



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:24 PM UTC

PDB ID : 7RTM / pdb\_00007rtm  
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](mailto: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>.

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

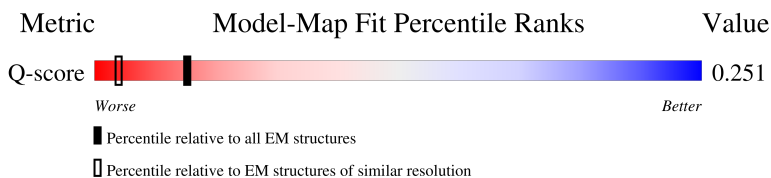
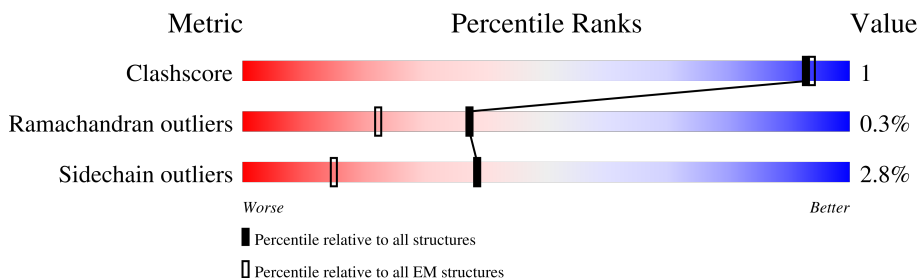
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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.



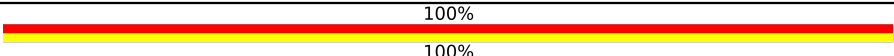
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 ( 2.90 - 3.90 )

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  $\geq 3$ , 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  $\leq 5\%$ . 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	
1	B	571	
2	C	3	

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Mol	Chain	Length	Quality of chain
2	D	3	 100%

## 2 Entry composition [i](#)

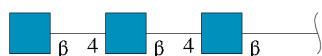
There are 5 unique types of molecules in this entry. The entry contains 9161 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S		
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
			Total	C	N	O		
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 (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).

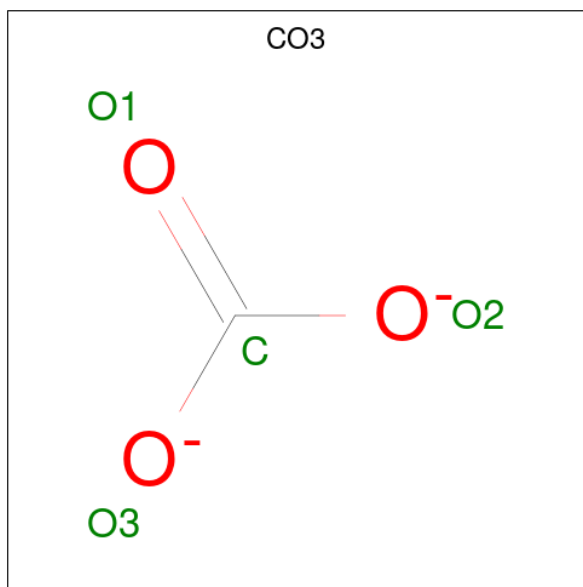


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	14	8	1	5	0
3	B	1	14	8	1	5	0

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

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

- Molecule 5 is CARBONATE ION (CCD ID: CO3) (formula: CO<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

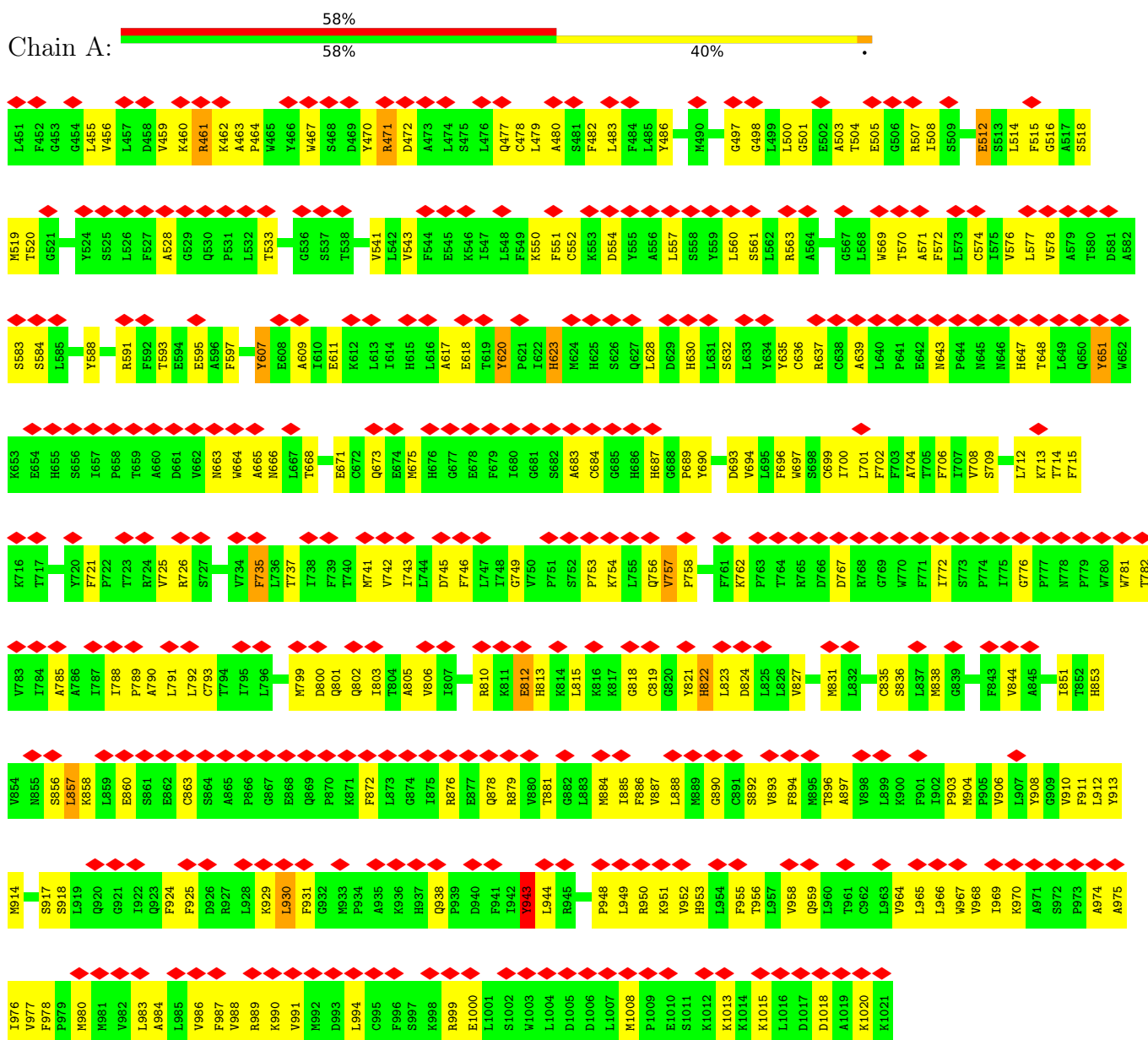


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			4	1	3	
5	B	1	Total	C	O	0
			4	1	3	

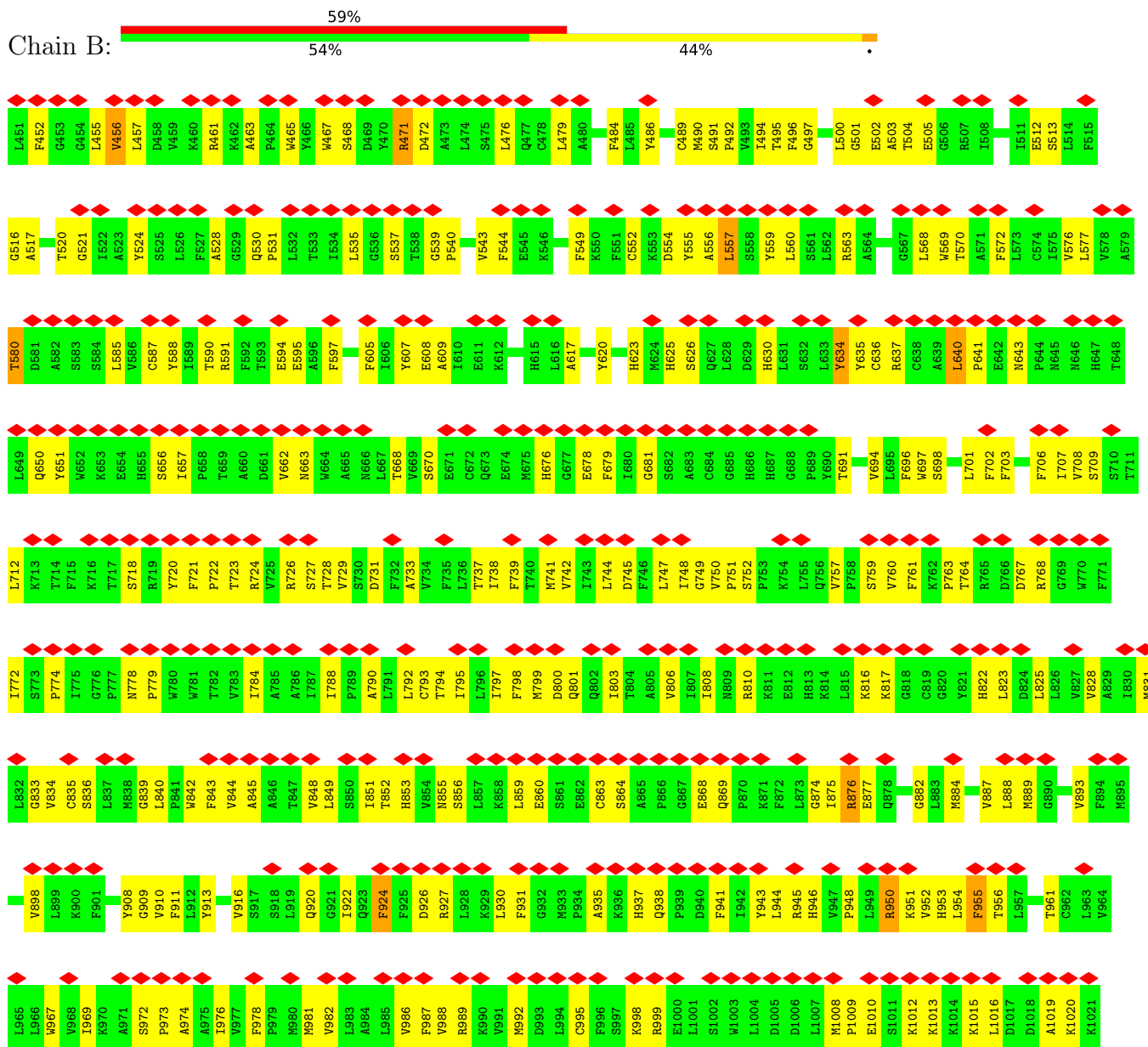
### 3 Residue-property plots

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.

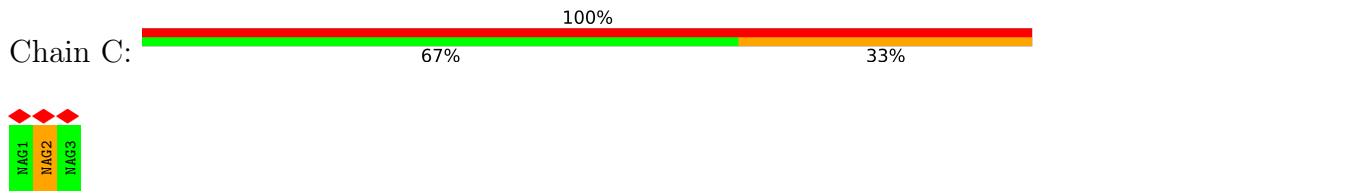
- Molecule 1: Electroneutral sodium bicarbonate exchanger 1



- Molecule 1: Electroneutral sodium bicarbonate exchanger 1



• 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



• 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





## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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 i

### 5.1 Standard geometry i

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

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	1.94	123/4647 (2.6%)	2.19	250/6319 (4.0%)
1	B	2.02	142/4646 (3.1%)	2.23	275/6318 (4.4%)
All	All	1.98	265/9293 (2.9%)	2.21	525/12637 (4.2%)

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 (265) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	501	GLY	CA-C	-11.87	1.39	1.52
1	A	471	ARG	NE-CZ	10.75	1.44	1.33
1	A	897	ALA	C-N	10.21	1.46	1.33
1	B	702	PHE	N-CA	-9.71	1.34	1.46
1	B	625	HIS	ND1-CE1	9.54	1.42	1.32
1	B	801	GLN	N-CA	-9.27	1.35	1.46
1	B	946	HIS	ND1-CE1	8.98	1.41	1.32
1	B	555	TYR	CA-C	-8.92	1.43	1.53
1	B	788	ILE	CA-C	8.91	1.60	1.52
1	A	668	THR	C-N	8.43	1.44	1.33
1	B	757	VAL	C-N	8.10	1.44	1.33
1	A	756	GLN	C-N	8.01	1.40	1.33
1	B	726	ARG	NE-CZ	7.93	1.41	1.33
1	B	853	HIS	CB-CG	7.88	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	530	GLN	C-N	-7.85	1.27	1.33
1	B	986	VAL	C-N	7.78	1.43	1.33
1	A	857	LEU	CA-CB	7.69	1.64	1.53
1	A	478	CYS	N-CA	-7.62	1.35	1.46
1	B	927	ARG	NE-CZ	7.58	1.41	1.33
1	A	480	ALA	CA-C	-7.51	1.43	1.52
1	A	623	HIS	ND1-CE1	7.48	1.40	1.32
1	B	520	THR	CA-C	-7.47	1.43	1.52
1	B	749	GLY	C-N	7.40	1.41	1.33
1	A	912	LEU	CA-CB	7.40	1.65	1.53
1	A	467	TRP	N-CA	-7.38	1.37	1.46
1	B	967	TRP	N-CA	-7.25	1.37	1.46
1	B	737	THR	N-CA	7.21	1.55	1.46
1	B	952	VAL	C-N	7.19	1.43	1.33
1	B	930	LEU	C-N	7.12	1.43	1.33
1	B	798	PHE	CA-CB	7.08	1.64	1.53
1	B	748	ILE	CA-C	-7.06	1.45	1.52
1	B	799	MET	C-N	6.93	1.42	1.33
1	A	785	ALA	C-N	6.93	1.43	1.33
1	B	851	ILE	CA-C	-6.92	1.43	1.52
1	A	858	LYS	CA-C	-6.91	1.44	1.52
1	B	726	ARG	C-N	6.91	1.43	1.33
1	A	460	LYS	C-N	6.89	1.43	1.33
1	B	720	TYR	C-N	6.88	1.40	1.33
1	A	550	LYS	CA-C	6.88	1.61	1.52
1	A	708	VAL	CA-CB	-6.87	1.45	1.54
1	A	896	THR	C-N	6.86	1.43	1.34
1	B	937	HIS	CB-CG	6.86	1.59	1.50
1	A	929	LYS	C-N	6.80	1.42	1.33
1	B	456	VAL	C-N	6.79	1.43	1.34
1	B	520	THR	N-CA	-6.79	1.38	1.46
1	B	749	GLY	CA-C	-6.76	1.42	1.51
1	A	953	HIS	ND1-CE1	6.71	1.39	1.32
1	A	673	GLN	N-CA	-6.68	1.37	1.46
1	B	845	ALA	N-CA	6.67	1.54	1.46
1	A	741	MET	CA-C	-6.63	1.43	1.52
1	A	758	PRO	C-N	6.63	1.43	1.33
1	B	797	ILE	CA-C	-6.62	1.44	1.52
1	A	1000	GLU	CA-CB	6.62	1.64	1.53
1	B	530	GLN	CA-C	-6.61	1.44	1.52
1	B	835	CYS	CA-CB	6.60	1.63	1.53
1	A	551	PHE	CA-C	6.59	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	924	PHE	N-CA	-6.58	1.38	1.46
1	A	563	ARG	C-N	6.57	1.42	1.33
1	B	637	ARG	NE-CZ	6.52	1.40	1.33
1	A	706	PHE	C-N	6.50	1.41	1.33
1	B	492	PRO	CA-C	-6.48	1.42	1.52
1	B	916	VAL	N-CA	-6.46	1.38	1.46
1	B	591	ARG	CD-NE	6.45	1.55	1.46
1	B	681	GLY	CA-C	-6.45	1.45	1.51
1	B	1015	LYS	N-CA	6.42	1.54	1.46
1	A	989	ARG	NE-CZ	6.41	1.40	1.33
1	B	792	LEU	CA-C	-6.41	1.44	1.52
1	B	513	SER	C-N	6.40	1.42	1.33
1	A	699	CYS	N-CA	-6.39	1.38	1.46
1	B	465	TRP	NE1-CE2	-6.39	1.30	1.37
1	B	504	THR	CA-CB	6.38	1.62	1.53
1	A	753	PRO	C-N	6.37	1.43	1.33
1	B	944	LEU	CA-C	-6.36	1.43	1.52
1	A	637	ARG	CA-C	-6.35	1.44	1.52
1	B	568	LEU	CA-CB	6.35	1.63	1.53
1	B	552	CYS	N-CA	-6.33	1.38	1.46
1	A	965	LEU	CA-CB	6.32	1.63	1.53
1	B	864	SER	CA-C	-6.32	1.44	1.52
1	B	822	HIS	ND1-CE1	6.27	1.38	1.32
1	B	779	PRO	CA-CB	6.26	1.62	1.53
1	A	917	SER	CA-C	-6.24	1.44	1.52
1	A	890	GLY	N-CA	-6.23	1.38	1.45
1	A	810	ARG	CD-NE	6.21	1.54	1.46
1	B	572	PHE	CA-CB	6.21	1.63	1.53
1	B	860	GLU	C-N	6.20	1.41	1.33
1	B	637	ARG	CD-NE	6.19	1.54	1.46
1	B	662	VAL	N-CA	6.18	1.54	1.46
1	A	818	GLY	CA-C	-6.13	1.44	1.51
1	B	595	GLU	N-CA	-6.13	1.38	1.46
1	A	578	VAL	C-N	6.11	1.42	1.33
1	B	608	GLU	CA-C	-6.11	1.44	1.52
1	B	745	ASP	CA-CB	6.07	1.63	1.53
1	B	825	LEU	C-N	6.07	1.41	1.33
1	A	958	VAL	C-N	6.05	1.42	1.33
1	A	694	VAL	CA-C	-6.03	1.45	1.52
1	A	788	ILE	C-N	6.03	1.42	1.34
1	A	863	CYS	CA-C	-6.02	1.44	1.52
1	B	724	ARG	CZ-NH2	6.01	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	950	ARG	CZ-NH1	6.00	1.41	1.32
1	B	973	PRO	N-CA	5.98	1.54	1.47
1	A	876	ARG	CA-CB	5.96	1.63	1.53
1	B	552	CYS	CA-CB	5.95	1.61	1.52
1	B	591	ARG	CZ-NH2	5.95	1.41	1.33
1	B	999	ARG	CA-CB	5.94	1.62	1.53
1	B	587	CYS	CA-CB	5.94	1.64	1.53
1	B	981	MET	CA-CB	5.94	1.63	1.53
1	B	503	ALA	N-CA	-5.94	1.39	1.46
1	B	988	VAL	CA-CB	-5.93	1.47	1.54
1	B	946	HIS	CG-CD2	5.91	1.42	1.35
1	B	467	TRP	CA-C	-5.91	1.45	1.52
1	B	543	VAL	CA-C	5.90	1.60	1.52
1	A	630	HIS	CA-CB	5.90	1.63	1.53
1	A	856	SER	C-N	-5.88	1.25	1.33
1	B	625	HIS	N-CA	-5.87	1.38	1.46
1	A	561	SER	C-N	5.85	1.41	1.33
1	A	635	TYR	CA-C	-5.84	1.45	1.52
1	B	617	ALA	N-CA	-5.83	1.38	1.46
1	A	853	HIS	CB-CG	5.82	1.58	1.50
1	A	684	CYS	CA-CB	5.82	1.61	1.53
1	A	630	HIS	ND1-CE1	5.82	1.38	1.32
1	B	950	ARG	CA-CB	5.82	1.62	1.53
1	B	810	ARG	CZ-NH1	5.79	1.40	1.32
1	B	924	PHE	CA-CB	5.78	1.62	1.53
1	A	461	ARG	CZ-NH1	5.76	1.40	1.32
1	B	726	ARG	CD-NE	5.76	1.54	1.46
1	A	838	MET	C-N	5.76	1.40	1.33
1	B	989	ARG	C-N	5.76	1.41	1.33
1	B	537	SER	N-CA	-5.75	1.38	1.45
1	A	803	ILE	N-CA	-5.74	1.39	1.46
1	A	810	ARG	CZ-NH2	5.74	1.41	1.33
1	B	909	GLY	CA-C	-5.73	1.45	1.52
1	B	694	VAL	CA-C	-5.73	1.45	1.52
1	A	884	MET	CA-CB	5.72	1.62	1.53
1	B	722	PRO	N-CD	5.72	1.55	1.47
1	A	507	ARG	NE-CZ	5.71	1.39	1.33
1	A	976	ILE	C-N	5.71	1.40	1.34
1	B	884	MET	C-O	-5.71	1.17	1.24
1	B	839	GLY	N-CA	5.70	1.53	1.45
1	A	497	GLY	N-CA	5.69	1.53	1.45
1	A	543	VAL	C-N	5.69	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	572	PHE	CA-CB	5.68	1.62	1.53
1	B	828	VAL	CA-C	5.68	1.59	1.52
1	A	498	GLY	CA-C	-5.67	1.45	1.52
1	A	503	ALA	C-N	5.66	1.40	1.33
1	A	986	VAL	CA-C	-5.65	1.45	1.52
1	B	856	SER	CA-CB	5.65	1.62	1.53
1	B	557	LEU	C-N	5.65	1.41	1.33
1	B	563	ARG	C-N	5.65	1.41	1.33
1	B	842	TRP	NE1-CE2	5.65	1.43	1.37
1	A	664	TRP	NE1-CE2	-5.63	1.31	1.37
1	A	762	LYS	N-CA	-5.62	1.40	1.46
1	A	651	TYR	N-CA	-5.62	1.39	1.46
1	B	747	LEU	CB-CG	5.62	1.64	1.53
1	B	800	ASP	CA-CB	5.61	1.62	1.53
1	A	974	ALA	CA-C	-5.58	1.45	1.52
1	A	821	TYR	CA-C	-5.57	1.45	1.52
1	B	810	ARG	CD-NE	5.57	1.54	1.46
1	A	835	CYS	CA-CB	5.56	1.61	1.53
1	A	888	LEU	C-N	5.55	1.41	1.34
1	A	607	TYR	CZ-OH	5.55	1.49	1.38
1	B	634	TYR	CA-CB	5.54	1.62	1.53
1	A	806	VAL	N-CA	5.54	1.53	1.46
1	A	793	CYS	CA-C	-5.54	1.45	1.52
1	B	788	ILE	C-N	5.54	1.41	1.34
1	B	888	LEU	C-N	5.54	1.41	1.34
1	A	822	HIS	CD2-NE2	5.53	1.44	1.37
1	A	977	VAL	C-N	5.52	1.41	1.33
1	B	910	VAL	CA-CB	5.49	1.61	1.54
1	B	708	VAL	C-N	5.48	1.41	1.33
1	A	607	TYR	CA-C	-5.47	1.45	1.52
1	B	559	TYR	CA-C	-5.47	1.45	1.52
1	B	844	VAL	C-O	-5.47	1.18	1.24
1	B	559	TYR	C-O	5.46	1.30	1.24
1	A	819	CYS	CA-C	-5.45	1.46	1.52
1	A	639	ALA	N-CA	-5.45	1.39	1.46
1	A	528	ALA	N-CA	-5.45	1.36	1.45
1	A	712	LEU	CA-C	-5.45	1.45	1.52
1	A	470	TYR	CA-C	-5.44	1.45	1.52
1	A	821	TYR	CZ-OH	5.43	1.49	1.38
1	A	552	CYS	C-N	5.43	1.41	1.33
1	B	852	THR	C-N	5.43	1.40	1.33
1	A	959	GLN	CA-CB	5.42	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	726	ARG	CD-NE	5.42	1.53	1.46
1	B	472	ASP	CA-CB	5.42	1.61	1.53
1	B	981	MET	CA-C	-5.41	1.45	1.52
1	B	724	ARG	NE-CZ	5.40	1.39	1.33
1	A	519	MET	C-N	5.40	1.40	1.33
1	B	486	TYR	N-CA	-5.40	1.40	1.46
1	B	768	ARG	CZ-NH2	5.39	1.40	1.33
1	A	713	LYS	C-N	5.39	1.41	1.33
1	A	702	PHE	C-N	5.38	1.41	1.33
1	B	723	THR	C-N	5.38	1.41	1.33
1	A	758	PRO	CA-C	5.38	1.57	1.52
1	B	594	GLU	CA-C	5.37	1.59	1.52
1	A	984	ALA	C-O	-5.37	1.17	1.24
1	B	544	PHE	N-CA	-5.37	1.40	1.46
1	A	569	TRP	CA-C	-5.36	1.45	1.52
1	B	982	VAL	C-N	5.36	1.40	1.33
1	B	1009	PRO	N-CD	-5.36	1.40	1.47
1	B	597	PHE	C-N	5.36	1.41	1.33
1	A	595	GLU	C-N	5.36	1.41	1.33
1	A	892	SER	C-N	5.35	1.39	1.33
1	B	636	CYS	CA-C	-5.35	1.46	1.52
1	B	528	ALA	N-CA	-5.35	1.39	1.46
1	A	648	THR	C-N	5.35	1.40	1.33
1	B	845	ALA	C-N	5.35	1.40	1.33
1	A	994	LEU	N-CA	-5.33	1.38	1.45
1	B	875	ILE	CA-C	-5.33	1.46	1.52
1	A	745	ASP	C-N	5.32	1.41	1.33
1	A	471	ARG	N-CA	-5.32	1.39	1.46
1	A	504	THR	N-CA	-5.31	1.40	1.46
1	B	676	HIS	ND1-CE1	5.30	1.37	1.32
1	A	860	GLU	CA-C	-5.28	1.46	1.52
1	A	872	PHE	C-N	5.28	1.41	1.33
1	A	560	LEU	C-N	5.28	1.40	1.33
1	A	482	PHE	C-N	5.27	1.40	1.33
1	A	853	HIS	CA-CB	5.26	1.61	1.53
1	A	706	PHE	N-CA	5.26	1.52	1.46
1	A	651	TYR	CA-CB	5.26	1.61	1.53
1	B	877	GLU	CA-CB	5.25	1.61	1.53
1	B	540	PRO	N-CA	-5.25	1.40	1.47
1	B	835	CYS	N-CA	-5.24	1.40	1.46
1	A	673	GLN	CA-C	5.24	1.59	1.52
1	A	709	SER	CA-CB	5.23	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	827	VAL	CA-C	5.22	1.59	1.52
1	B	851	ILE	N-CA	-5.22	1.40	1.46
1	A	887	VAL	CA-C	-5.21	1.46	1.52
1	B	560	LEU	C-O	-5.21	1.18	1.24
1	A	505	GLU	CA-CB	5.21	1.62	1.53
1	A	636	CYS	N-CA	-5.20	1.40	1.46
1	B	489	CYS	CA-C	-5.20	1.45	1.52
1	B	803	ILE	C-N	5.19	1.40	1.33
1	B	457	LEU	N-CA	-5.19	1.39	1.46
1	A	504	THR	C-N	5.18	1.41	1.33
1	B	969	ILE	CA-C	5.18	1.59	1.52
1	A	835	CYS	N-CA	-5.17	1.40	1.46
1	B	623	HIS	CD2-NE2	5.16	1.43	1.37
1	B	635	TYR	CA-C	-5.16	1.46	1.52
1	B	728	THR	C-N	5.14	1.39	1.33
1	B	836	SER	CA-C	5.14	1.59	1.52
1	B	531	PRO	CA-CB	5.13	1.60	1.53
1	B	860	GLU	CA-C	5.13	1.58	1.52
1	A	999	ARG	C-O	-5.12	1.18	1.24
1	A	518	SER	CA-C	-5.12	1.46	1.52
1	A	515	PHE	N-CA	-5.11	1.40	1.46
1	A	516	GLY	C-O	-5.10	1.17	1.23
1	A	966	LEU	C-N	5.09	1.40	1.33
1	B	823	LEU	N-CA	-5.09	1.40	1.46
1	B	972	SER	CA-C	5.09	1.59	1.53
1	B	620	TYR	CZ-OH	5.09	1.48	1.38
1	A	987	PHE	C-N	5.08	1.40	1.33
1	B	580	THR	CA-CB	-5.08	1.44	1.53
1	B	595	GLU	CA-C	5.07	1.59	1.52
1	B	630	HIS	ND1-CE1	5.06	1.37	1.32
1	B	718	SER	N-CA	-5.05	1.39	1.45
1	A	699	CYS	C-N	5.04	1.40	1.33
1	B	998	LYS	N-CA	-5.04	1.39	1.46
1	B	587	CYS	N-CA	-5.04	1.39	1.46
1	B	822	HIS	N-CA	-5.04	1.40	1.46
1	B	697	TRP	N-CA	-5.04	1.40	1.46
1	A	910	VAL	CA-CB	5.04	1.60	1.54
1	A	479	LEU	C-O	-5.03	1.18	1.24
1	B	798	PHE	CA-C	-5.03	1.46	1.52
1	A	749	GLY	C-O	-5.02	1.16	1.23
1	A	737	THR	N-CA	5.01	1.52	1.46

All (525) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	893	VAL	N-CA-C	-11.04	102.71	113.53
1	B	463	ALA	CA-C-O	-9.73	108.90	118.34
1	B	920	GLN	N-CA-C	-9.62	101.30	113.23
1	B	1010	GLU	N-CA-C	9.56	122.71	111.71
1	B	926	ASP	CA-C-N	9.40	132.88	120.28
1	B	926	ASP	C-N-CA	9.40	132.88	120.28
1	B	656	SER	N-CA-C	9.33	124.58	111.52
1	A	812	GLU	N-CA-C	-9.32	101.90	113.28
1	B	640	LEU	CA-C-N	9.23	129.31	119.89
1	B	640	LEU	C-N-CA	9.23	129.31	119.89
1	B	922	ILE	N-CA-C	-8.98	94.87	107.99
1	A	471	ARG	CA-C-N	8.98	132.31	120.28
1	A	471	ARG	C-N-CA	8.98	132.31	120.28
1	B	884	MET	N-CA-C	8.97	121.14	111.36
1	B	909	GLY	O-C-N	8.96	130.79	122.19
1	A	700	ILE	CA-C-O	-8.88	111.71	120.95
1	A	507	ARG	NE-CZ-NH2	8.84	127.15	119.20
1	A	835	CYS	CA-C-O	-8.78	111.60	120.82
1	B	668	THR	N-CA-CB	8.75	122.77	110.26
1	A	554	ASP	CA-CB-CG	8.72	121.32	112.60
1	B	731	ASP	CA-CB-CG	8.71	121.31	112.60
1	B	490	MET	N-CA-C	8.70	120.76	111.28
1	A	904	MET	CA-C-O	-8.69	109.91	118.34
1	A	693	ASP	CA-CB-CG	-8.40	104.19	112.60
1	B	559	TYR	O-C-N	8.38	131.00	122.12
1	B	1013	LYS	CA-C-O	-8.35	111.57	120.42
1	A	983	LEU	CA-C-N	8.26	131.35	120.28
1	A	983	LEU	C-N-CA	8.26	131.35	120.28
1	A	501	GLY	O-C-N	8.22	130.08	122.19
1	A	746	PHE	CA-C-N	8.21	131.79	120.63
1	A	746	PHE	C-N-CA	8.21	131.79	120.63
1	B	1015	LYS	CA-C-N	8.13	131.69	120.63
1	B	1015	LYS	C-N-CA	8.13	131.69	120.63
1	B	568	LEU	CA-C-O	-8.03	112.04	120.55
1	B	840	LEU	CA-C-N	7.96	127.98	119.78
1	B	840	LEU	C-N-CA	7.96	127.98	119.78
1	A	482	PHE	CA-CB-CG	7.92	121.72	113.80
1	B	961	THR	N-CA-CB	7.90	121.73	110.12
1	B	516	GLY	CA-C-N	7.89	130.70	120.44
1	B	516	GLY	C-N-CA	7.89	130.70	120.44
1	A	894	PHE	N-CA-C	-7.88	101.80	113.61
1	B	708	VAL	N-CA-C	7.81	118.61	110.72
1	A	583	SER	N-CA-C	7.80	119.86	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	853	HIS	CA-CB-CG	7.80	121.60	113.80
1	A	467	TRP	O-C-N	-7.78	112.11	122.23
1	A	822	HIS	CB-CG-CD2	-7.78	121.08	131.20
1	A	456	VAL	CA-C-O	-7.77	112.87	120.95
1	A	503	ALA	CA-C-O	-7.69	112.27	120.42
1	B	981	MET	N-CA-CB	7.68	122.19	110.28
1	A	663	ASN	N-CA-C	-7.67	104.05	113.41
1	A	715	PHE	CA-CB-CG	7.63	121.43	113.80
1	A	835	CYS	O-C-N	7.61	129.91	122.07
1	A	968	VAL	CA-C-N	7.58	130.85	120.46
1	A	968	VAL	C-N-CA	7.58	130.85	120.46
1	B	559	TYR	CA-C-O	-7.54	112.56	120.55
1	A	990	LYS	N-CA-C	7.53	120.44	111.33
1	A	701	LEU	CA-C-N	7.52	130.57	120.65
1	A	701	LEU	C-N-CA	7.52	130.57	120.65
1	A	785	ALA	CA-C-O	7.50	128.57	119.49
1	A	886	PHE	CA-CB-CG	-7.44	106.36	113.80
1	B	679	PHE	N-CA-C	-7.43	96.44	108.41
1	B	833	GLY	O-C-N	-7.43	115.04	122.18
1	A	943	TYR	N-CA-C	7.43	120.25	111.71
1	A	948	PRO	CA-C-N	7.42	130.97	120.28
1	A	948	PRO	C-N-CA	7.42	130.97	120.28
1	A	944	LEU	N-CA-C	7.41	119.36	111.28
1	B	501	GLY	CA-C-O	-7.35	113.06	121.00
1	A	951	LYS	CA-C-O	-7.35	112.63	120.42
1	B	643	ASN	CA-C-N	7.33	127.31	119.76
1	B	643	ASN	C-N-CA	7.33	127.31	119.76
1	A	1008	MET	N-CA-C	-7.28	96.74	109.48
1	B	948	PRO	N-CA-C	7.26	122.66	111.11
1	B	585	LEU	CA-C-O	7.23	126.71	118.47
1	A	463	ALA	CA-C-N	7.22	127.22	119.28
1	A	463	ALA	C-N-CA	7.22	127.22	119.28
1	A	757	VAL	N-CA-C	-7.21	103.28	109.19
1	A	507	ARG	NE-CZ-NH1	-7.20	114.31	121.50
1	A	851	ILE	CA-C-O	-7.19	113.22	120.85
1	A	930	LEU	O-C-N	-7.19	113.49	122.19
1	B	887	VAL	CA-C-O	-7.19	113.55	121.17
1	B	539	GLY	CA-C-O	-7.18	111.25	121.52
1	A	851	ILE	N-CA-C	7.16	117.95	110.72
1	B	591	ARG	N-CA-C	7.16	119.08	111.28
1	A	611	GLU	N-CA-CB	7.15	120.74	110.16
1	A	956	THR	N-CA-CB	7.15	120.63	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	898	VAL	N-CA-C	7.13	117.89	110.62
1	B	859	LEU	O-C-N	-7.12	115.22	123.27
1	A	799	MET	CA-C-N	7.10	129.68	120.44
1	A	799	MET	C-N-CA	7.10	129.68	120.44
1	B	793	CYS	CA-C-O	-7.09	113.03	120.55
1	B	767	ASP	CA-C-O	7.08	126.63	119.97
1	A	904	MET	O-C-N	7.07	127.36	120.71
1	A	785	ALA	O-C-N	-7.07	113.20	122.39
1	A	1018	ASP	CA-CB-CG	-7.07	105.53	112.60
1	A	512	GLU	N-CA-C	-7.05	103.59	111.28
1	A	665	ALA	N-CA-C	-7.05	103.53	111.14
1	A	609	ALA	CA-C-O	7.01	128.18	120.82
1	A	823	LEU	CA-C-N	6.99	129.98	120.54
1	A	823	LEU	C-N-CA	6.99	129.98	120.54
1	A	541	VAL	N-CA-C	6.98	117.74	110.62
1	B	623	HIS	CE1-NE2-CD2	-6.96	102.04	109.00
1	A	831	MET	CA-C-N	6.95	129.48	120.44
1	A	831	MET	C-N-CA	6.95	129.48	120.44
1	A	461	ARG	CA-C-O	-6.91	110.92	119.28
1	B	495	THR	CA-C-N	6.90	129.41	120.44
1	B	495	THR	C-N-CA	6.90	129.41	120.44
1	A	518	SER	CA-C-O	-6.90	113.58	120.82
1	A	853	HIS	CA-CB-CG	6.90	120.70	113.80
1	B	505	GLU	N-CA-C	6.88	120.89	111.39
1	A	958	VAL	N-CA-CB	6.88	119.89	110.54
1	A	533	THR	N-CA-C	-6.87	98.49	109.76
1	B	721	PHE	O-C-N	-6.87	117.31	121.71
1	A	938	GLN	CA-C-N	6.86	126.84	119.78
1	A	938	GLN	C-N-CA	6.86	126.84	119.78
1	B	597	PHE	CA-C-N	6.86	129.77	120.44
1	B	597	PHE	C-N-CA	6.86	129.77	120.44
1	B	774	PRO	N-CA-C	6.86	121.84	111.14
1	A	838	MET	CA-C-O	6.85	127.36	119.35
1	B	950	ARG	NE-CZ-NH2	-6.84	113.04	119.20
1	A	886	PHE	N-CA-C	-6.84	103.61	112.23
1	B	855	ASN	N-CA-C	6.84	118.81	111.36
1	A	1020	LYS	N-CA-C	-6.83	105.07	113.41
1	B	989	ARG	CA-C-O	6.83	127.99	120.82
1	B	641	PRO	N-CA-CB	6.82	109.05	103.32
1	B	843	PHE	CA-CB-CG	-6.78	107.02	113.80
1	A	500	LEU	N-CA-C	-6.77	104.03	112.90
1	A	823	LEU	N-CA-C	6.76	118.65	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	ASP	CA-C-N	6.75	130.30	120.71
1	A	472	ASP	C-N-CA	6.75	130.30	120.71
1	A	908	TYR	O-C-N	-6.74	114.47	122.15
1	B	703	PHE	CA-C-O	-6.74	113.28	120.42
1	A	632	SER	N-CA-C	6.72	121.08	113.01
1	B	556	ALA	CA-C-N	6.70	129.81	120.29
1	B	556	ALA	C-N-CA	6.70	129.81	120.29
1	A	690	TYR	CA-C-N	6.66	129.65	120.39
1	A	690	TYR	C-N-CA	6.66	129.65	120.39
1	A	478	CYS	CA-C-N	6.66	129.10	120.44
1	A	478	CYS	C-N-CA	6.66	129.10	120.44
1	A	597	PHE	CA-C-N	6.64	129.72	120.29
1	A	597	PHE	C-N-CA	6.64	129.72	120.29
1	B	938	GLN	OE1-CD-NE2	6.61	129.21	122.60
1	A	767	ASP	N-CA-C	-6.61	104.38	114.16
1	A	805	ALA	CA-C-N	6.61	128.89	120.56
1	A	805	ALA	C-N-CA	6.61	128.89	120.56
1	A	620	TYR	CA-C-N	6.60	126.58	119.78
1	A	620	TYR	C-N-CA	6.60	126.58	119.78
1	A	782	THR	CA-C-N	6.57	129.47	120.46
1	A	782	THR	C-N-CA	6.57	129.47	120.46
1	B	491	SER	CA-C-O	-6.57	112.30	118.73
1	B	944	LEU	N-CA-C	-6.56	105.84	114.31
1	B	1008	MET	CA-C-N	6.55	127.09	120.14
1	B	1008	MET	C-N-CA	6.55	127.09	120.14
1	A	801	GLN	CA-C-N	6.54	129.57	120.29
1	A	801	GLN	C-N-CA	6.54	129.57	120.29
1	B	723	THR	CA-C-N	6.53	129.03	120.28
1	B	723	THR	C-N-CA	6.53	129.03	120.28
1	B	810	ARG	N-CA-CB	6.51	120.45	110.49
1	A	885	ILE	N-CA-C	6.50	116.99	110.23
1	A	908	TYR	CA-C-O	6.50	127.31	120.42
1	A	563	ARG	NE-CZ-NH1	-6.50	115.00	121.50
1	B	479	LEU	CA-C-N	6.50	128.99	120.28
1	B	479	LEU	C-N-CA	6.50	128.99	120.28
1	A	554	ASP	N-CA-C	-6.48	98.64	109.07
1	B	471	ARG	NE-CZ-NH2	6.48	125.03	119.20
1	A	461	ARG	NE-CZ-NH1	-6.47	115.03	121.50
1	B	512	GLU	N-CA-C	6.46	118.33	111.28
1	B	843	PHE	N-CA-C	-6.46	98.09	109.06
1	B	759	SER	CB-CA-C	-6.44	99.33	110.09
1	B	637	ARG	O-C-N	-6.43	115.33	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	663	ASN	CA-CB-CG	6.42	119.02	112.60
1	A	735	PHE	CA-CB-CG	-6.42	107.38	113.80
1	B	607	TYR	CA-C-O	6.42	127.56	120.82
1	B	882	GLY	CA-C-N	6.41	129.11	120.65
1	B	882	GLY	C-N-CA	6.41	129.11	120.65
1	B	517	ALA	CA-C-N	6.41	128.77	120.44
1	B	517	ALA	C-N-CA	6.41	128.77	120.44
1	B	784	ILE	CA-C-O	6.40	127.64	120.85
1	A	931	PHE	CA-CB-CG	6.40	120.20	113.80
1	B	570	THR	CA-C-O	-6.39	112.62	119.97
1	A	782	THR	N-CA-C	6.38	118.24	111.28
1	A	822	HIS	CE1-NE2-CD2	-6.38	102.62	109.00
1	B	733	ALA	N-CA-C	6.37	118.75	111.11
1	B	626	SER	N-CA-C	6.36	118.21	111.28
1	B	739	PHE	CA-C-O	-6.35	114.15	120.82
1	A	576	VAL	O-C-N	6.34	128.97	121.80
1	A	643	ASN	CA-C-N	6.33	126.28	119.76
1	A	643	ASN	C-N-CA	6.33	126.28	119.76
1	B	727	SER	O-C-N	6.32	128.81	122.12
1	A	803	ILE	CA-C-O	-6.30	114.17	120.85
1	B	913	TYR	CA-C-N	6.28	129.01	120.54
1	B	913	TYR	C-N-CA	6.28	129.01	120.54
1	A	690	TYR	CB-CG-CD1	6.27	130.21	120.80
1	A	467	TRP	CA-C-N	6.26	130.62	120.60
1	A	467	TRP	C-N-CA	6.26	130.62	120.60
1	A	989	ARG	CA-C-N	6.26	128.96	120.38
1	A	989	ARG	C-N-CA	6.26	128.96	120.38
1	A	477	GLN	N-CA-C	-6.25	104.24	113.61
1	A	964	VAL	CA-C-N	6.25	128.65	120.28
1	A	964	VAL	C-N-CA	6.25	128.65	120.28
1	B	676	HIS	CG-CD2-NE2	6.25	113.44	107.20
1	A	950	ARG	CA-C-N	6.24	129.15	120.29
1	A	950	ARG	C-N-CA	6.24	129.15	120.29
1	B	869	GLN	CA-C-N	6.24	126.21	119.78
1	B	869	GLN	C-N-CA	6.24	126.21	119.78
1	B	605	PHE	CA-CB-CG	-6.23	107.57	113.80
1	B	794	THR	CA-C-N	6.22	128.40	120.56
1	B	794	THR	C-N-CA	6.22	128.40	120.56
1	A	988	VAL	CA-C-N	6.22	128.53	120.44
1	A	988	VAL	C-N-CA	6.22	128.53	120.44
1	B	554	ASP	CA-CB-CG	6.21	118.81	112.60
1	B	696	PHE	N-CA-C	6.20	120.04	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	914	MET	CA-C-O	-6.19	114.32	120.82
1	A	455	LEU	CA-C-N	6.18	128.93	120.46
1	A	455	LEU	C-N-CA	6.18	128.93	120.46
1	A	623	HIS	CE1-NE2-CD2	-6.18	102.82	109.00
1	A	628	LEU	N-CA-C	6.16	123.92	110.80
1	B	764	THR	N-CA-C	6.16	119.18	110.50
1	A	704	ALA	N-CA-CB	6.13	119.12	110.12
1	B	876	ARG	CD-NE-CZ	-6.12	115.83	124.40
1	B	935	ALA	N-CA-C	6.12	120.88	113.17
1	A	1013	LYS	CA-C-N	6.11	128.39	120.44
1	A	1013	LYS	C-N-CA	6.11	128.39	120.44
1	A	822	HIS	N-CA-CB	6.11	119.20	110.16
1	A	700	ILE	O-C-N	6.11	127.79	121.87
1	A	918	SER	N-CA-C	6.10	118.01	111.36
1	A	950	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	B	822	HIS	O-C-N	-6.08	115.22	122.15
1	B	452	PHE	N-CA-CB	6.07	119.06	109.71
1	B	795	ILE	CA-C-O	-6.06	114.74	121.17
1	B	724	ARG	N-CA-C	6.06	117.88	111.28
1	A	789	PRO	CA-C-N	6.04	129.49	120.31
1	A	789	PRO	C-N-CA	6.04	129.49	120.31
1	A	800	ASP	CA-C-N	6.03	128.68	120.54
1	A	800	ASP	C-N-CA	6.03	128.68	120.54
1	B	549	PHE	CA-CB-CG	-6.03	107.77	113.80
1	B	494	ILE	N-CA-C	6.03	116.77	110.62
1	B	731	ASP	N-CA-C	-6.03	107.16	114.75
1	A	503	ALA	CB-CA-C	-6.02	100.62	110.85
1	A	528	ALA	CB-CA-C	-6.01	103.69	113.37
1	B	778	ASN	CA-C-N	-6.01	113.58	119.78
1	B	778	ASN	C-N-CA	-6.01	113.58	119.78
1	B	630	HIS	CE1-NE2-CD2	-6.00	103.00	109.00
1	A	925	PHE	CA-C-O	-6.00	114.19	120.55
1	B	504	THR	O-C-N	5.99	129.91	122.19
1	B	588	TYR	CB-CG-CD1	5.98	129.77	120.80
1	B	790	ALA	CA-C-N	5.97	128.76	120.29
1	B	790	ALA	C-N-CA	5.97	128.76	120.29
1	A	514	LEU	N-CA-C	-5.94	104.80	111.28
1	A	673	GLN	N-CA-C	5.94	120.14	113.01
1	A	790	ALA	N-CA-CB	5.93	119.48	110.28
1	B	500	LEU	CA-C-N	5.93	126.53	119.94
1	B	500	LEU	C-N-CA	5.93	126.53	119.94
1	B	607	TYR	O-C-N	-5.93	115.96	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	951	LYS	CA-C-N	5.93	128.03	120.56
1	B	951	LYS	C-N-CA	5.93	128.03	120.56
1	B	752	SER	CA-C-N	5.90	126.23	119.92
1	B	752	SER	C-N-CA	5.90	126.23	119.92
1	A	903	PRO	CB-CA-C	-5.90	103.22	110.95
1	B	763	PRO	CA-C-O	-5.90	114.41	121.48
1	B	630	HIS	ND1-CE1-NE2	5.89	114.29	108.40
1	B	729	VAL	N-CA-C	-5.89	105.34	111.58
1	A	623	HIS	CG-CD2-NE2	5.88	113.08	107.20
1	A	712	LEU	CA-C-O	-5.87	114.33	120.55
1	B	634	TYR	N-CA-CB	5.87	118.59	109.97
1	A	593	THR	CA-C-N	5.86	128.61	120.29
1	A	593	THR	C-N-CA	5.86	128.61	120.29
1	B	924	PHE	CA-C-N	5.85	128.39	120.38
1	B	924	PHE	C-N-CA	5.85	128.39	120.38
1	A	584	SER	N-CA-C	5.85	117.65	111.28
1	A	876	ARG	NE-CZ-NH1	-5.84	115.66	121.50
1	B	501	GLY	O-C-N	5.84	127.78	122.18
1	B	1012	LYS	CA-C-N	5.83	128.58	120.29
1	B	1012	LYS	C-N-CA	5.83	128.58	120.29
1	B	931	PHE	CA-CB-CG	5.83	119.63	113.80
1	B	1016	LEU	N-CA-C	-5.82	104.57	111.03
1	A	725	VAL	CA-C-N	5.82	128.54	120.63
1	A	725	VAL	C-N-CA	5.82	128.54	120.63
1	B	751	PRO	CA-C-N	5.81	128.47	120.39
1	B	751	PRO	C-N-CA	5.81	128.47	120.39
1	A	696	PHE	CA-CB-CG	-5.81	107.99	113.80
1	A	813	HIS	N-CA-C	-5.81	105.51	112.59
1	B	868	GLU	N-CA-C	5.81	117.55	110.41
1	B	835	CYS	N-CA-CB	5.80	118.64	110.12
1	A	863	CYS	N-CA-C	-5.79	106.37	113.50
1	A	836	SER	CA-C-O	-5.79	114.42	120.55
1	A	588	TYR	CA-CB-CG	-5.79	103.49	113.90
1	B	831	MET	CG-SD-CE	5.79	113.63	100.90
1	B	742	VAL	CA-CB-CG2	-5.78	100.57	110.40
1	B	822	HIS	ND1-CE1-NE2	5.78	114.18	108.40
1	B	568	LEU	CA-C-N	5.78	127.95	120.44
1	B	568	LEU	C-N-CA	5.78	127.95	120.44
1	B	834	VAL	N-CA-C	5.78	116.56	110.72
1	A	528	ALA	CA-C-O	-5.78	114.65	120.77
1	B	945	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	B	956	THR	N-CA-C	5.77	117.57	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	663	ASN	N-CA-CB	5.75	118.87	110.47
1	B	706	PHE	CA-CB-CG	-5.75	108.05	113.80
1	A	591	ARG	N-CA-C	5.74	117.54	111.28
1	B	698	SER	N-CA-CB	5.73	118.64	110.16
1	B	798	PHE	N-CA-C	5.73	117.20	111.07
1	B	941	PHE	CA-C-O	-5.72	115.02	122.45
1	B	504	THR	CA-C-N	5.71	130.47	122.36
1	B	504	THR	C-N-CA	5.71	130.47	122.36
1	B	726	ARG	NE-CZ-NH2	5.71	124.33	119.20
1	B	953	HIS	O-C-N	5.71	128.17	122.12
1	A	464	PRO	CB-CA-C	-5.70	103.31	112.21
1	B	588	TYR	CB-CG-CD2	-5.70	112.25	120.80
1	B	797	ILE	N-CA-C	5.70	116.43	110.62
1	A	952	VAL	N-CA-CB	5.69	117.86	110.57
1	B	835	CYS	CB-CA-C	-5.68	101.36	110.79
1	A	791	LEU	N-CA-CB	5.68	118.56	110.16
1	A	978	PHE	CA-C-N	5.68	125.04	118.85
1	A	978	PHE	C-N-CA	5.68	125.04	118.85
1	B	889	MET	CA-C-N	5.68	126.28	119.98
1	B	889	MET	C-N-CA	5.68	126.28	119.98
1	A	903	PRO	N-CD-CG	5.67	111.71	103.20
1	B	848	VAL	CA-C-O	-5.67	115.06	120.95
1	A	743	ILE	O-C-N	5.66	127.79	121.90
1	B	999	ARG	N-CA-CB	5.66	118.54	110.16
1	A	671	GLU	CA-C-N	5.66	127.86	120.28
1	A	671	GLU	C-N-CA	5.66	127.86	120.28
1	A	955	PHE	CA-C-O	-5.65	114.89	120.82
1	A	914	MET	CA-C-N	5.65	126.25	119.98
1	A	914	MET	C-N-CA	5.65	126.25	119.98
1	A	758	PRO	N-CA-CB	5.64	106.08	102.92
1	B	570	THR	N-CA-CB	5.64	119.02	110.28
1	B	1020	LYS	N-CA-C	-5.63	106.57	113.50
1	B	724	ARG	NE-CZ-NH1	5.63	127.13	121.50
1	B	502	GLU	CA-C-N	5.63	128.10	120.44
1	B	502	GLU	C-N-CA	5.63	128.10	120.44
1	B	953	HIS	CE1-NE2-CD2	-5.63	103.37	109.00
1	B	467	TRP	N-CA-C	5.62	117.49	111.36
1	B	503	ALA	N-CA-C	5.61	117.19	111.14
1	B	585	LEU	CA-C-N	5.61	128.38	120.42
1	B	585	LEU	C-N-CA	5.61	128.38	120.42
1	B	670	SER	CA-C-N	5.60	127.78	120.28
1	B	670	SER	C-N-CA	5.60	127.78	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	THR	CA-C-N	5.60	126.19	119.98
1	A	881	THR	C-N-CA	5.60	126.19	119.98
1	A	892	SER	N-CA-CB	5.59	119.94	110.49
1	A	721	PHE	CA-CB-CG	5.59	119.39	113.80
1	B	543	VAL	CA-C-N	5.58	127.69	120.44
1	B	543	VAL	C-N-CA	5.58	127.69	120.44
1	B	869	GLN	N-CA-C	5.58	122.14	109.81
1	A	903	PRO	CA-C-O	-5.58	114.94	122.08
1	B	569	TRP	N-CA-C	-5.57	105.11	111.07
1	B	741	MET	CG-SD-CE	-5.57	88.65	100.90
1	A	617	ALA	CA-C-O	5.57	126.37	119.97
1	A	790	ALA	CA-C-N	5.57	128.19	120.29
1	A	790	ALA	C-N-CA	5.57	128.19	120.29
1	A	968	VAL	N-CA-CB	5.56	120.84	110.77
1	A	694	VAL	N-CA-C	5.56	116.29	110.62
1	B	893	VAL	O-C-N	5.55	128.08	121.80
1	B	709	SER	N-CA-CB	5.55	118.27	110.12
1	B	822	HIS	CE1-NE2-CD2	-5.54	103.45	109.00
1	B	497	GLY	CA-C-N	5.54	126.13	119.98
1	B	497	GLY	C-N-CA	5.54	126.13	119.98
1	A	977	VAL	CA-C-N	5.54	127.02	120.09
1	A	977	VAL	C-N-CA	5.54	127.02	120.09
1	A	844	VAL	N-CA-C	-5.54	99.83	108.86
1	A	671	GLU	N-CA-C	5.53	116.99	111.07
1	B	954	LEU	CA-C-O	-5.53	114.56	120.42
1	B	982	VAL	CA-CB-CG1	5.53	119.80	110.40
1	B	697	TRP	CA-C-O	-5.53	114.69	120.55
1	A	872	PHE	CA-C-N	5.52	132.08	121.54
1	A	872	PHE	C-N-CA	5.52	132.08	121.54
1	A	876	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	B	955	PHE	CA-CB-CG	5.50	119.30	113.80
1	B	974	ALA	N-CA-C	-5.50	99.08	110.80
1	A	618	GLU	N-CA-CB	5.49	118.29	110.16
1	B	721	PHE	CA-C-O	5.49	125.55	120.50
1	B	816	LYS	CB-CG-CD	5.49	123.94	111.30
1	A	949	LEU	N-CA-C	-5.49	105.40	111.71
1	B	461	ARG	O-C-N	-5.49	114.27	122.39
1	B	590	THR	CA-C-N	5.48	127.62	120.28
1	B	590	THR	C-N-CA	5.48	127.62	120.28
1	A	951	LYS	O-C-N	5.47	128.39	122.15
1	B	708	VAL	CA-C-N	5.47	127.61	120.28
1	B	708	VAL	C-N-CA	5.47	127.61	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	893	VAL	N-CA-CB	5.46	119.50	112.12
1	B	956	THR	N-CA-CB	5.46	118.15	110.12
1	A	577	LEU	CA-C-N	5.46	129.71	120.64
1	A	577	LEU	C-N-CA	5.46	129.71	120.64
1	A	462	LYS	CA-C-N	5.46	127.58	120.26
1	A	462	LYS	C-N-CA	5.46	127.58	120.26
1	B	808	ILE	CA-C-N	5.46	132.01	122.95
1	B	808	ILE	C-N-CA	5.46	132.01	122.95
1	B	937	HIS	O-C-N	-5.46	115.64	122.24
1	B	797	ILE	CA-C-N	5.45	127.52	120.44
1	B	797	ILE	C-N-CA	5.45	127.52	120.44
1	A	754	LYS	CA-C-O	-5.42	114.77	121.11
1	B	521	GLY	CA-C-O	-5.42	115.17	120.75
1	B	608	GLU	N-CA-C	5.42	119.61	112.89
1	B	741	MET	N-CA-C	-5.42	105.54	111.82
1	A	959	GLN	CA-C-N	5.41	127.98	120.29
1	A	959	GLN	C-N-CA	5.41	127.98	120.29
1	B	496	PHE	CA-C-N	5.41	125.95	119.94
1	B	496	PHE	C-N-CA	5.41	125.95	119.94
1	B	560	LEU	CA-C-N	5.41	127.53	120.28
1	B	560	LEU	C-N-CA	5.41	127.53	120.28
1	B	650	GLN	N-CA-CB	5.41	117.86	110.01
1	B	543	VAL	N-CA-C	5.41	116.19	110.72
1	B	953	HIS	CA-C-N	5.41	127.97	120.29
1	B	953	HIS	C-N-CA	5.41	127.97	120.29
1	B	863	CYS	N-CA-CB	5.41	119.69	110.87
1	B	712	LEU	CA-C-O	-5.39	115.16	120.82
1	B	701	LEU	CA-C-N	5.39	127.77	120.65
1	B	701	LEU	C-N-CA	5.39	127.77	120.65
1	A	1015	LYS	CA-C-O	-5.38	114.84	120.55
1	A	503	ALA	N-CA-CB	5.38	118.12	110.16
1	B	884	MET	CA-C-O	5.37	126.11	120.42
1	B	992	MET	N-CA-C	5.37	119.31	112.87
1	B	535	LEU	CA-C-O	-5.37	115.71	121.56
1	B	1019	ALA	CB-CA-C	-5.37	99.92	110.11
1	B	856	SER	N-CA-C	5.36	117.13	111.28
1	B	721	PHE	CA-CB-CG	-5.36	108.44	113.80
1	A	822	HIS	CB-CA-C	-5.35	101.76	110.85
1	A	980	MET	N-CA-CB	5.34	119.25	110.39
1	A	991	VAL	N-CA-CB	5.33	117.80	110.54
1	A	969	ILE	CA-C-N	5.33	127.42	120.28
1	A	969	ILE	C-N-CA	5.33	127.42	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	577	LEU	N-CA-C	5.32	117.16	111.36
1	B	817	LYS	N-CA-CB	5.32	119.89	111.43
1	B	745	ASP	CA-C-N	5.32	127.85	120.29
1	B	745	ASP	C-N-CA	5.32	127.85	120.29
1	A	737	THR	N-CA-CB	5.32	117.72	110.01
1	B	698	SER	O-C-N	5.31	128.21	122.15
1	B	922	ILE	CA-C-O	5.30	126.37	120.59
1	A	689	PRO	CB-CA-C	5.30	118.01	111.23
1	B	952	VAL	O-C-N	5.30	127.10	121.91
1	A	569	TRP	O-C-N	-5.29	116.51	122.12
1	B	728	THR	CA-C-N	5.29	129.91	121.34
1	B	728	THR	C-N-CA	5.29	129.91	121.34
1	A	742	VAL	CA-C-N	5.29	127.33	120.56
1	A	742	VAL	C-N-CA	5.29	127.33	120.56
1	B	537	SER	CA-C-N	5.29	130.77	122.21
1	B	537	SER	C-N-CA	5.29	130.77	122.21
1	A	714	THR	CA-C-N	5.28	129.06	120.60
1	A	714	THR	C-N-CA	5.28	129.06	120.60
1	A	818	GLY	O-C-N	-5.27	118.12	122.92
1	B	768	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	B	953	HIS	CA-C-O	-5.27	114.97	120.55
1	B	709	SER	CA-C-N	5.25	128.30	120.31
1	B	709	SER	C-N-CA	5.25	128.30	120.31
1	A	630	HIS	CA-CB-CG	5.24	119.04	113.80
1	B	806	VAL	CA-C-N	5.24	127.64	120.46
1	B	806	VAL	C-N-CA	5.24	127.64	120.46
1	A	571	ALA	CA-C-N	5.24	127.29	120.28
1	A	571	ALA	C-N-CA	5.24	127.29	120.28
1	B	496	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	595	GLU	CA-C-N	5.23	127.28	120.28
1	A	595	GLU	C-N-CA	5.23	127.28	120.28
1	A	570	THR	O-C-N	-5.22	115.84	122.27
1	A	697	TRP	O-C-N	-5.22	116.20	122.15
1	B	569	TRP	CA-C-O	-5.22	115.34	120.82
1	A	975	ALA	CA-C-N	5.21	129.26	120.29
1	A	975	ALA	C-N-CA	5.21	129.26	120.29
1	B	737	THR	CA-C-O	-5.21	115.03	120.55
1	A	576	VAL	CA-C-O	-5.21	114.85	120.47
1	A	483	LEU	CA-C-O	-5.20	115.03	120.55
1	B	860	GLU	N-CA-C	-5.20	101.17	109.23
1	A	687	HIS	N-CA-C	5.20	116.95	111.28
1	B	707	ILE	CA-C-N	5.20	127.80	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	707	ILE	C-N-CA	5.20	127.80	120.42
1	A	647	HIS	CA-CB-CG	-5.19	108.61	113.80
1	A	623	HIS	ND1-CE1-NE2	5.19	113.59	108.40
1	B	484	PHE	O-C-N	5.19	127.41	122.07
1	A	463	ALA	CA-C-O	-5.18	113.65	118.73
1	A	683	ALA	N-CA-CB	-5.17	102.33	110.46
1	B	760	VAL	CA-C-N	5.17	129.65	122.77
1	B	760	VAL	C-N-CA	5.17	129.65	122.77
1	B	927	ARG	CD-NE-CZ	-5.17	117.17	124.40
1	A	694	VAL	O-C-N	-5.16	116.86	121.87
1	A	802	GLN	N-CA-CB	5.16	117.80	110.16
1	A	890	GLY	O-C-N	5.16	127.14	122.18
1	B	937	HIS	CB-CG-ND1	5.16	130.44	122.70
1	B	999	ARG	CA-C-O	5.16	125.89	120.42
1	A	792	LEU	CA-C-O	5.16	125.89	120.42
1	B	995	CYS	N-CA-C	-5.16	105.74	111.36
1	A	930	LEU	CA-C-O	5.16	125.56	119.48
1	B	744	LEU	N-CA-CB	5.15	117.68	110.12
1	B	738	ILE	O-C-N	-5.14	116.87	121.91
1	B	750	VAL	N-CA-C	-5.14	97.77	108.88
1	A	618	GLU	CB-CA-C	-5.14	102.12	110.85
1	B	489	CYS	N-CA-CB	5.14	118.21	110.30
1	B	950	ARG	N-CA-C	-5.13	105.58	111.07
1	A	911	PHE	CA-CB-CG	5.13	118.93	113.80
1	B	952	VAL	N-CA-C	5.13	115.34	110.42
1	A	726	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	A	822	HIS	ND1-CE1-NE2	5.12	113.52	108.40
1	B	516	GLY	CA-C-O	-5.12	115.48	120.75
1	B	853	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
1	A	459	VAL	CB-CA-C	-5.10	105.25	112.14
1	B	650	GLN	CA-C-N	5.10	127.37	120.38
1	B	650	GLN	C-N-CA	5.10	127.37	120.38
1	A	951	LYS	CA-C-N	5.10	127.09	120.56
1	A	951	LYS	C-N-CA	5.10	127.09	120.56
1	B	678	GLU	N-CA-CB	5.09	117.75	110.06
1	A	967	TRP	N-CA-CB	5.09	117.39	110.01
1	B	650	GLN	O-C-N	-5.08	116.83	122.07
1	B	609	ALA	CA-C-O	5.07	126.14	120.82
1	A	949	LEU	CA-C-N	5.07	127.33	120.44
1	A	949	LEU	C-N-CA	5.07	127.33	120.44
1	B	761	PHE	CA-CB-CG	5.05	118.85	113.80
1	B	953	HIS	ND1-CE1-NE2	5.05	113.45	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	SER	CA-C-N	5.05	130.60	122.83
1	B	468	SER	C-N-CA	5.05	130.60	122.83
1	B	784	ILE	O-C-N	-5.05	116.63	121.83
1	A	737	THR	CA-CB-OG1	5.04	117.16	109.60
1	B	737	THR	N-CA-CB	5.04	117.53	110.12
1	A	574	CYS	CA-C-O	-5.03	114.19	119.97
1	B	978	PHE	N-CA-C	5.03	120.44	113.45
1	B	825	LEU	CA-C-N	5.03	126.97	120.44
1	B	825	LEU	C-N-CA	5.03	126.97	120.44
1	B	874	GLY	CA-C-O	-5.03	114.73	122.52
1	B	877	GLU	N-CA-C	-5.03	100.10	108.34
1	A	781	TRP	N-CA-C	5.02	117.48	111.71
1	B	641	PRO	CA-N-CD	-5.02	104.97	112.00
1	A	970	LYS	O-C-N	5.02	127.44	122.12
1	A	956	THR	CA-C-O	-5.01	115.23	120.55
1	B	1009	PRO	CA-C-O	-5.01	115.75	121.86
1	B	517	ALA	O-C-N	-5.01	116.91	122.07
1	A	824	ASP	O-C-N	-5.00	116.89	122.09
1	A	1015	LYS	CA-C-N	5.00	127.44	120.63
1	A	1015	LYS	C-N-CA	5.00	127.44	120.63

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

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Mol	Chain	Res	Type	Group
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	59
1	B	569/571 (100%)	530 (93%)	38 (7%)	1 (0%)	43	71
All	All	1138/1142 (100%)	1058 (93%)	77 (7%)	3 (0%)	37	65

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%)	485 (97%)	16 (3%)	34	58
1	B	500/501 (100%)	488 (98%)	12 (2%)	43	62
All	All	1001/1002 (100%)	973 (97%)	28 (3%)	38	60

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	508	ILE
1	A	512	GLU
1	A	520	THR

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Mol	Chain	Res	Type
1	A	557	LEU
1	A	623	HIS
1	A	666	ASN
1	A	675	MET
1	A	757	VAL
1	A	812	GLU
1	A	815	LEU
1	A	857	LEU
1	A	878	GLN
1	A	879	ARG
1	A	906	VAL
1	A	930	LEU
1	A	943	TYR
1	B	455	LEU
1	B	456	VAL
1	B	476	LEU
1	B	557	LEU
1	B	576	VAL
1	B	580	THR
1	B	640	LEU
1	B	657	ILE
1	B	691	THR
1	B	772	ILE
1	B	849	LEU
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(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	11.12	127.09	112.19
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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:

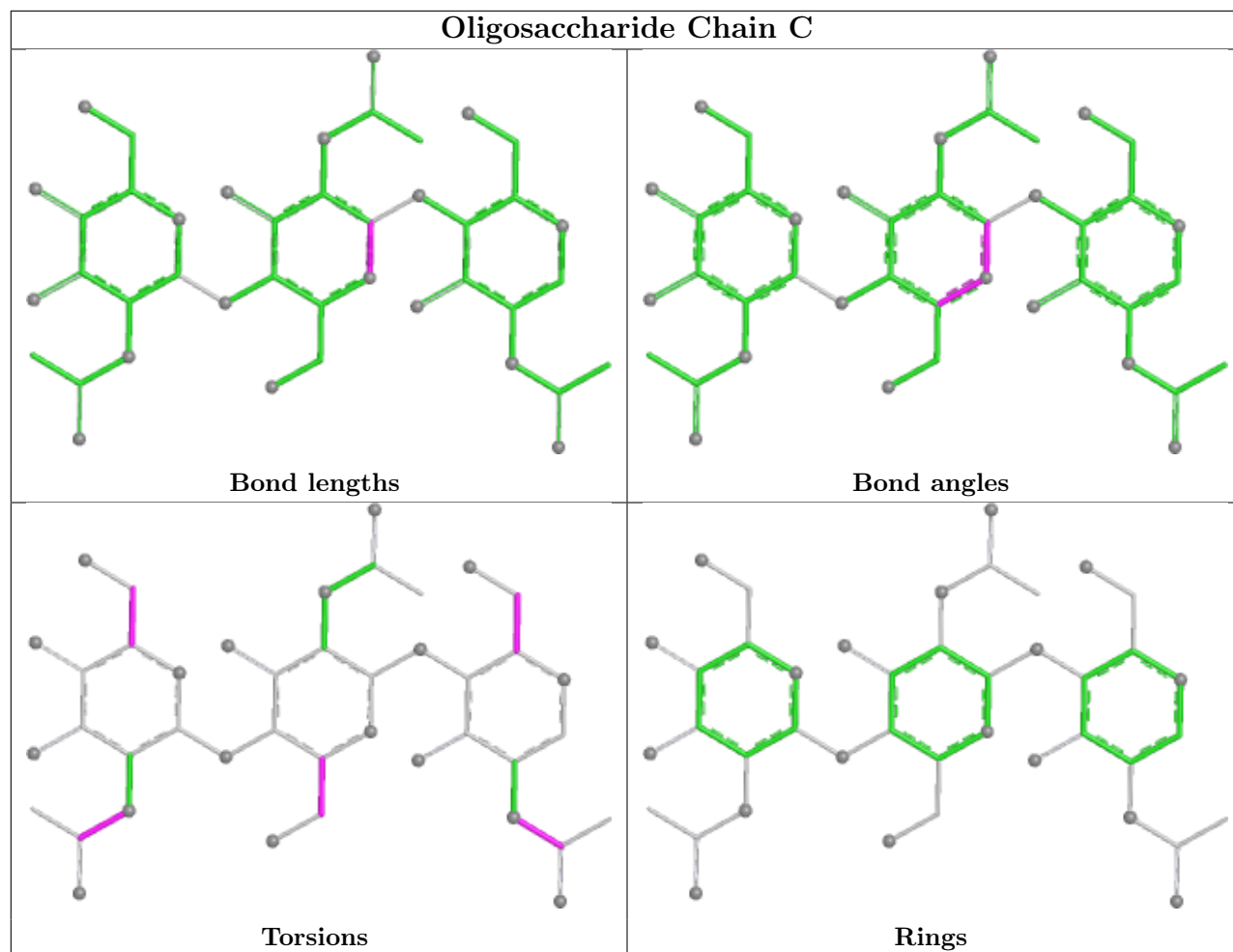
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	D	3	NAG	C1-C2-N2-C7
2	D	3	NAG	C8-C7-N2-C2
2	D	3	NAG	O7-C7-N2-C2
2	C	3	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	3	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2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

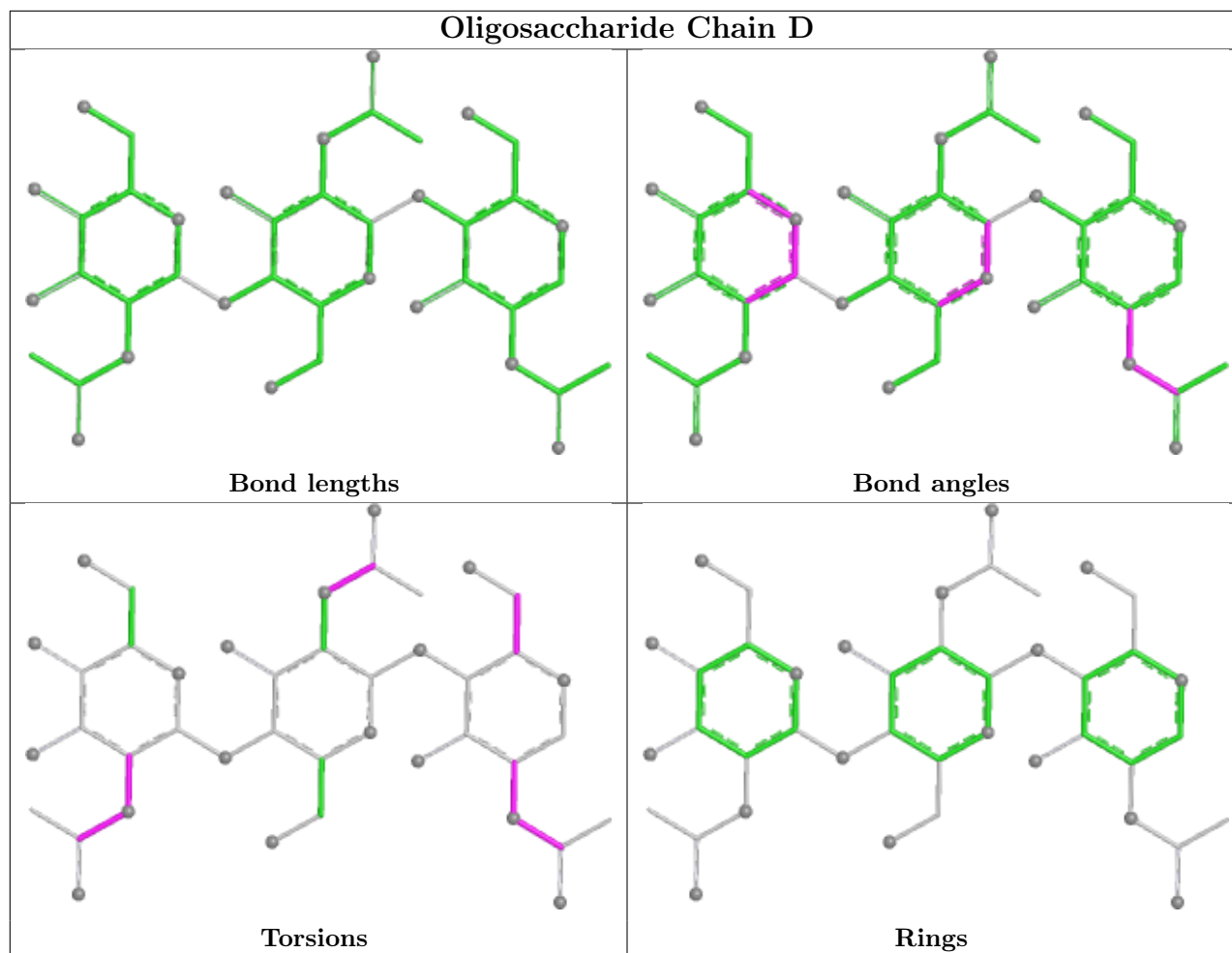
There are no ring outliers.

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.





## 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$
5	CO3	B	1103	4	3,3,3	0.80	0	2,3,3	0.06	0
5	CO3	A	1103	4	3,3,3	0.79	0	2,3,3	0.07	0
3	NAG	A	1101	-	14,14,15	0.24	0	17,19,21	0.35	0
3	NAG	B	1101	-	14,14,15	0.22	0	17,19,21	0.37	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	A	1101	-	-	4/6/23/26	0/1/1/1
3	NAG	B	1101	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

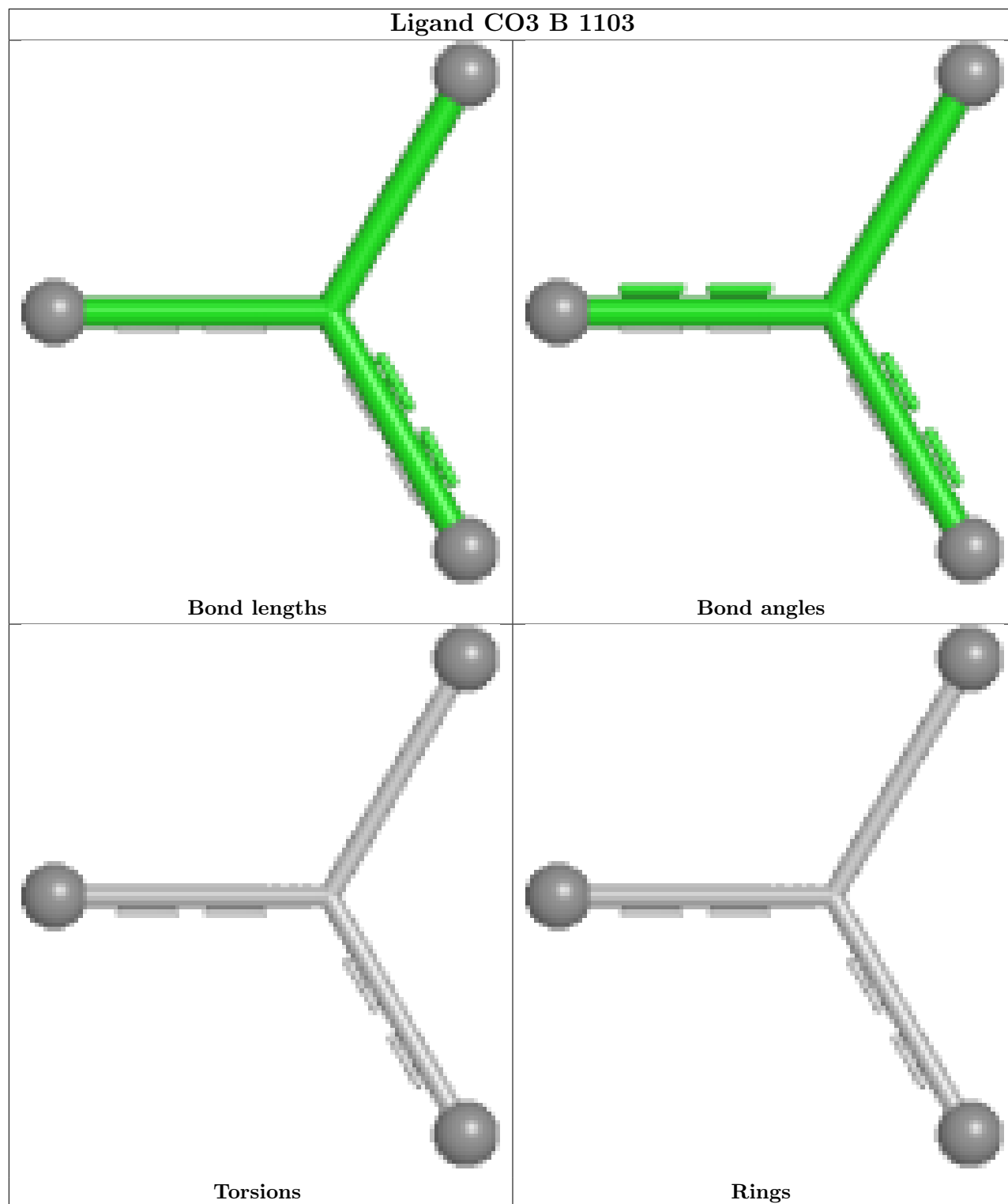
All (6) torsion outliers are listed below:

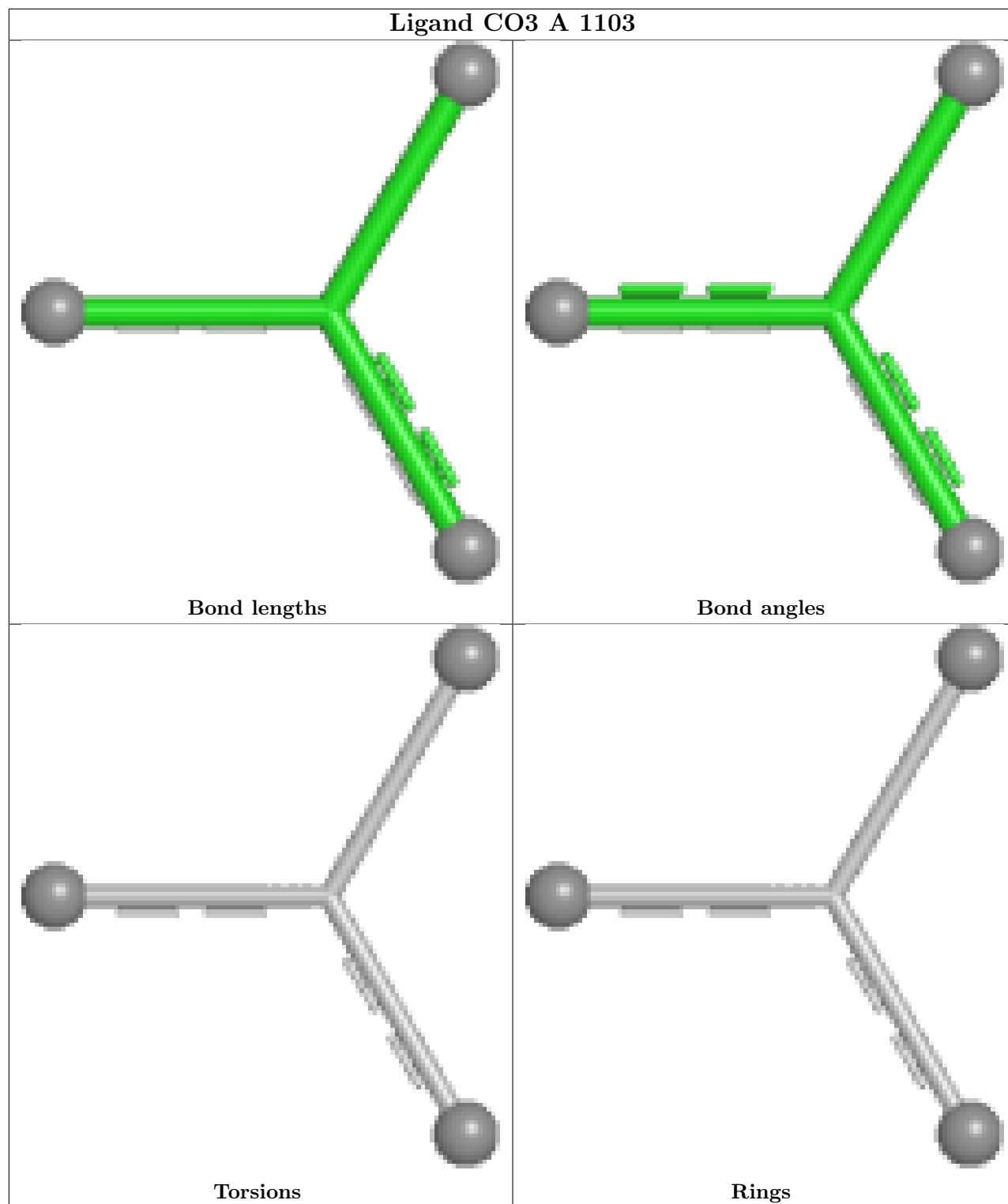
Mol	Chain	Res	Type	Atoms
3	B	1101	NAG	C4-C5-C6-O6
3	B	1101	NAG	O5-C5-C6-O6
3	A	1101	NAG	O5-C5-C6-O6
3	A	1101	NAG	C4-C5-C6-O6
3	A	1101	NAG	C8-C7-N2-C2
3	A	1101	NAG	O7-C7-N2-C2

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 than 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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

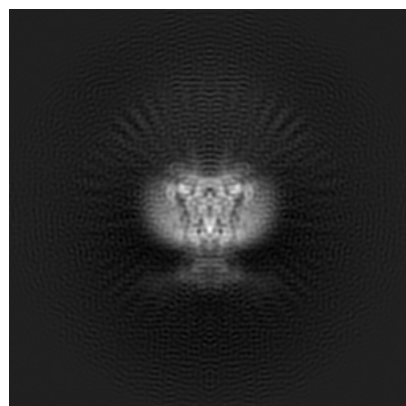
## 6 Map visualisation [i](#)

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.

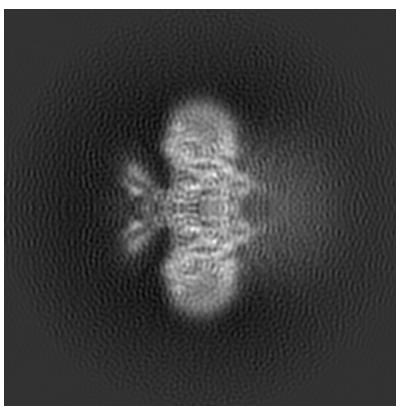
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

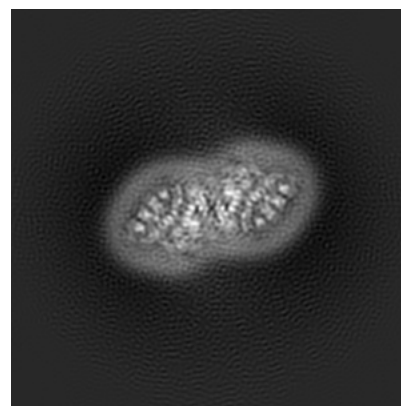
#### 6.1.1 Primary map



X

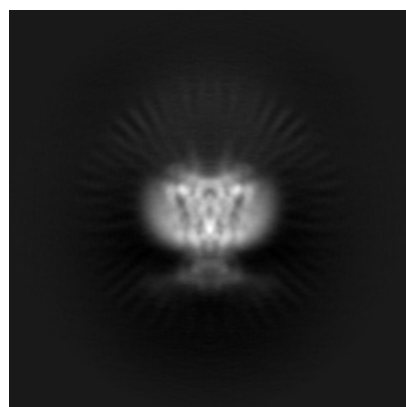


Y

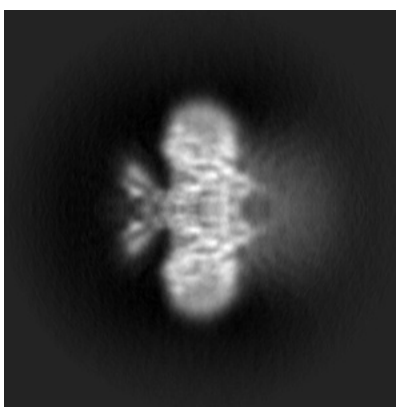


Z

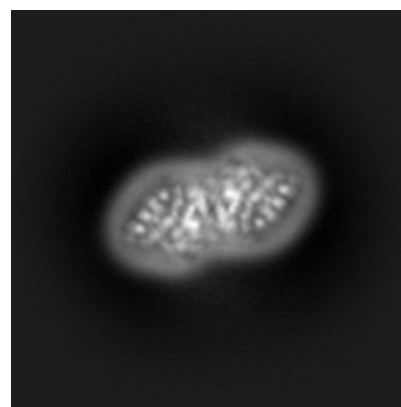
#### 6.1.2 Raw map



X



Y

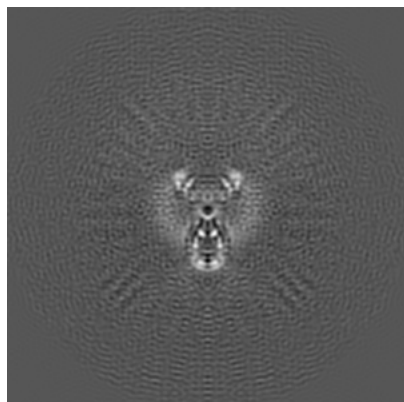


Z

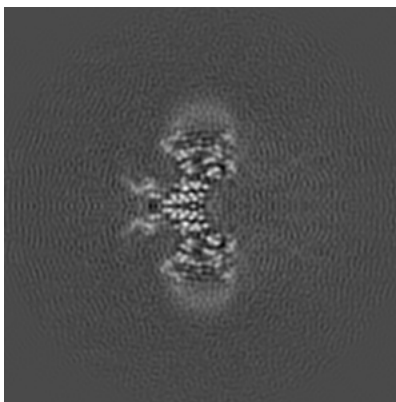
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

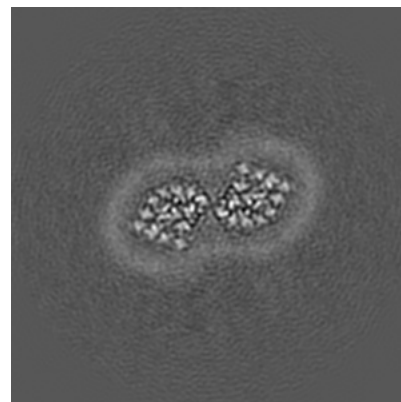
### 6.2.1 Primary map



X Index: 124

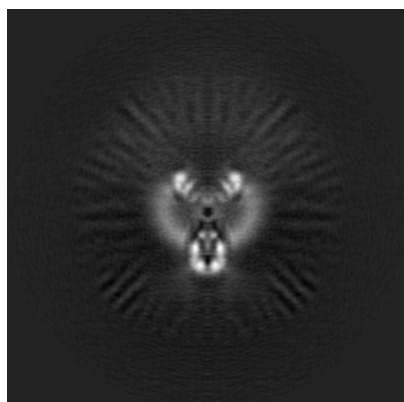


Y Index: 124

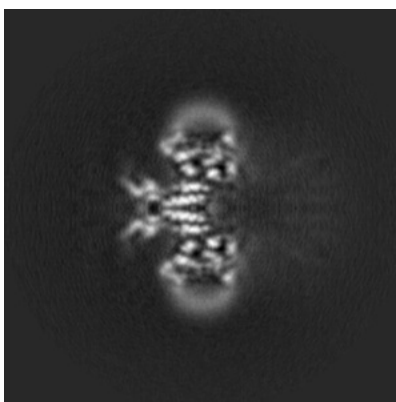


Z Index: 124

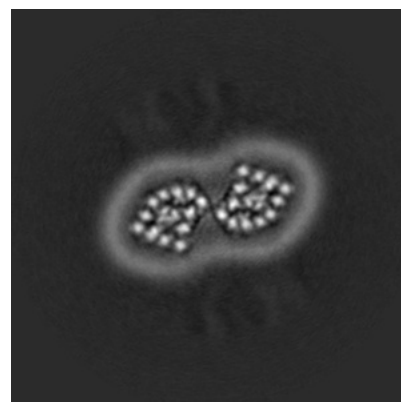
### 6.2.2 Raw map



X Index: 124



Y Index: 124

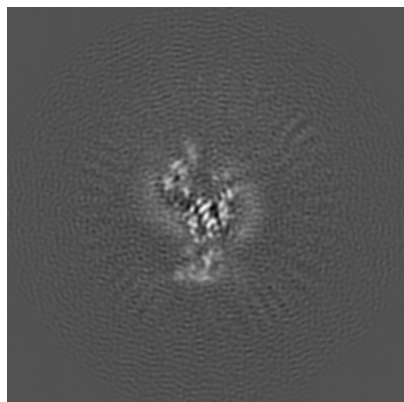


Z Index: 124

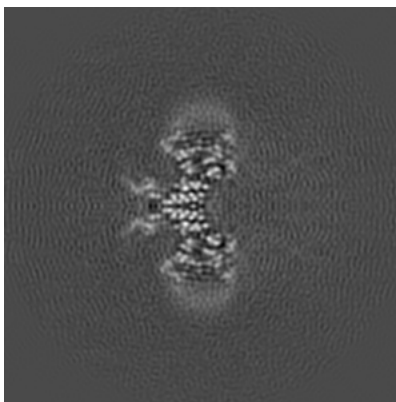
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

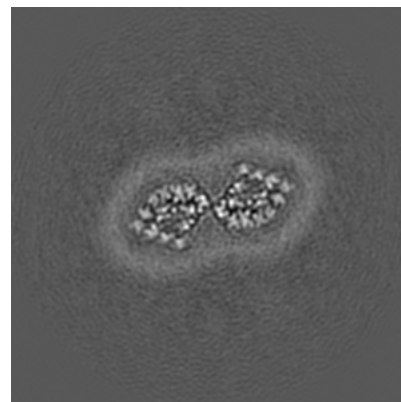
### 6.3.1 Primary map



X Index: 112

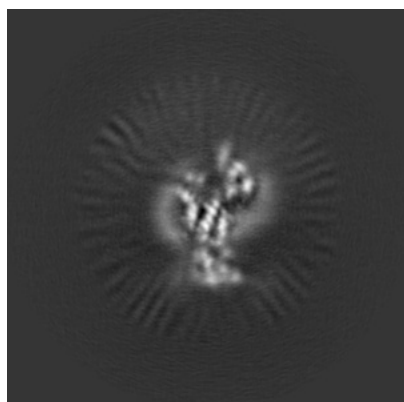


Y Index: 124

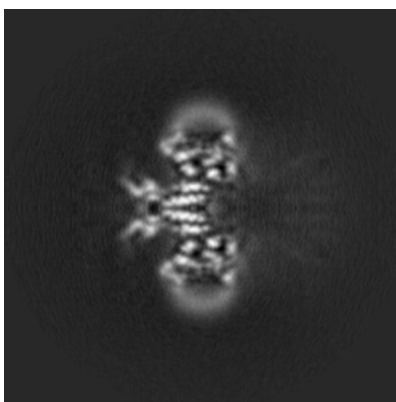


Z Index: 123

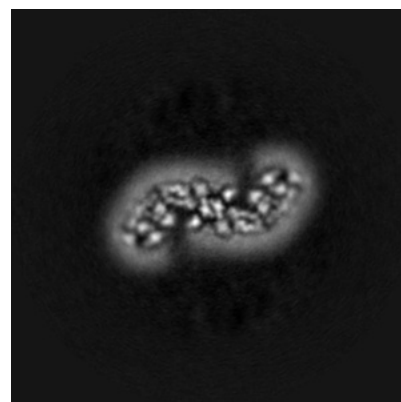
### 6.3.2 Raw map



X Index: 136



Y Index: 124

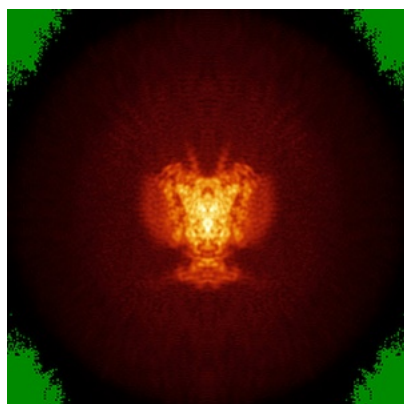


Z Index: 108

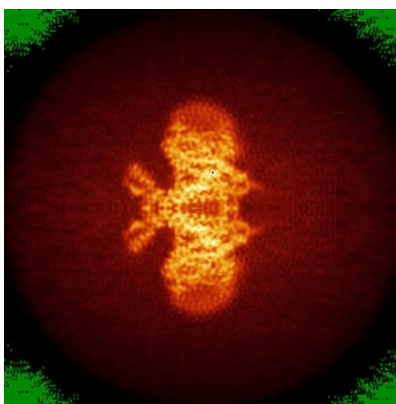
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

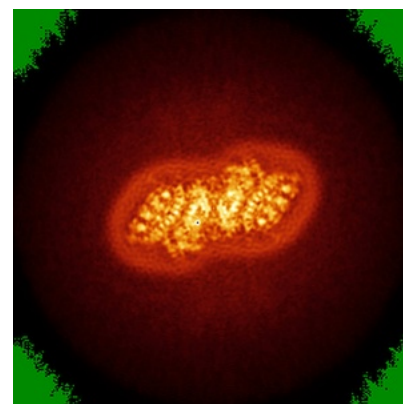
### 6.4.1 Primary map



X

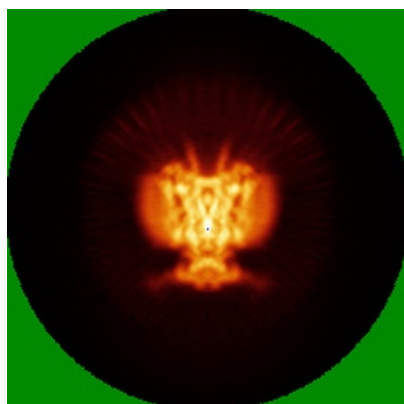


Y



Z

### 6.4.2 Raw map



X



Y

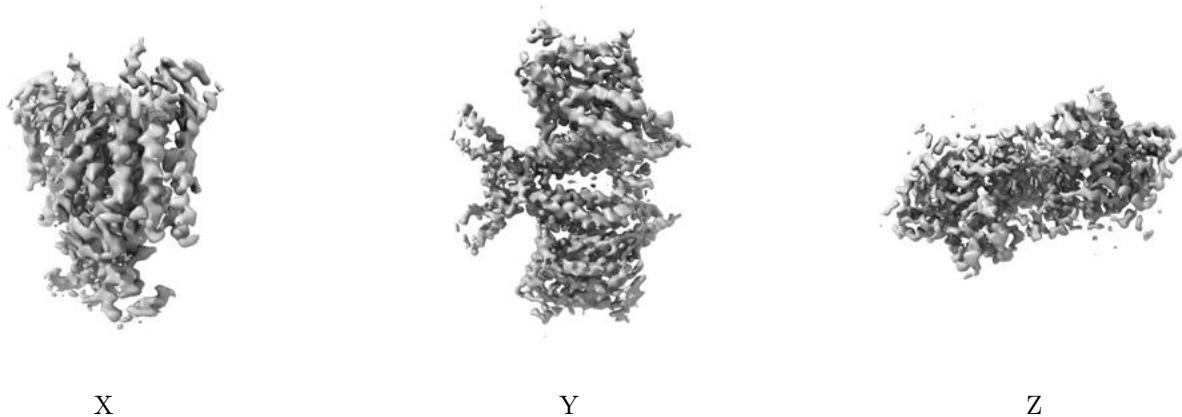


Z

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.

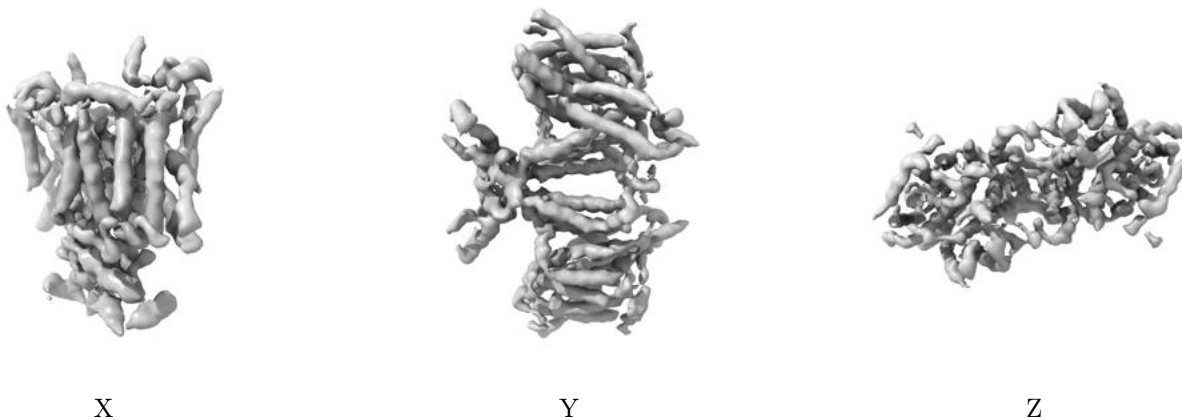
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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



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.

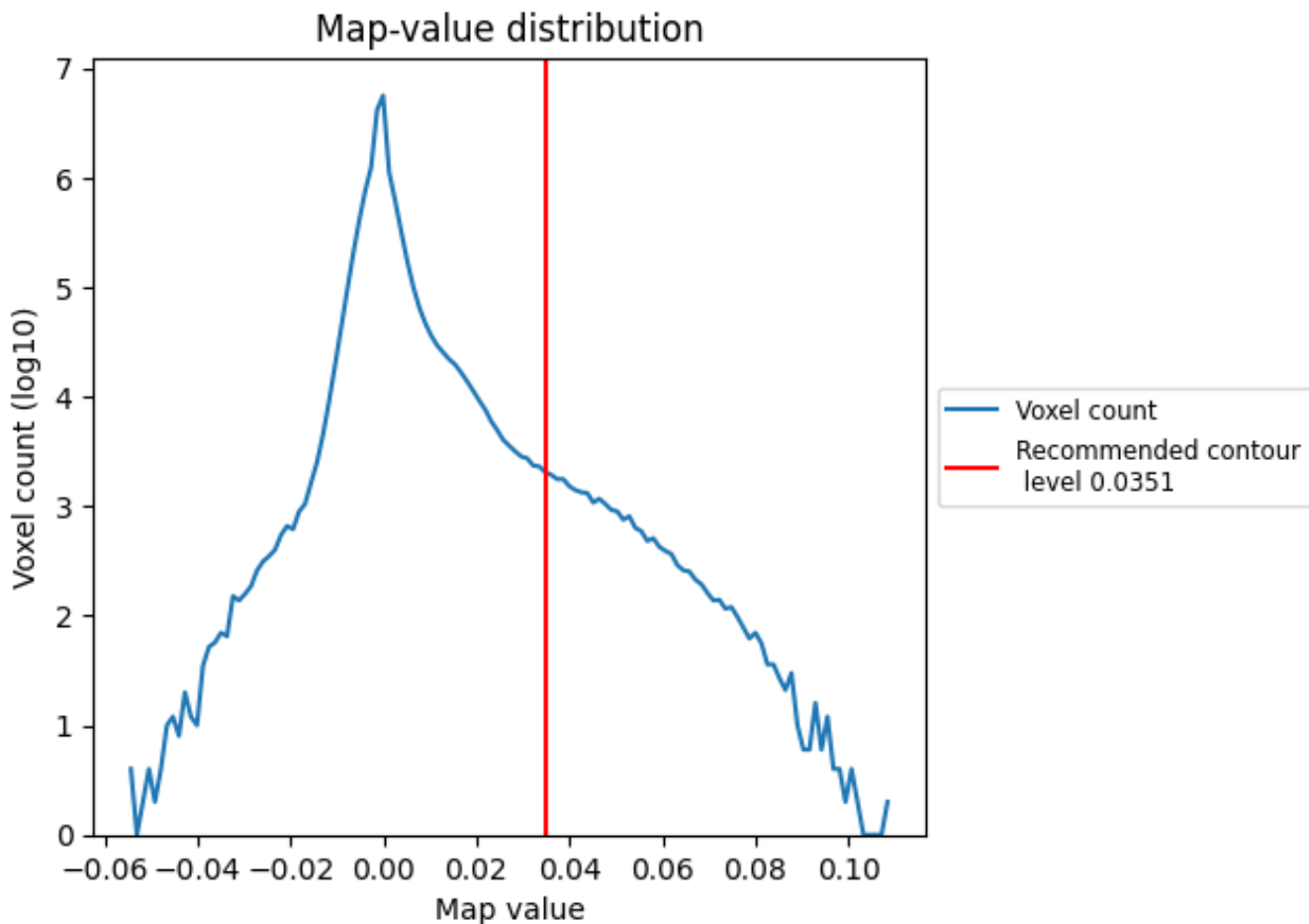
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

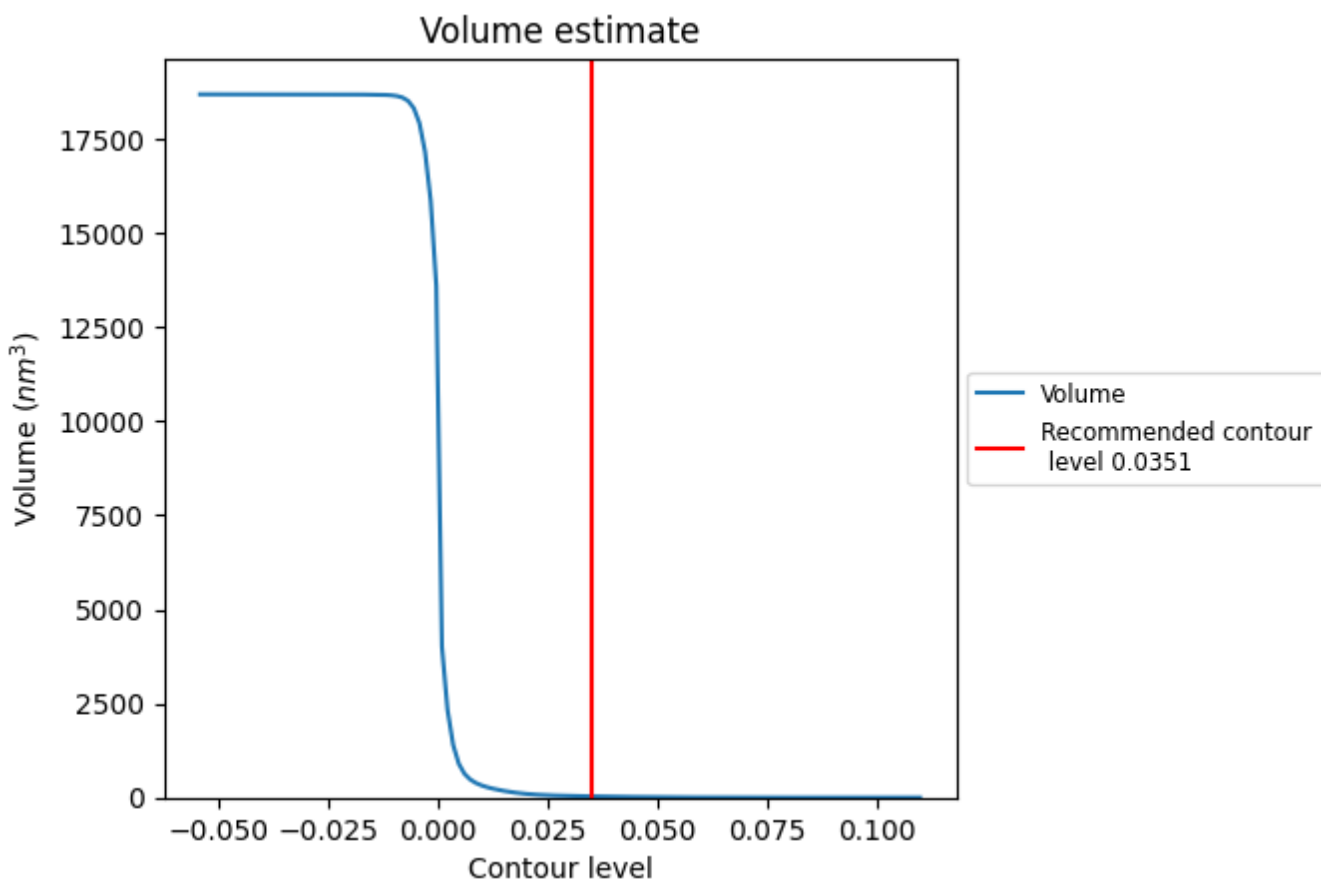
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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.

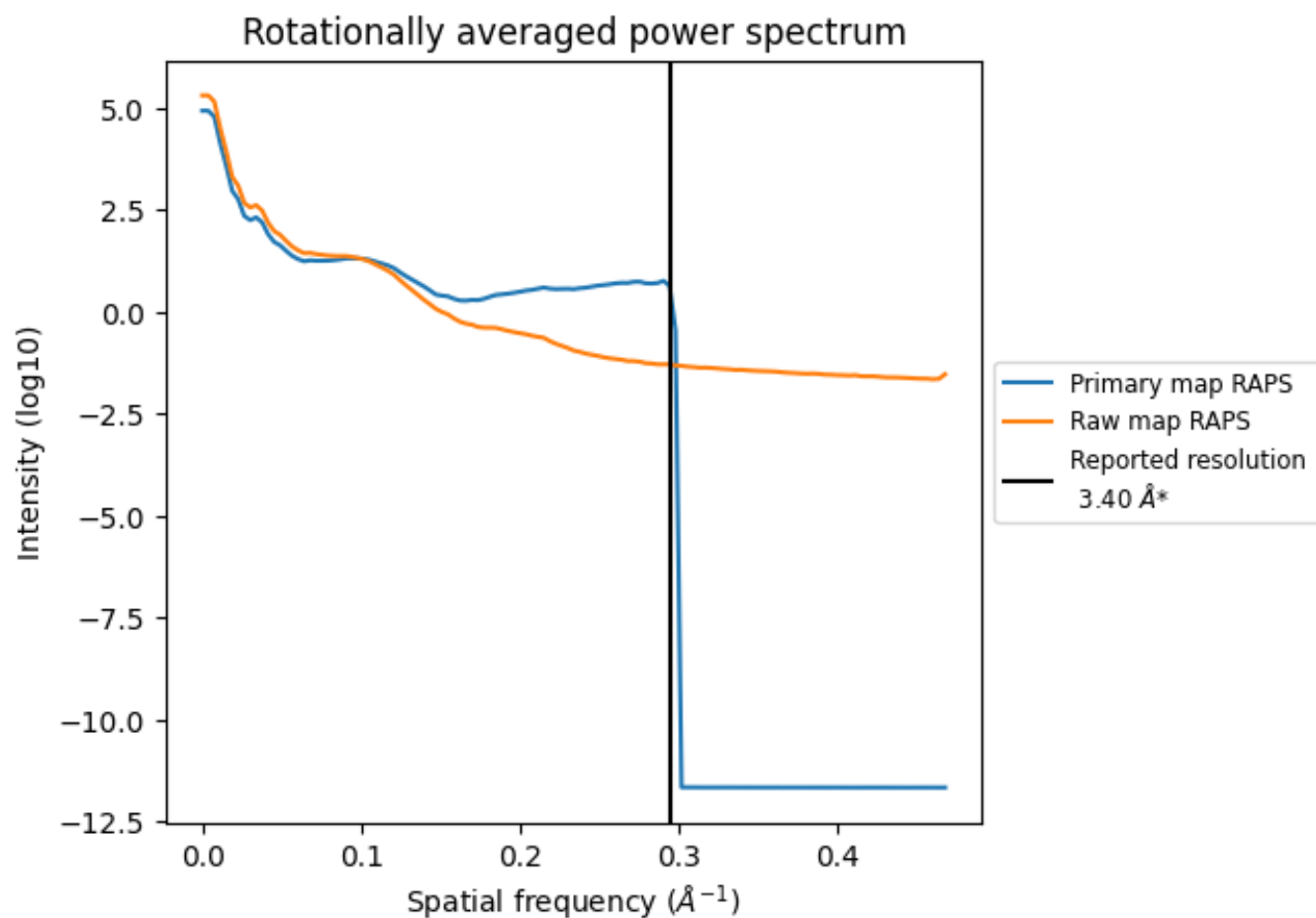
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 31 nm<sup>3</sup>; 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](#)

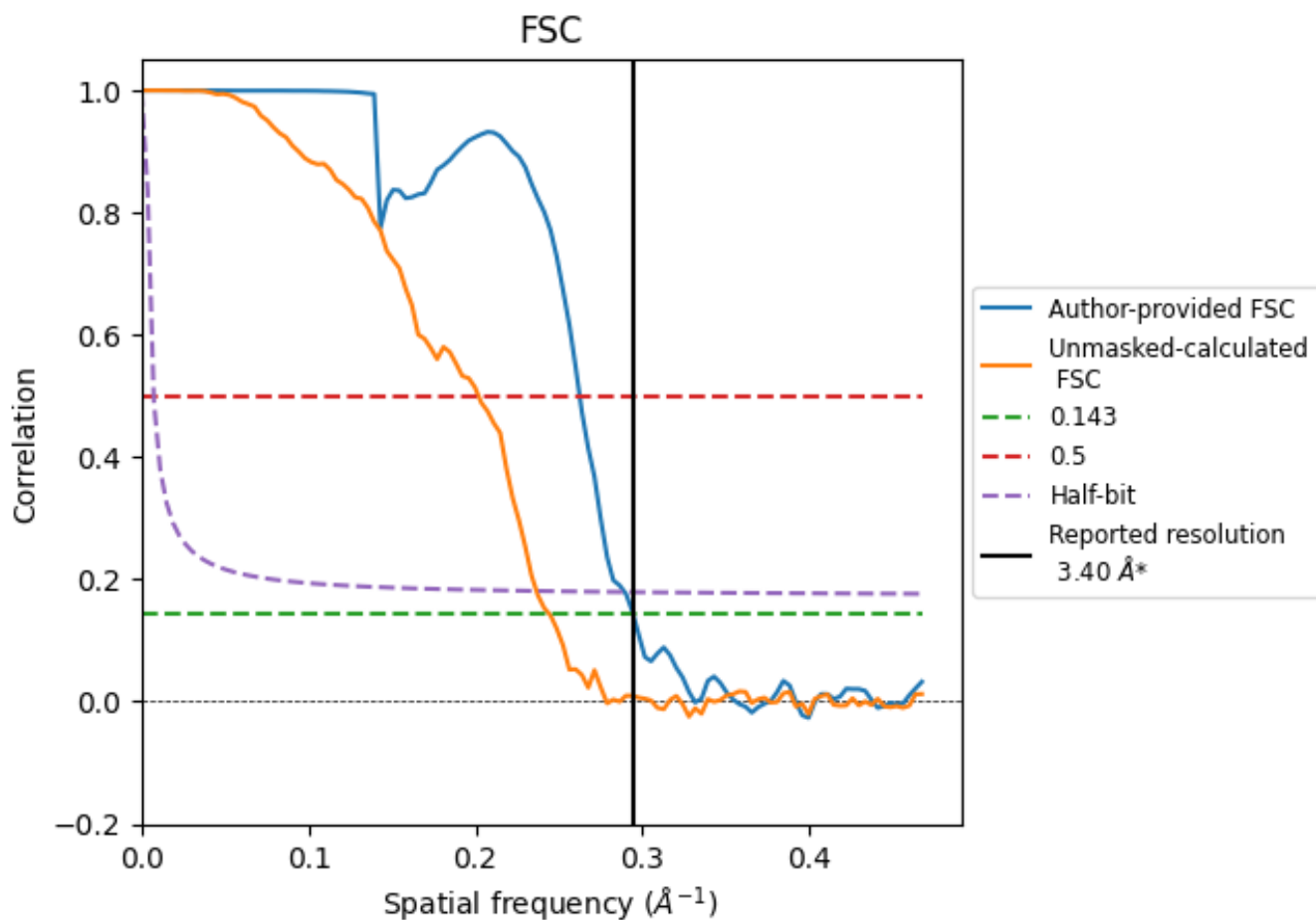


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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 %

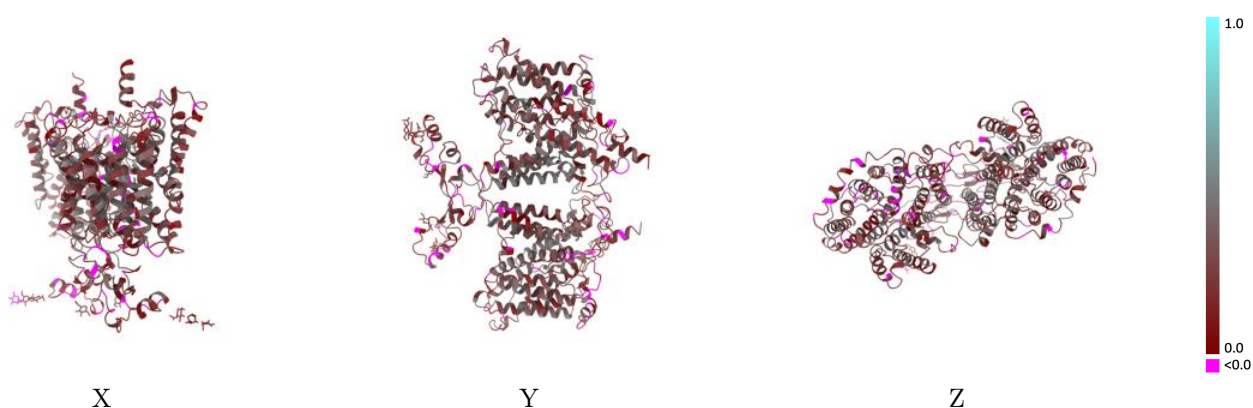
## 9 Map-model fit [i](#)

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 7.

### 9.1 Map-model overlay [i](#)

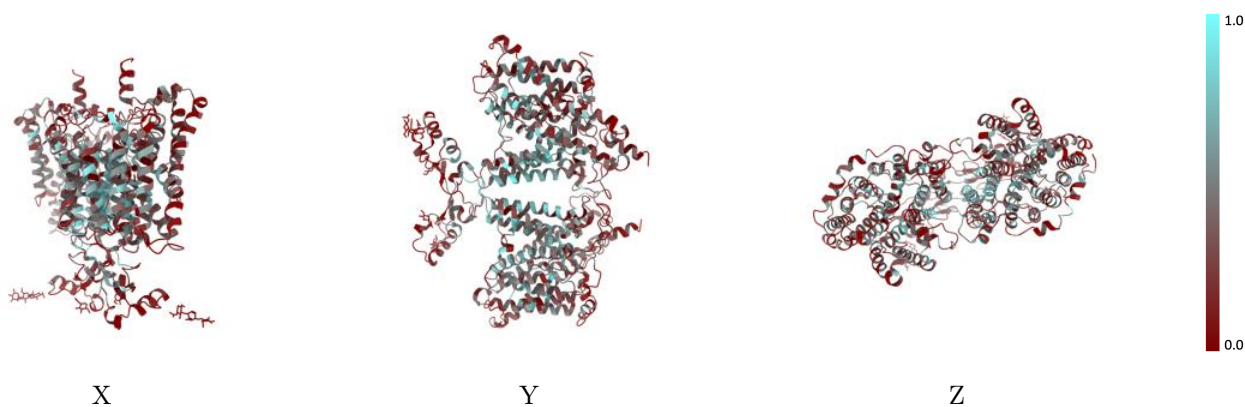
This section was not generated.

### 9.2 Q-score mapped to coordinate model [i](#)



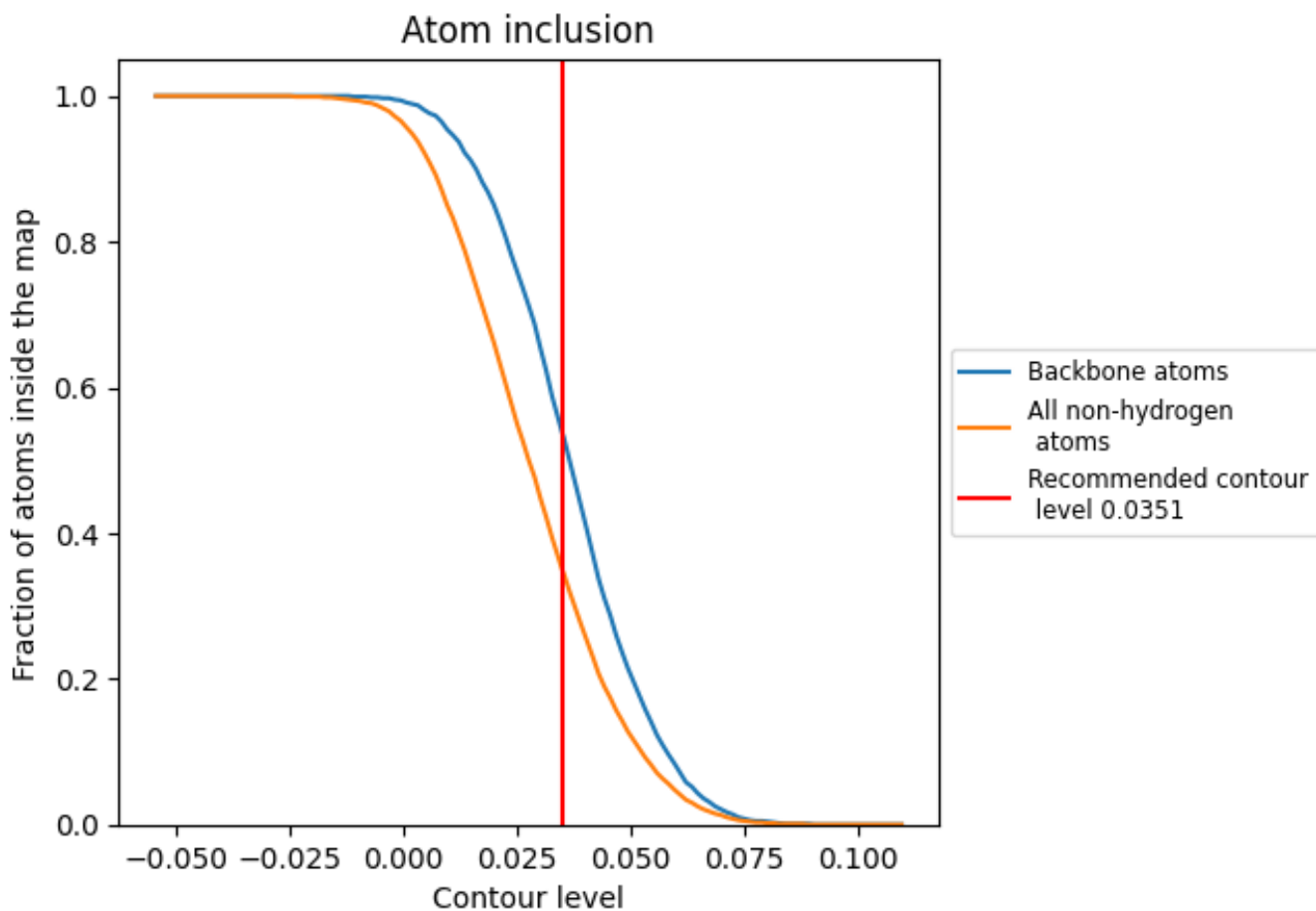
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 [i](#)

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

