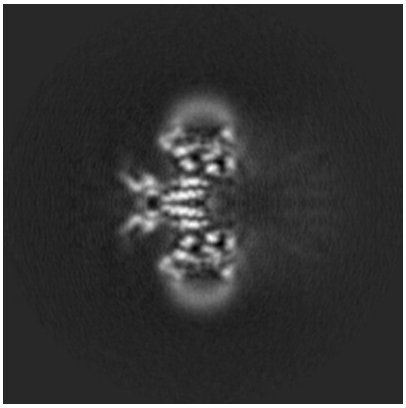


Z Index: 123

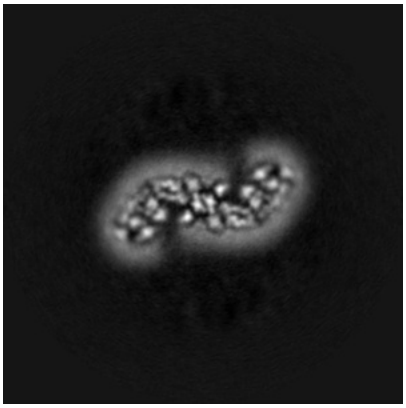
6.3.2 Raw map



X Index: 136



Y Index: 124

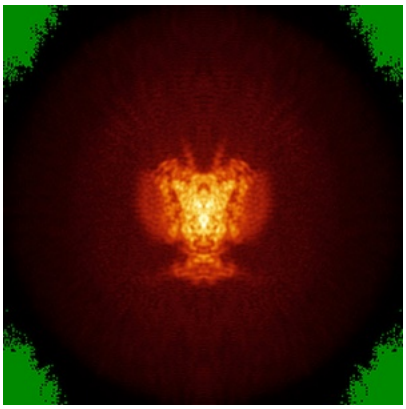


Z Index: 108

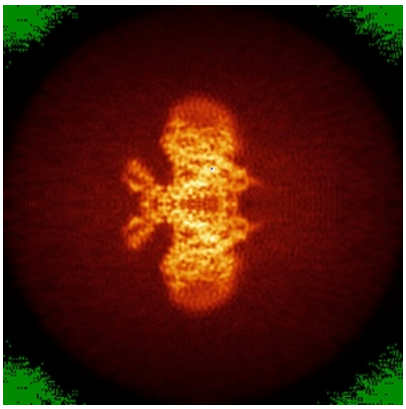
The images above show the largest variance slices of the map in three orthogonal directions.

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

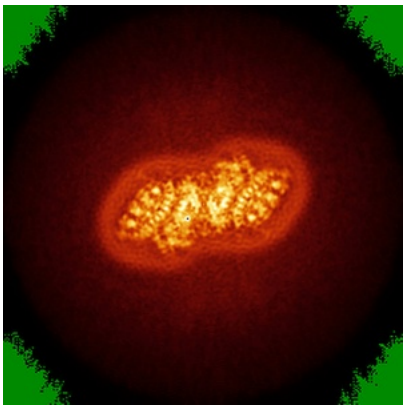
6.4.1 Primary map



X

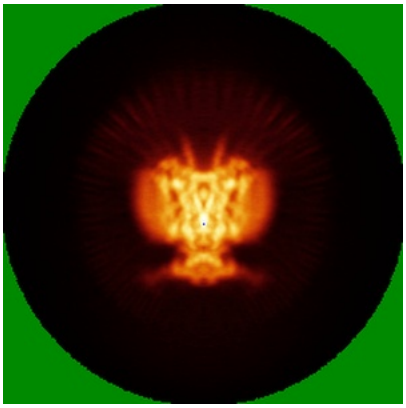


Y

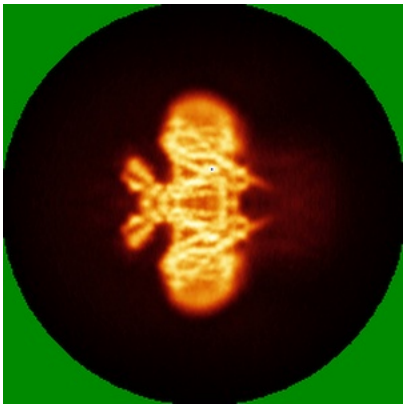


Z

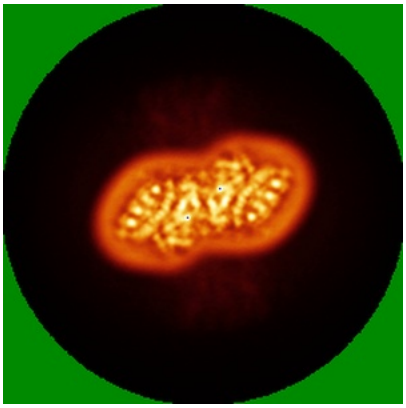
6.4.2 Raw map



X



Y

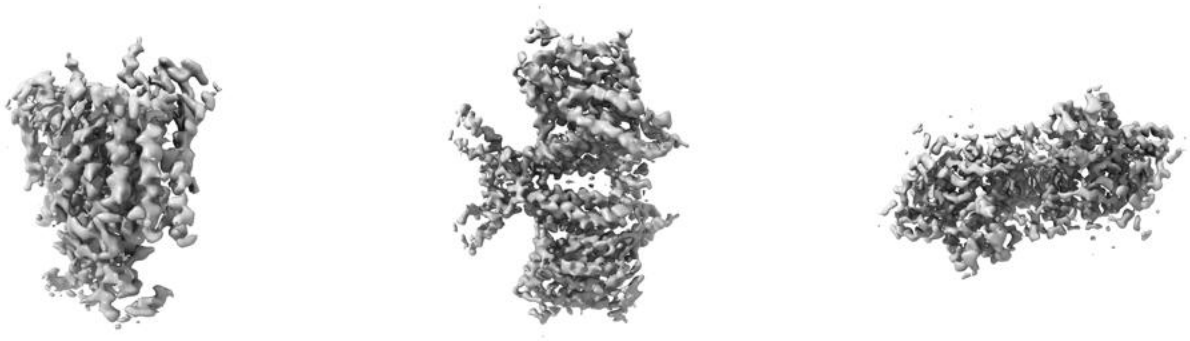


Z

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)

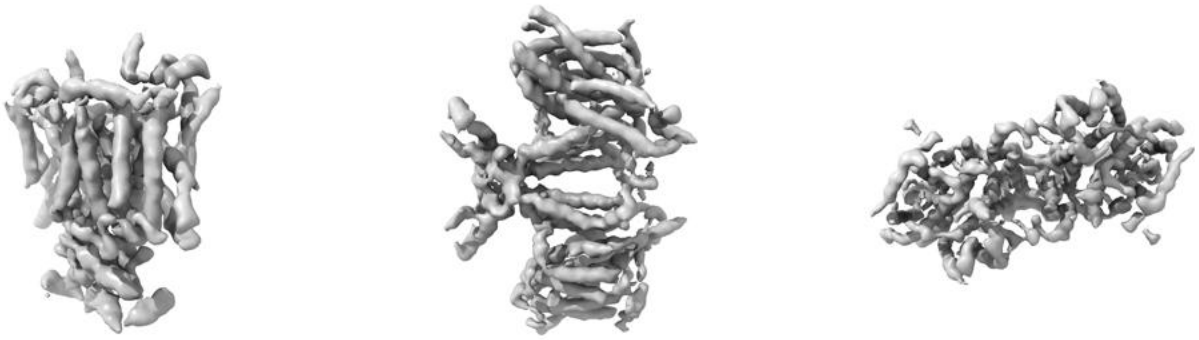
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0351. 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.

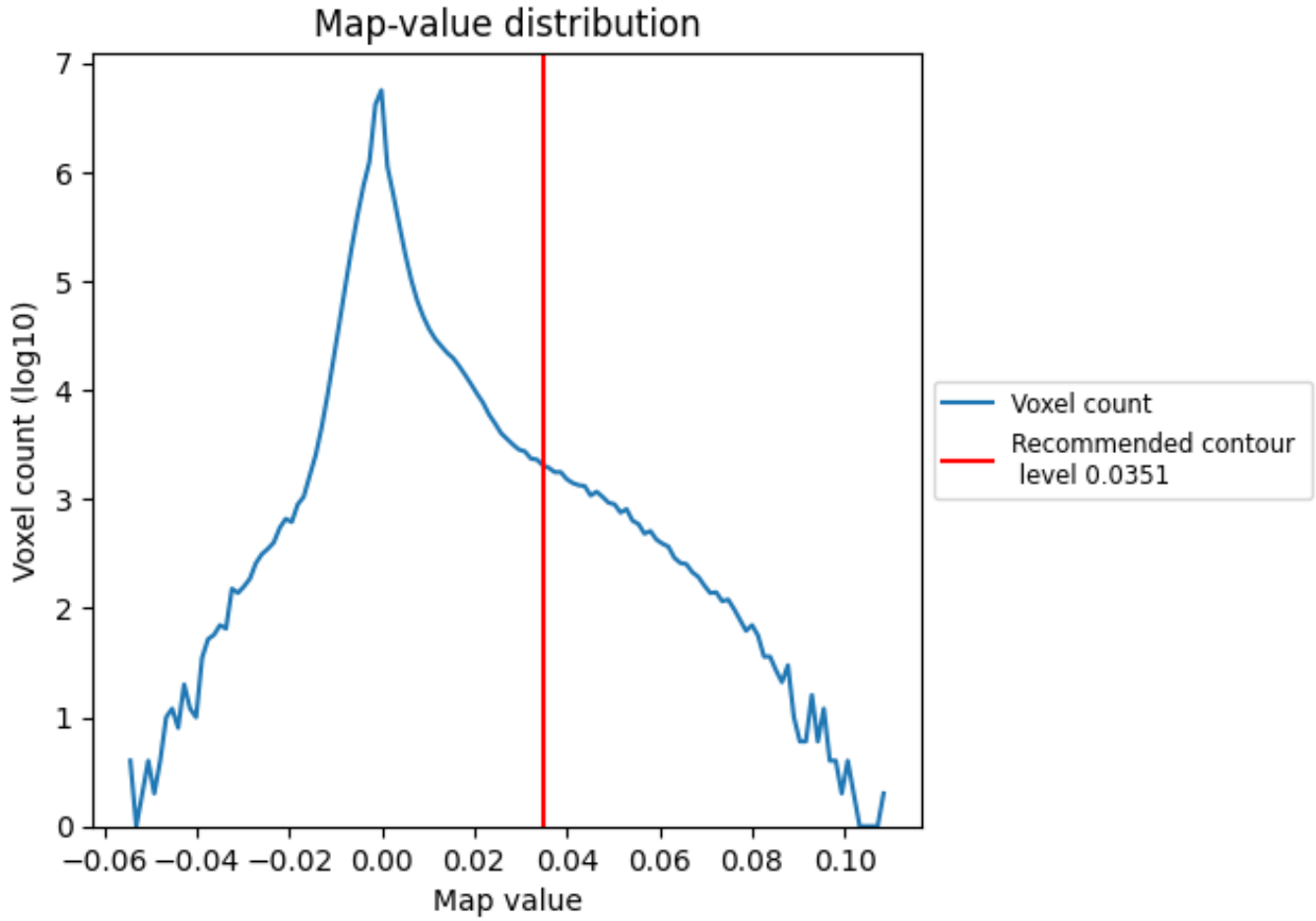
6.6 Mask visualisation (i)

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

7 Map analysis

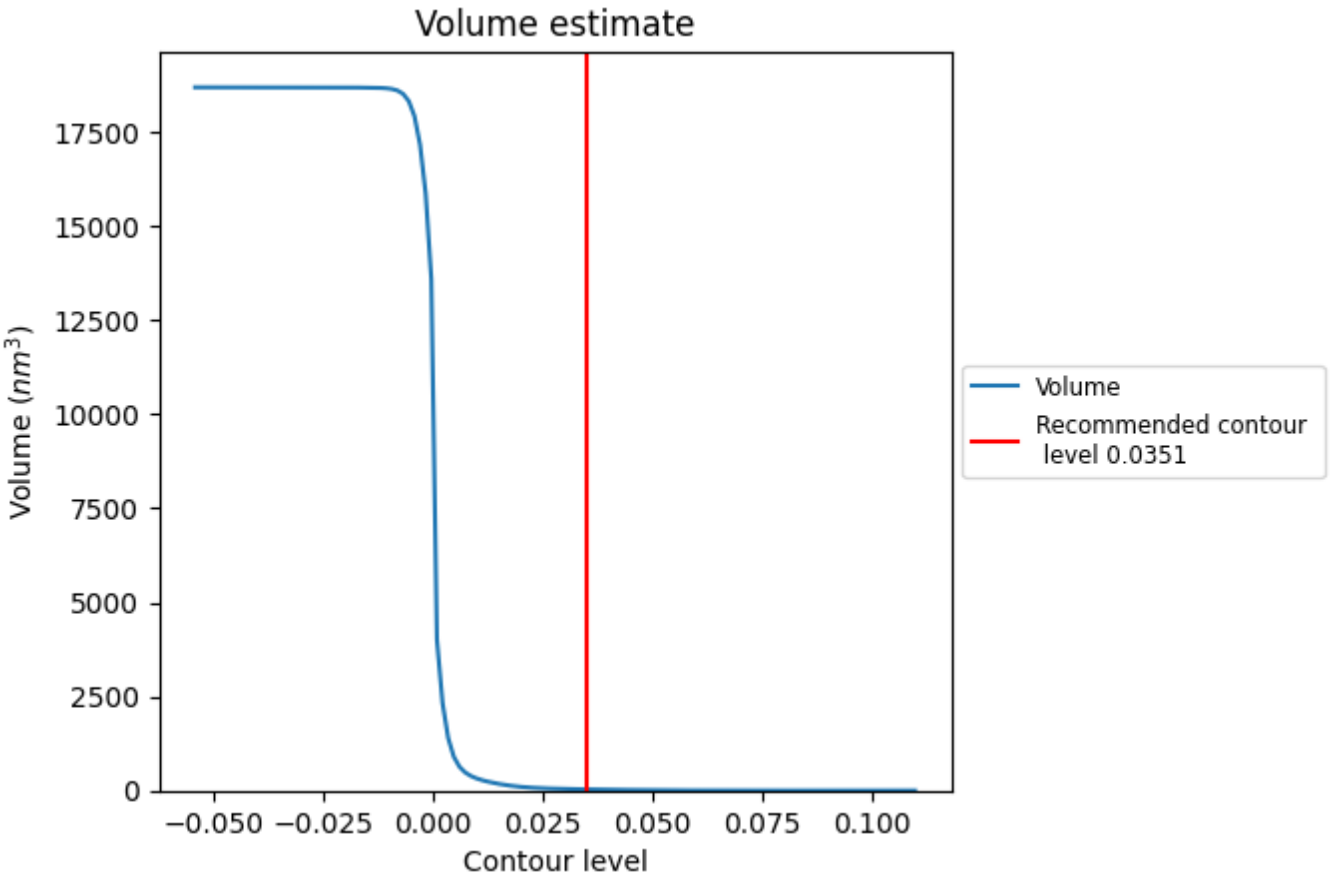
This section contains the results of statistical analysis of the map.

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.

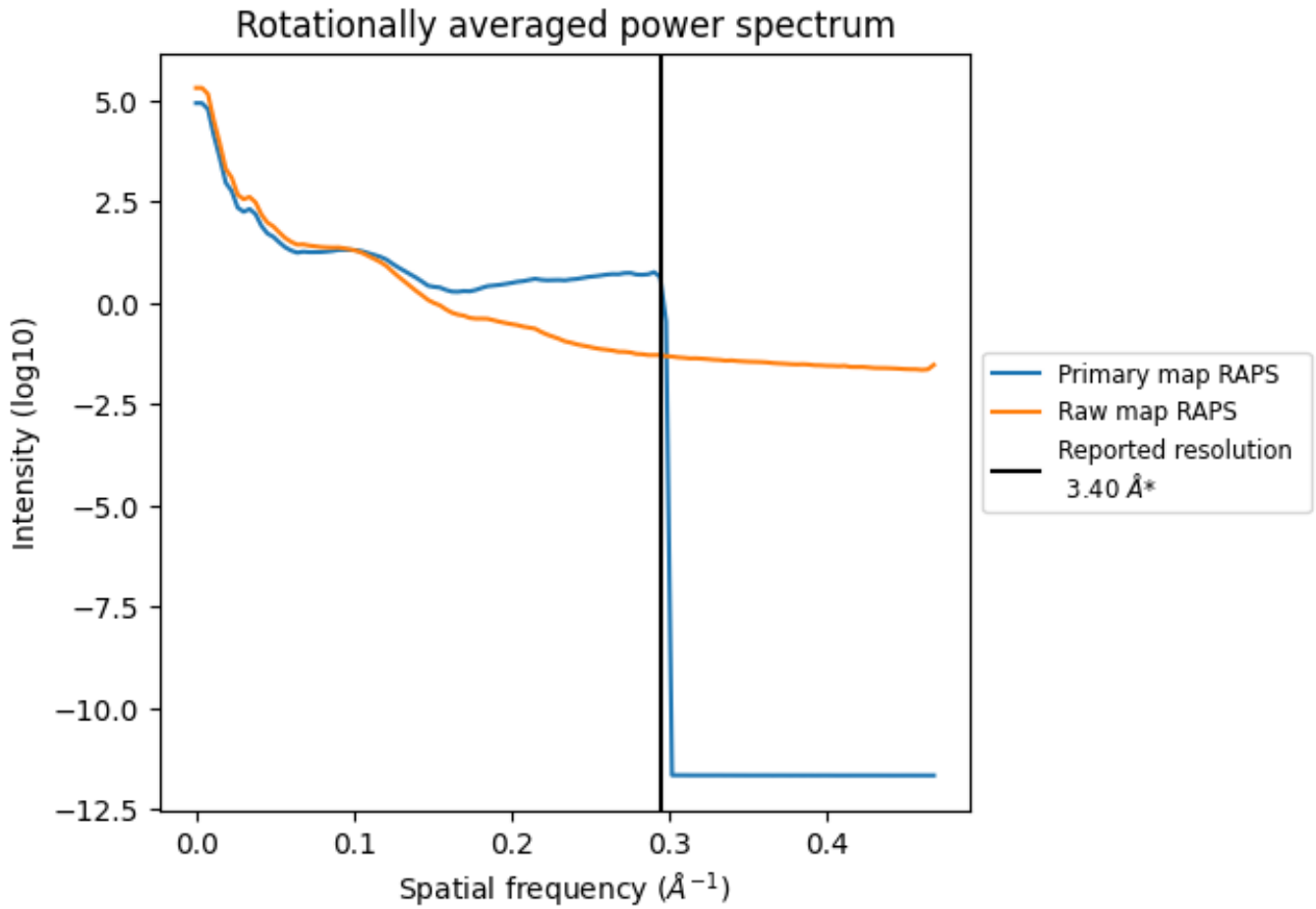
7.2 Volume estimate



The volume at the recommended contour level is 31 nm^3; this corresponds to an approximate mass of 28 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)

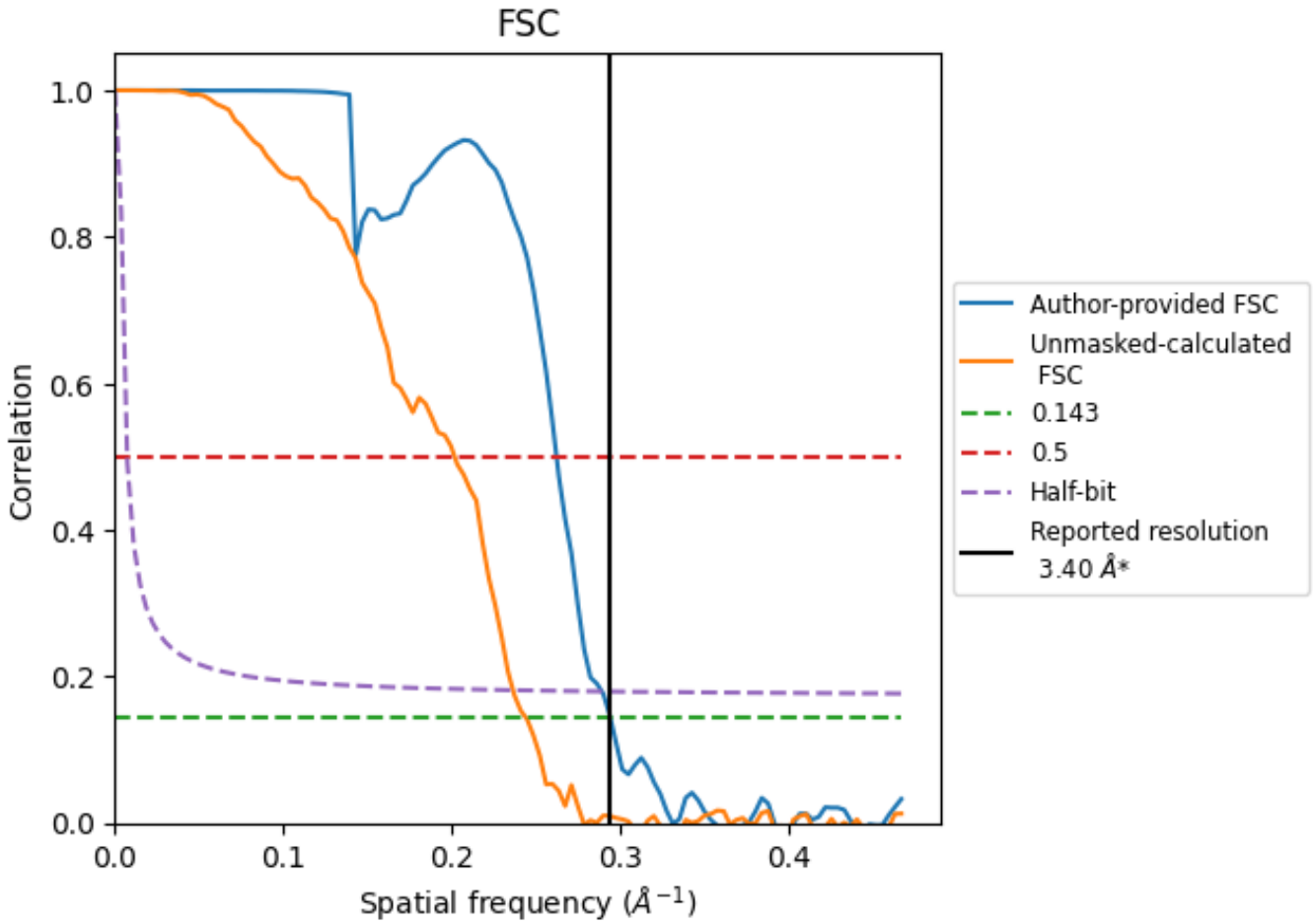


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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)

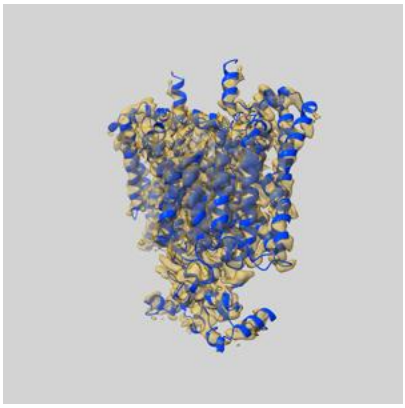
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.81	3.46
Unmasked-calculated*	4.09	4.95	4.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.4 by more than 10 %

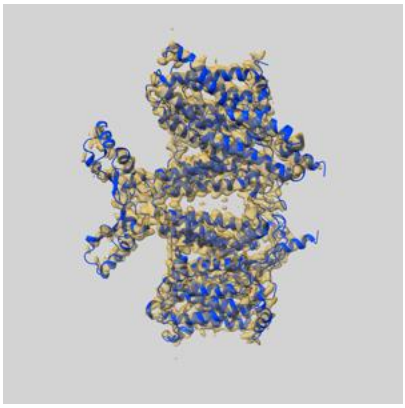
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24683 and PDB model 7RTM. Per-residue inclusion information can be found in section 3 on page 6.

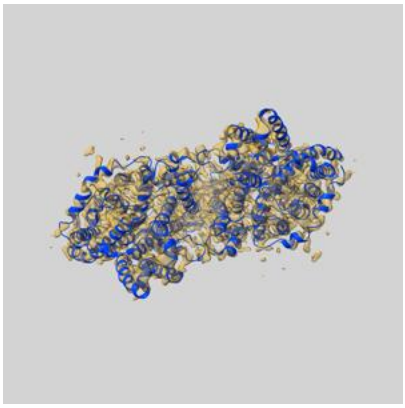
9.1 Map-model overlay



X



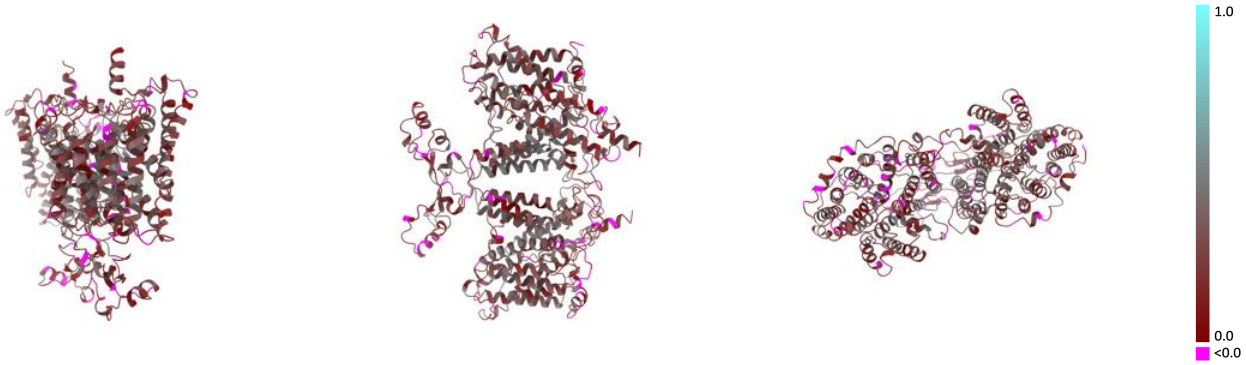
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0351 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

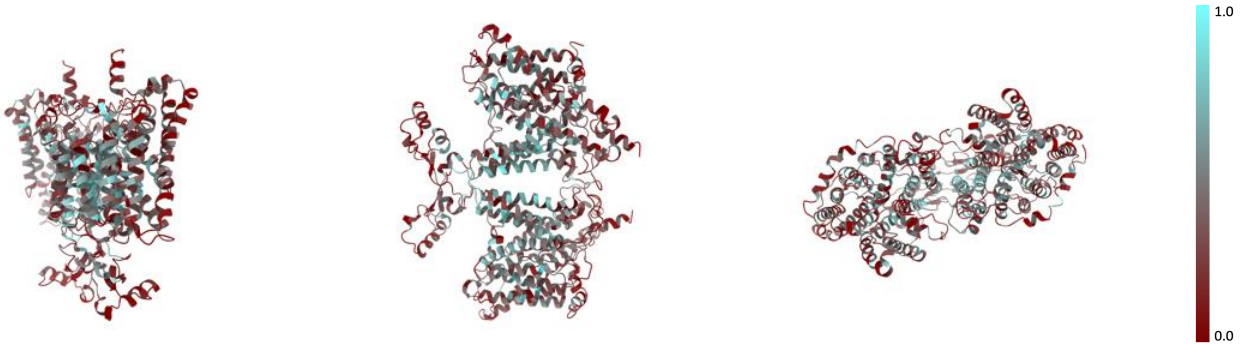
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

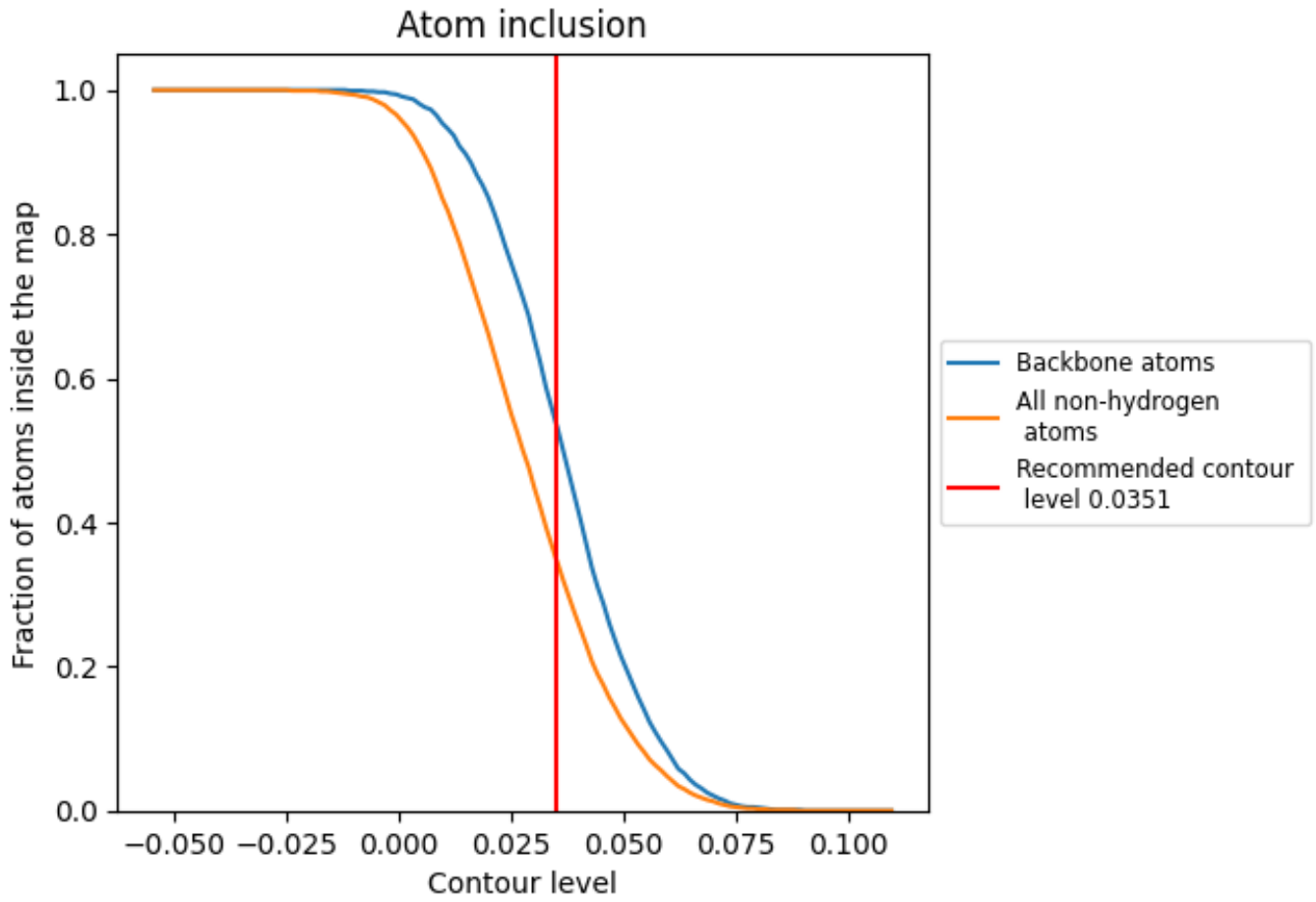
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0351).

9.4 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 35% 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 (0.0351) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3490	0.2510
A	0.3540	0.2620
B	0.3500	0.2420
C	0.0000	0.1730
D	0.0000	0.0350