



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:08 AM UTC

PDB ID : 9ARF / pdb_00009arf
EMDB ID : EMD-43780
Title : Rat GluN1-GluN2B NMDA receptor channel in complex with glycine, glutamate, and EU-1622-A, in nonactive1 conformation
Authors : Chou, T.-H.; Furukawa, H.
Deposited on : 2024-02-23
Resolution : 3.13 Å(reported)
Based on initial model : 7SAA

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

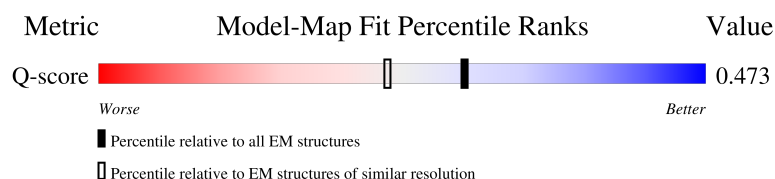
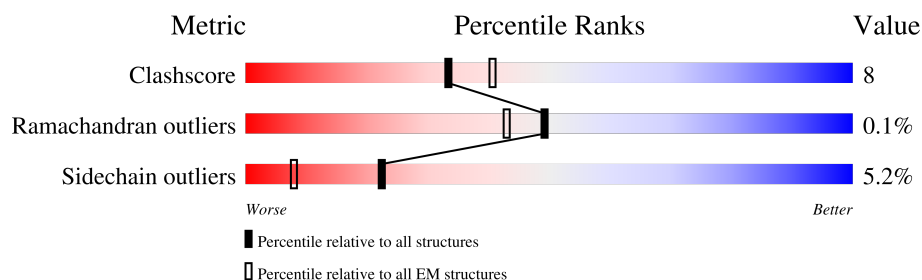
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.13 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	14478 (2.63 - 3.63)

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 $\leq 5\%$. 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	847	
1	C	847	
2	B	883	
2	D	883	

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Mol	Chain	Length	Quality of chain
3	E	2	 100%
3	F	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23032 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	796	Total	C	N	O	S	0	0
			5775	3698	978	1069	30		
1	C	796	Total	C	N	O	S	0	0
			5775	3698	978	1069	30		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	CYS	conflict	UNP P35439
A	61	GLN	ASN	conflict	UNP P35439
A	239	ASP	ASN	conflict	UNP P35439
A	350	GLN	ASN	conflict	UNP P35439
A	471	GLN	ASN	conflict	UNP P35439
A	491	GLN	ASN	conflict	UNP P35439
A	771	GLN	ASN	conflict	UNP P35439
A	844	ASN	ARG	conflict	UNP P35439
A	845	GLY	ARG	conflict	UNP P35439
A	846	ALA	LYS	conflict	UNP P35439
C	22	SER	CYS	conflict	UNP P35439
C	61	GLN	ASN	conflict	UNP P35439
C	239	ASP	ASN	conflict	UNP P35439
C	350	GLN	ASN	conflict	UNP P35439
C	471	GLN	ASN	conflict	UNP P35439
C	491	GLN	ASN	conflict	UNP P35439
C	771	GLN	ASN	conflict	UNP P35439
C	844	ASN	ARG	conflict	UNP P35439
C	845	GLY	ARG	conflict	UNP P35439
C	846	ALA	LYS	conflict	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	785	Total 5684	C 3671	N 922	O 1061	S 30	0	0
2	D	785	Total 5684	C 3671	N 922	O 1061	S 30	0	0

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-30	MET	-	expression tag	UNP Q00960
B	-29	GLY	-	expression tag	UNP Q00960
B	-28	THR	-	expression tag	UNP Q00960
B	-27	MET	-	expression tag	UNP Q00960
B	-26	ARG	-	expression tag	UNP Q00960
B	-25	LEU	-	expression tag	UNP Q00960
B	-24	PHE	-	expression tag	UNP Q00960
B	-23	LEU	-	expression tag	UNP Q00960
B	-22	LEU	-	expression tag	UNP Q00960
B	-21	ALA	-	expression tag	UNP Q00960
B	-20	VAL	-	expression tag	UNP Q00960
B	-19	LEU	-	expression tag	UNP Q00960
B	-18	PHE	-	expression tag	UNP Q00960
B	-17	LEU	-	expression tag	UNP Q00960
B	-16	PHE	-	expression tag	UNP Q00960
B	-15	SER	-	expression tag	UNP Q00960
B	-14	PHE	-	expression tag	UNP Q00960
B	-13	ALA	-	expression tag	UNP Q00960
B	-12	ARG	-	expression tag	UNP Q00960
B	-11	ALA	-	expression tag	UNP Q00960
B	-10	THR	-	expression tag	UNP Q00960
B	-9	GLY	-	expression tag	UNP Q00960
B	-8	TRP	-	expression tag	UNP Q00960
B	-7	SER	-	expression tag	UNP Q00960
B	-6	HIS	-	expression tag	UNP Q00960
B	-5	PRO	-	expression tag	UNP Q00960
B	-4	GLN	-	expression tag	UNP Q00960
B	-3	PHE	-	expression tag	UNP Q00960
B	-2	GLU	-	expression tag	UNP Q00960
B	-1	LYS	-	expression tag	UNP Q00960
B	0	GLY	-	expression tag	UNP Q00960
B	1	GLY	-	expression tag	UNP Q00960
B	2	GLY	-	expression tag	UNP Q00960
B	3	SER	-	expression tag	UNP Q00960
B	4	GLY	-	expression tag	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	GLY	-	expression tag	UNP Q00960
B	6	GLY	-	expression tag	UNP Q00960
B	7	SER	-	expression tag	UNP Q00960
B	8	GLY	-	expression tag	UNP Q00960
B	9	GLY	-	expression tag	UNP Q00960
B	10	SER	-	expression tag	UNP Q00960
B	11	ALA	-	expression tag	UNP Q00960
B	12	TRP	-	expression tag	UNP Q00960
B	13	SER	-	expression tag	UNP Q00960
B	14	HIS	-	expression tag	UNP Q00960
B	15	PRO	-	expression tag	UNP Q00960
B	16	GLN	-	expression tag	UNP Q00960
B	17	PHE	-	expression tag	UNP Q00960
B	18	GLU	-	expression tag	UNP Q00960
B	19	LYS	-	expression tag	UNP Q00960
B	20	GLY	-	expression tag	UNP Q00960
B	21	ALA	-	expression tag	UNP Q00960
B	22	LEU	-	expression tag	UNP Q00960
B	23	VAL	-	expression tag	UNP Q00960
B	24	PRO	-	expression tag	UNP Q00960
B	25	ARG	-	expression tag	UNP Q00960
B	26	GLY	-	expression tag	UNP Q00960
B	849	SER	CYS	conflict	UNP Q00960
D	-30	MET	-	expression tag	UNP Q00960
D	-29	GLY	-	expression tag	UNP Q00960
D	-28	THR	-	expression tag	UNP Q00960
D	-27	MET	-	expression tag	UNP Q00960
D	-26	ARG	-	expression tag	UNP Q00960
D	-25	LEU	-	expression tag	UNP Q00960
D	-24	PHE	-	expression tag	UNP Q00960
D	-23	LEU	-	expression tag	UNP Q00960
D	-22	LEU	-	expression tag	UNP Q00960
D	-21	ALA	-	expression tag	UNP Q00960
D	-20	VAL	-	expression tag	UNP Q00960
D	-19	LEU	-	expression tag	UNP Q00960
D	-18	PHE	-	expression tag	UNP Q00960
D	-17	LEU	-	expression tag	UNP Q00960
D	-16	PHE	-	expression tag	UNP Q00960
D	-15	SER	-	expression tag	UNP Q00960
D	-14	PHE	-	expression tag	UNP Q00960
D	-13	ALA	-	expression tag	UNP Q00960
D	-12	ARG	-	expression tag	UNP Q00960

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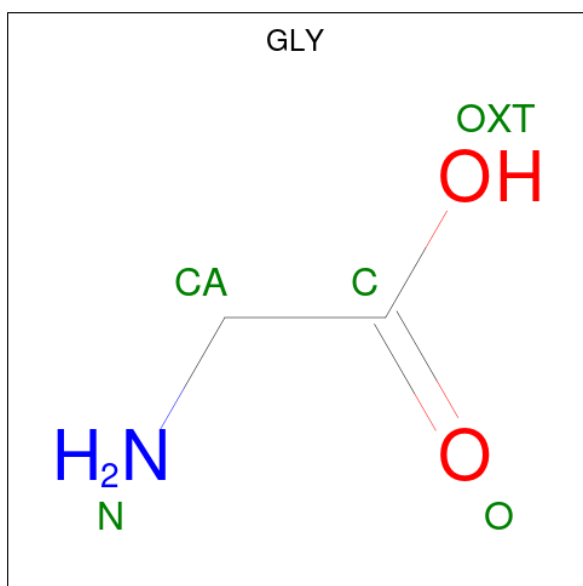
Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	ALA	-	expression tag	UNP Q00960
D	-10	THR	-	expression tag	UNP Q00960
D	-9	GLY	-	expression tag	UNP Q00960
D	-8	TRP	-	expression tag	UNP Q00960
D	-7	SER	-	expression tag	UNP Q00960
D	-6	HIS	-	expression tag	UNP Q00960
D	-5	PRO	-	expression tag	UNP Q00960
D	-4	GLN	-	expression tag	UNP Q00960
D	-3	PHE	-	expression tag	UNP Q00960
D	-2	GLU	-	expression tag	UNP Q00960
D	-1	LYS	-	expression tag	UNP Q00960
D	0	GLY	-	expression tag	UNP Q00960
D	1	GLY	-	expression tag	UNP Q00960
D	2	GLY	-	expression tag	UNP Q00960
D	3	SER	-	expression tag	UNP Q00960
D	4	GLY	-	expression tag	UNP Q00960
D	5	GLY	-	expression tag	UNP Q00960
D	6	GLY	-	expression tag	UNP Q00960
D	7	SER	-	expression tag	UNP Q00960
D	8	GLY	-	expression tag	UNP Q00960
D	9	GLY	-	expression tag	UNP Q00960
D	10	SER	-	expression tag	UNP Q00960
D	11	ALA	-	expression tag	UNP Q00960
D	12	TRP	-	expression tag	UNP Q00960
D	13	SER	-	expression tag	UNP Q00960
D	14	HIS	-	expression tag	UNP Q00960
D	15	PRO	-	expression tag	UNP Q00960
D	16	GLN	-	expression tag	UNP Q00960
D	17	PHE	-	expression tag	UNP Q00960
D	18	GLU	-	expression tag	UNP Q00960
D	19	LYS	-	expression tag	UNP Q00960
D	20	GLY	-	expression tag	UNP Q00960
D	21	ALA	-	expression tag	UNP Q00960
D	22	LEU	-	expression tag	UNP Q00960
D	23	VAL	-	expression tag	UNP Q00960
D	24	PRO	-	expression tag	UNP Q00960
D	25	ARG	-	expression tag	UNP Q00960
D	26	GLY	-	expression tag	UNP Q00960
D	849	SER	CYS	conflict	UNP Q00960

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



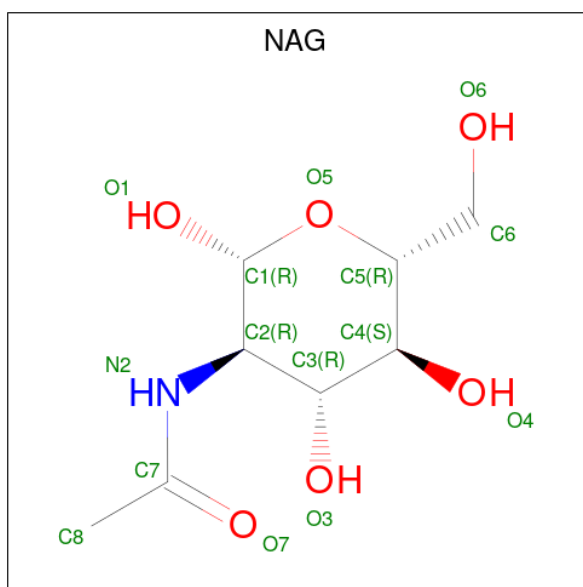
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$) (labeled as "Ligand of Interest" by depositor).



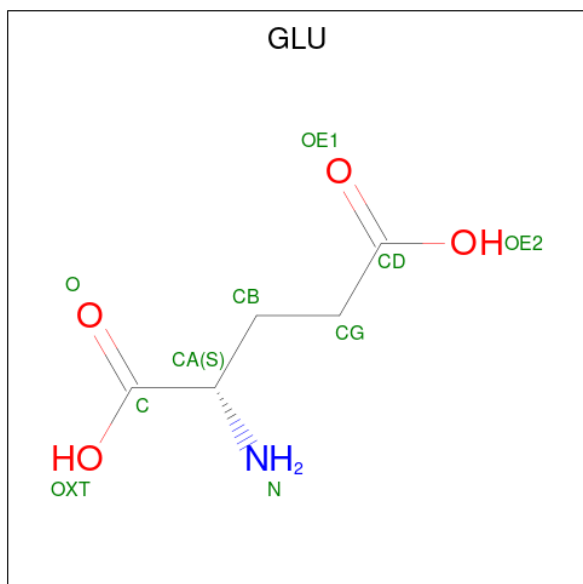
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			5	2	1	2	
4	C	1	Total	C	N	O	0
			5	2	1	2	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			10	5	1	4	

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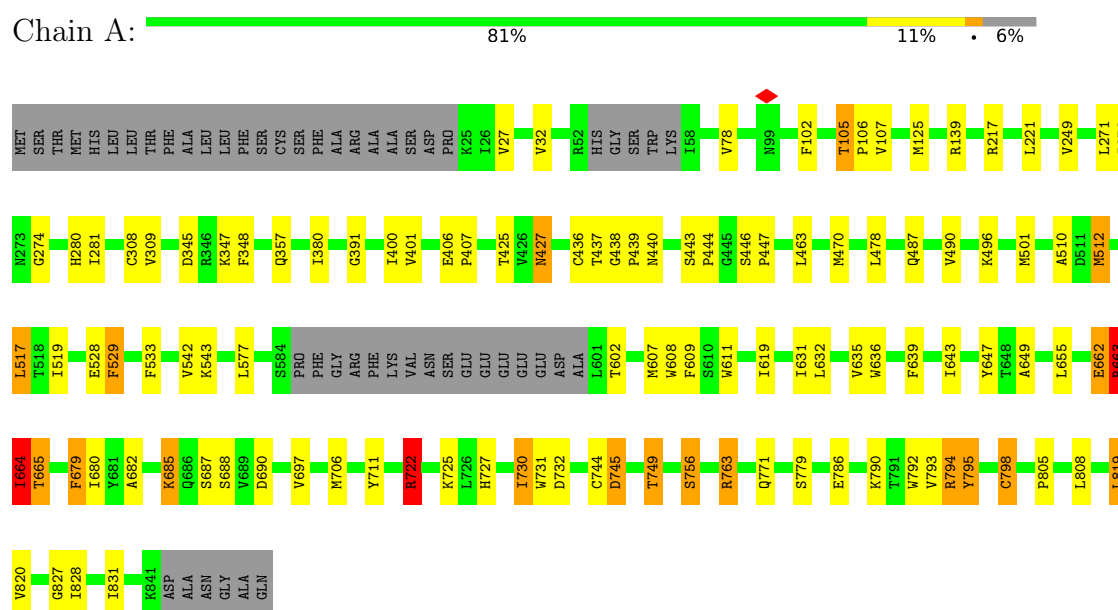
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	D	1	10	5	1	4	0

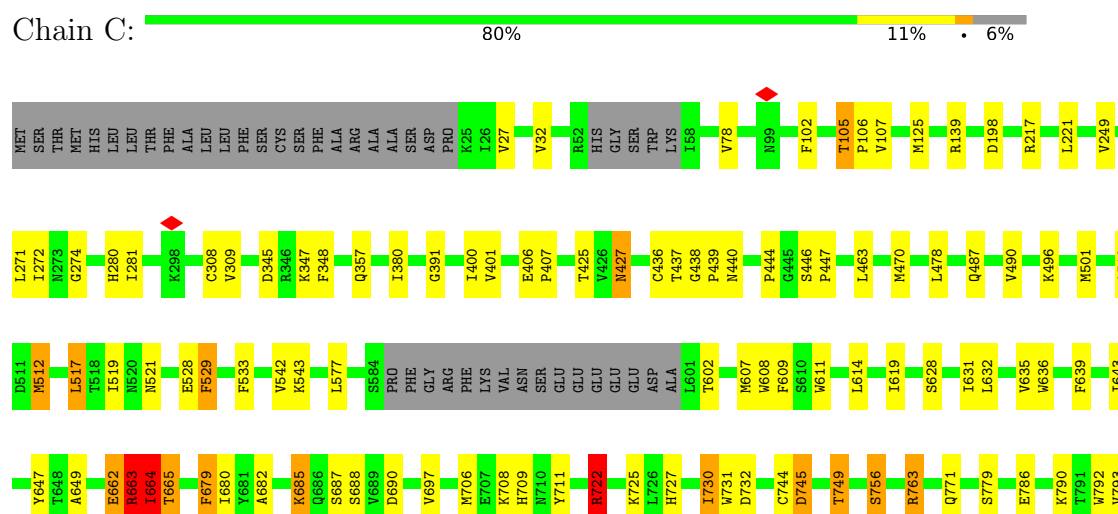
3 Residue-property plots

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.

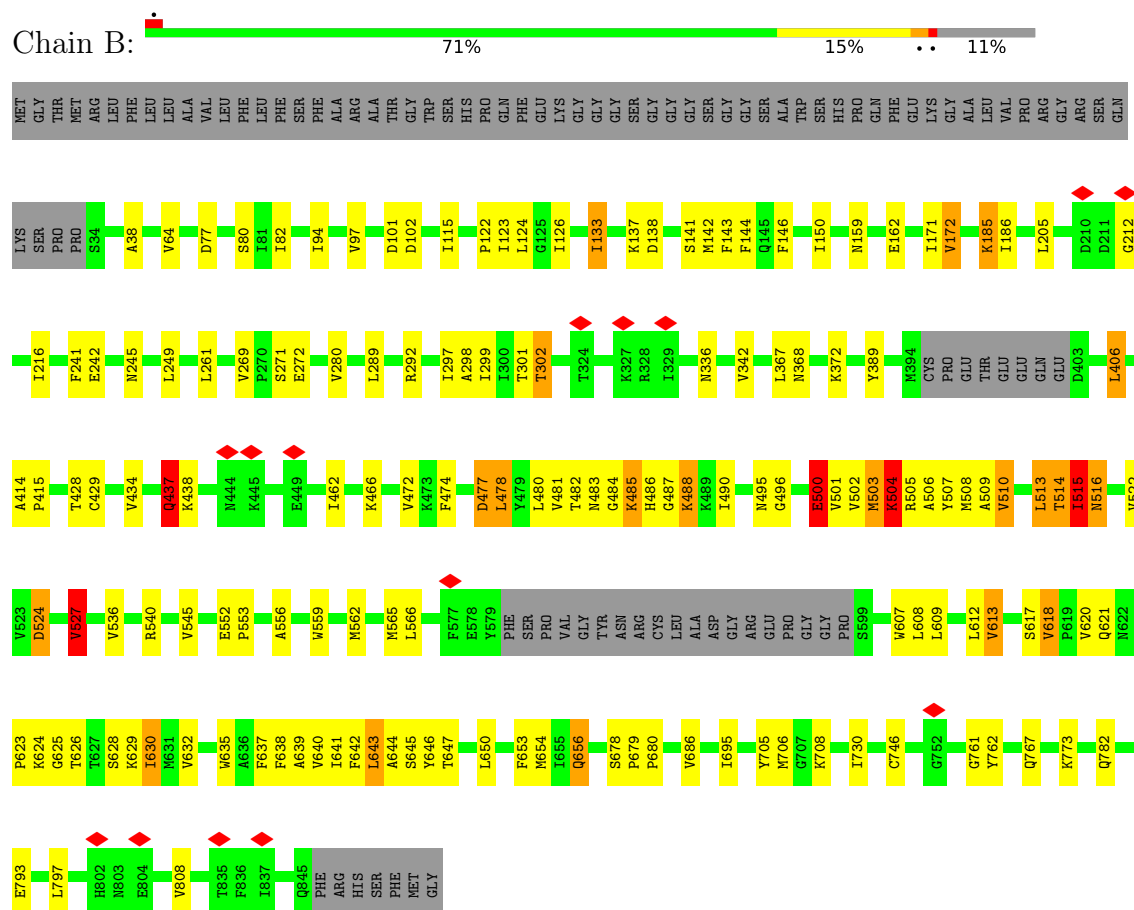
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



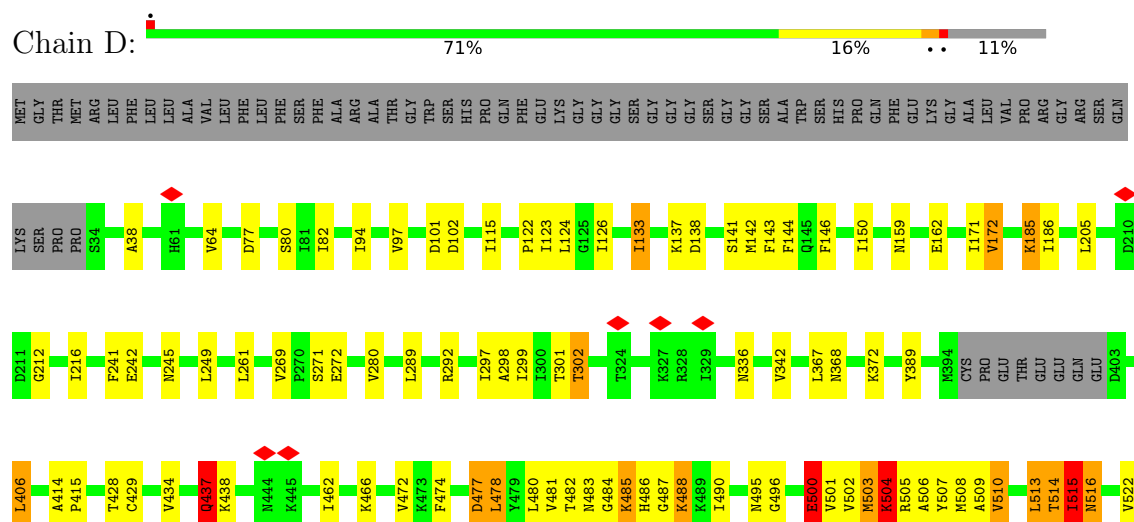
- Molecule 1: Glutamate receptor ionotropic, NMDA 1

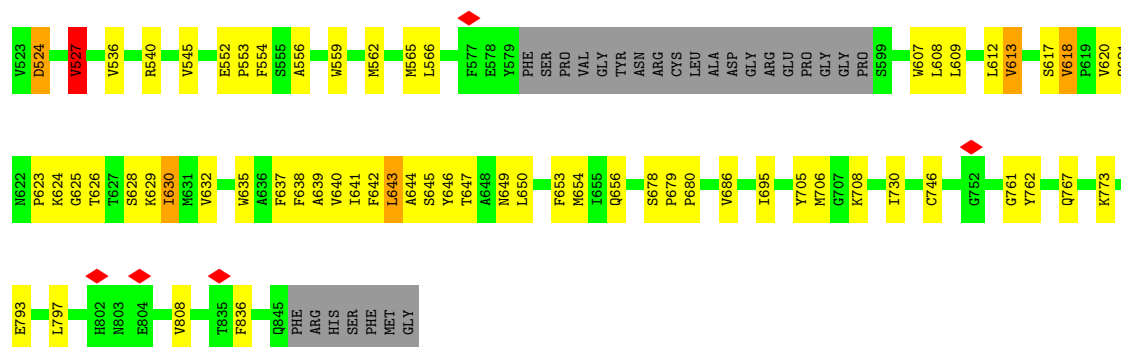


- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



- Molecule 2: Glutamate receptor ionotropic, NMDA 2B





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	396327	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 ($e^-/\text{\AA}^2$)	66.3	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.671	Depositor
Minimum map value	-1.173	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.0704	Depositor
Map size ($\text{\AA}$)	344.4, 344.4, 344.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.861, 0.861, 0.861	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: 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	0.68	16/5900 (0.3%)	0.74	23/8062 (0.3%)
1	C	0.68	16/5900 (0.3%)	0.74	23/8062 (0.3%)
2	B	0.84	30/5801 (0.5%)	0.81	35/7929 (0.4%)
2	D	0.84	30/5801 (0.5%)	0.81	35/7929 (0.4%)
All	All	0.76	92/23402 (0.4%)	0.77	116/31982 (0.4%)

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	1
1	C	0	1
2	B	0	3
2	D	0	3
All	All	0	8

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	512	MET	C-O	-15.77	1.04	1.23
1	A	512	MET	C-O	-15.74	1.04	1.23
2	B	508	MET	C-O	-15.06	1.04	1.23
2	D	508	MET	C-O	-15.06	1.04	1.23
2	D	509	ALA	C-O	-14.47	1.06	1.24
2	B	509	ALA	C-O	-14.44	1.06	1.24
2	B	485	LYS	C-O	-14.44	1.11	1.23
2	D	485	LYS	C-O	-14.34	1.12	1.23
2	D	500	GLU	C-O	-13.43	1.08	1.24
2	B	500	GLU	C-O	-13.39	1.08	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	528	GLU	C-O	-13.32	1.08	1.24
1	A	528	GLU	C-O	-13.28	1.08	1.24
2	B	488	LYS	C-O	-12.55	1.08	1.23
2	D	488	LYS	C-O	-12.53	1.08	1.23
2	B	506	ALA	C-O	-12.35	1.08	1.24
2	D	506	ALA	C-O	-12.31	1.08	1.24
1	C	690	ASP	C-O	-11.38	1.10	1.24
1	A	690	ASP	C-O	-11.32	1.10	1.24
1	A	779	SER	C-O	-10.95	1.09	1.24
1	C	779	SER	C-O	-10.93	1.09	1.24
2	D	510	VAL	C-O	-10.92	1.12	1.24
2	B	510	VAL	C-O	-10.92	1.12	1.24
2	D	495	ASN	C-O	-10.81	1.11	1.23
2	B	495	ASN	C-O	-10.80	1.11	1.23
2	B	515	ILE	C-O	-10.69	1.13	1.24
2	D	515	ILE	C-O	-10.66	1.13	1.24
1	A	730	ILE	C-O	-10.24	1.12	1.24
1	C	730	ILE	C-O	-10.19	1.12	1.24
2	B	524	ASP	C-O	-9.74	1.09	1.23
2	D	524	ASP	C-O	-9.72	1.09	1.23
1	C	786	GLU	C-O	-9.65	1.11	1.24
1	A	786	GLU	C-O	-9.63	1.11	1.24
2	D	513	LEU	C-O	-9.53	1.12	1.24
2	B	513	LEU	C-O	-9.47	1.12	1.24
1	A	519	ILE	C-O	-9.21	1.13	1.23
1	C	519	ILE	C-O	-9.21	1.13	1.23
1	C	533	PHE	C-O	-9.11	1.11	1.24
1	A	533	PHE	C-O	-9.09	1.11	1.24
2	B	478	LEU	C-O	-9.05	1.11	1.23
2	D	478	LEU	C-O	-9.03	1.11	1.23
2	B	486	HIS	C-O	-8.92	1.13	1.24
2	D	486	HIS	C-O	-8.90	1.13	1.24
2	D	501	VAL	C-O	-8.48	1.14	1.24
2	B	501	VAL	C-O	-8.47	1.14	1.24
2	B	487	GLY	C-O	-8.39	1.12	1.23
1	C	529	PHE	C-O	-8.39	1.13	1.23
2	D	487	GLY	C-O	-8.39	1.12	1.23
1	A	529	PHE	C-O	-8.37	1.13	1.23
1	C	749	THR	C-O	-8.37	1.14	1.24
1	A	749	THR	C-O	-8.36	1.14	1.24
2	D	514	THR	C-O	-8.32	1.14	1.23
1	A	517	LEU	C-O	-8.31	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	517	LEU	C-O	-8.30	1.13	1.24
2	D	437	GLN	C-O	-8.27	1.14	1.24
2	B	514	THR	C-O	-8.25	1.14	1.23
2	B	522	VAL	C-O	-8.23	1.14	1.24
2	B	437	GLN	C-O	-8.22	1.14	1.24
2	D	522	VAL	C-O	-8.19	1.14	1.24
1	A	664	ILE	C-O	-8.10	1.16	1.24
1	A	756	SER	C-O	-8.10	1.13	1.23
1	C	664	ILE	C-O	-8.08	1.16	1.24
1	C	756	SER	C-O	-8.08	1.13	1.23
2	B	503	MET	C-O	-8.00	1.14	1.24
2	D	503	MET	C-O	-7.97	1.14	1.24
2	D	406	LEU	C-O	-7.93	1.13	1.23
2	B	406	LEU	C-O	-7.93	1.13	1.23
1	A	688	SER	CA-CB	-7.81	1.39	1.53
1	C	688	SER	CA-CB	-7.79	1.39	1.53
2	D	484	GLY	C-O	-7.61	1.13	1.23
2	B	484	GLY	C-O	-7.57	1.13	1.23
2	D	516	ASN	C-O	-7.46	1.14	1.23
2	B	516	ASN	C-O	-7.40	1.14	1.23
1	A	779	SER	CA-CB	-7.35	1.40	1.53
1	C	779	SER	CA-CB	-7.33	1.40	1.53
2	B	507	TYR	C-O	-6.89	1.15	1.24
2	D	507	TYR	C-O	-6.84	1.15	1.24
1	A	763	ARG	C-O	-6.35	1.15	1.23
2	B	527	VAL	C-O	-6.34	1.16	1.24
2	D	527	VAL	C-O	-6.34	1.16	1.24
1	C	763	ARG	C-O	-6.33	1.15	1.23
2	B	502	VAL	C-O	-6.09	1.16	1.24
2	D	502	VAL	C-O	-6.07	1.17	1.24
2	B	643	LEU	C-O	-5.90	1.17	1.24
2	D	643	LEU	C-O	-5.86	1.17	1.24
2	D	482	THR	C-O	-5.65	1.17	1.24
2	B	482	THR	C-O	-5.63	1.17	1.24
2	D	645	SER	CA-CB	-5.62	1.44	1.53
2	B	645	SER	CA-CB	-5.57	1.44	1.53
2	D	506	ALA	CA-CB	-5.35	1.46	1.54
2	B	506	ALA	CA-CB	-5.32	1.46	1.54
2	D	481	VAL	C-O	-5.10	1.17	1.24
2	B	481	VAL	C-O	-5.05	1.17	1.24

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	495	ASN	CB-CA-C	-13.22	81.69	113.15
2	D	495	ASN	CB-CA-C	-13.21	81.70	113.15
1	C	690	ASP	CB-CA-C	-13.07	89.10	110.79
1	A	690	ASP	CB-CA-C	-13.06	89.11	110.79
2	B	500	GLU	CB-CA-C	-9.27	95.10	110.85
2	D	500	GLU	CB-CA-C	-9.25	95.13	110.85
2	D	524	ASP	CA-CB-CG	8.37	120.97	112.60
2	D	437	GLN	N-CA-CB	-8.34	97.48	110.65
2	B	437	GLN	N-CA-CB	-8.33	97.49	110.65
2	B	524	ASP	CA-CB-CG	8.33	120.93	112.60
1	A	685	LYS	CB-CA-C	-8.32	95.81	109.53
1	C	685	LYS	CB-CA-C	-8.31	95.81	109.53
2	D	506	ALA	CA-C-O	-7.75	109.77	118.69
2	B	506	ALA	CA-C-O	-7.72	109.81	118.69
1	C	533	PHE	CA-CB-CG	7.50	121.30	113.80
1	A	533	PHE	CA-CB-CG	7.48	121.28	113.80
1	A	722	ARG	CB-CG-CD	-7.36	94.38	111.30
1	C	722	ARG	CB-CG-CD	-7.34	94.41	111.30
2	D	478	LEU	N-CA-CB	-7.10	100.65	110.38
2	B	478	LEU	N-CA-CB	-7.08	100.67	110.38
1	A	662	GLU	CB-CA-C	6.99	124.34	110.42
2	D	516	ASN	CB-CA-C	6.99	126.26	110.67
1	C	662	GLU	CB-CA-C	6.99	124.33	110.42
2	B	516	ASN	CB-CA-C	6.97	126.22	110.67
1	C	722	ARG	CG-CD-NE	6.96	127.31	112.00
1	A	722	ARG	CG-CD-NE	6.95	127.30	112.00
2	B	500	GLU	CA-C-O	-6.83	113.18	120.42
2	D	500	GLU	CA-C-O	-6.79	113.22	120.42
2	D	515	ILE	N-CA-CB	-6.74	103.33	110.82
2	B	647	THR	CB-CA-C	-6.73	99.61	110.79
2	D	647	THR	CB-CA-C	-6.73	99.62	110.79
2	B	515	ILE	N-CA-CB	-6.72	103.36	110.82
1	C	679	PHE	CA-C-O	-6.71	113.13	120.24
1	A	679	PHE	CA-C-O	-6.69	113.15	120.24
2	B	504	LYS	N-CA-C	6.66	120.11	108.52
2	D	504	LYS	N-CA-C	6.64	120.07	108.52
2	D	501	VAL	CA-C-N	6.61	129.81	120.42
2	D	501	VAL	C-N-CA	6.61	129.81	120.42
2	B	501	VAL	CA-C-N	6.60	129.80	120.42
2	B	501	VAL	C-N-CA	6.60	129.80	120.42
2	D	524	ASP	N-CA-CB	-6.59	100.90	111.58
2	B	524	ASP	N-CA-CB	-6.59	100.90	111.58
2	B	482	THR	CA-C-N	6.45	129.44	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	482	THR	C-N-CA	6.45	129.44	120.29
2	D	482	THR	CA-C-N	6.42	129.41	120.29
2	D	482	THR	C-N-CA	6.42	129.41	120.29
1	C	528	GLU	CB-CG-CD	6.29	123.29	112.60
1	A	528	GLU	CB-CG-CD	6.28	123.28	112.60
1	C	786	GLU	CB-CA-C	6.10	121.93	109.55
2	D	483	ASN	N-CA-C	6.10	118.01	111.36
1	A	786	GLU	CB-CA-C	6.10	121.92	109.55
1	C	687	SER	CA-C-N	-6.09	111.36	122.38
1	C	687	SER	C-N-CA	-6.09	111.36	122.38
1	A	687	SER	CA-C-N	-6.08	111.38	122.38
1	A	687	SER	C-N-CA	-6.08	111.38	122.38
2	B	483	ASN	N-CA-C	6.07	117.97	111.36
1	A	794	ARG	CA-C-N	-5.99	114.53	122.85
1	A	794	ARG	C-N-CA	-5.99	114.53	122.85
1	C	794	ARG	CA-C-N	-5.97	114.55	122.85
1	C	794	ARG	C-N-CA	-5.97	114.55	122.85
1	A	528	GLU	CB-CA-C	-5.94	100.45	110.19
1	C	528	GLU	CB-CA-C	-5.93	100.47	110.19
1	C	730	ILE	CA-C-O	-5.85	114.22	120.59
1	A	730	ILE	CA-C-O	-5.82	114.25	120.59
2	D	505	ARG	CA-C-O	-5.69	112.69	119.35
2	B	505	ARG	CA-C-O	-5.67	112.72	119.35
2	D	501	VAL	CA-C-O	-5.60	114.92	120.85
2	B	501	VAL	CA-C-O	-5.58	114.94	120.85
1	A	730	ILE	N-CA-CB	-5.55	104.72	111.21
2	B	477	ASP	O-C-N	-5.53	117.15	123.40
2	D	477	ASP	O-C-N	-5.52	117.16	123.40
1	C	730	ILE	N-CA-CB	-5.52	104.75	111.21
1	C	665	THR	CA-C-N	5.49	132.17	121.41
1	C	665	THR	C-N-CA	5.49	132.17	121.41
1	A	665	THR	CA-C-N	5.48	132.16	121.41
1	A	665	THR	C-N-CA	5.48	132.16	121.41
1	C	607	MET	CA-C-N	-5.47	112.99	120.44
1	C	607	MET	C-N-CA	-5.47	112.99	120.44
2	B	482	THR	CA-CB-OG1	-5.47	101.39	109.60
1	A	607	MET	CA-C-N	-5.45	113.03	120.44
1	A	607	MET	C-N-CA	-5.45	113.03	120.44
2	D	482	THR	CA-CB-OG1	-5.45	101.42	109.60
2	B	515	ILE	O-C-N	5.44	128.92	122.66
2	B	502	VAL	CA-C-O	-5.40	115.13	120.85
2	D	515	ILE	O-C-N	5.39	128.86	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	VAL	CA-C-O	-5.36	115.17	120.85
2	B	503	MET	CA-C-N	-5.33	113.73	122.26
2	B	503	MET	C-N-CA	-5.33	113.73	122.26
2	B	486	HIS	CA-C-O	-5.31	114.79	120.42
1	C	543	LYS	CB-CA-C	-5.31	100.53	109.72
2	D	478	LEU	CA-C-N	5.31	131.96	122.09
2	D	478	LEU	C-N-CA	5.31	131.96	122.09
2	D	503	MET	CA-C-N	-5.30	113.77	122.26
2	D	503	MET	C-N-CA	-5.30	113.77	122.26
2	D	486	HIS	CA-C-O	-5.30	114.80	120.42
2	B	478	LEU	CA-C-N	5.30	131.94	122.09
2	B	478	LEU	C-N-CA	5.30	131.94	122.09
1	A	543	LYS	CB-CA-C	-5.28	100.58	109.72
2	D	640	VAL	CA-C-N	-5.17	113.07	120.42
2	D	640	VAL	C-N-CA	-5.17	113.07	120.42
2	B	640	VAL	CA-C-N	-5.16	113.09	120.42
2	B	640	VAL	C-N-CA	-5.16	113.09	120.42
2	D	644	ALA	CA-C-N	-5.15	112.12	121.14
2	D	644	ALA	C-N-CA	-5.15	112.12	121.14
2	B	644	ALA	CA-C-N	-5.14	112.15	121.14
2	B	644	ALA	C-N-CA	-5.14	112.15	121.14
2	B	488	LYS	CB-CA-C	-5.11	99.06	109.94
2	D	488	LYS	CB-CA-C	-5.11	99.06	109.94
2	B	505	ARG	O-C-N	5.06	128.67	122.34
1	C	662	GLU	CA-C-O	-5.06	113.27	120.51
1	A	662	GLU	CA-C-O	-5.06	113.28	120.51
2	D	505	ARG	O-C-N	5.05	128.65	122.34
1	C	519	ILE	CB-CA-C	-5.04	105.79	111.23
1	A	519	ILE	CB-CA-C	-5.03	105.79	111.23
2	D	509	ALA	CA-C-O	-5.01	114.95	120.36
2	B	509	ALA	CA-C-O	-5.00	114.95	120.36

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	792	TRP	Mainchain
2	B	500	GLU	Mainchain
2	B	503	MET	Mainchain
2	B	527	VAL	Mainchain
1	C	792	TRP	Mainchain
2	D	500	GLU	Mainchain

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Mol	Chain	Res	Type	Group
2	D	503	MET	Mainchain
2	D	527	VAL	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5775	0	5408	88	0
1	C	5775	0	5408	87	0
2	B	5684	0	5339	115	0
2	D	5684	0	5339	122	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	5	0	2	1	0
4	C	5	0	2	1	0
5	B	14	0	13	0	0
5	D	14	0	13	0	0
6	B	10	0	5	0	0
6	D	10	0	5	0	0
All	All	23032	0	21584	371	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 8.

All (371) 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:D:297:ILE:O	2:D:301:THR:HG23	1.09	1.25
2:B:297:ILE:O	2:B:301:THR:HG23	1.09	1.22
2:B:297:ILE:O	2:B:301:THR:CG2	1.99	1.11
2:B:608:LEU:HD13	2:B:620:VAL:HG11	1.28	1.11
2:D:297:ILE:O	2:D:301:THR:CG2	1.99	1.10
2:D:608:LEU:HD13	2:D:620:VAL:HG11	1.28	1.09
2:D:298:ALA:O	2:D:302:THR:HG22	1.55	1.07
2:B:298:ALA:O	2:B:302:THR:HG22	1.55	1.04
2:D:623:PRO:HB2	2:D:628:SER:OG	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:623:PRO:HB2	2:B:628:SER:OG	1.62	0.98
2:B:608:LEU:CD1	2:B:620:VAL:HG11	1.94	0.97
2:D:608:LEU:CD1	2:D:620:VAL:HG11	1.94	0.96
2:B:608:LEU:HD13	2:B:620:VAL:CG1	1.95	0.96
2:D:552:GLU:CB	2:D:653:PHE:CE2	2.48	0.96
2:D:608:LEU:HD13	2:D:620:VAL:CG1	1.95	0.95
2:B:552:GLU:CB	2:B:653:PHE:CE2	2.48	0.95
1:A:647:TYR:OH	2:D:641:ILE:CD1	2.15	0.94
1:C:798:CYS:SG	1:C:798:CYS:O	2.27	0.91
1:A:798:CYS:O	1:A:798:CYS:SG	2.27	0.91
2:B:641:ILE:CD1	1:C:647:TYR:OH	2.21	0.89
1:A:664:ILE:HD11	1:A:679:PHE:CZ	2.10	0.87
1:C:664:ILE:HD11	1:C:679:PHE:CZ	2.10	0.87
1:C:347:LYS:HD2	1:C:348:PHE:CD2	2.10	0.86
1:A:608:TRP:HH2	2:D:630:ILE:HD11	1.41	0.85
1:A:347:LYS:HD2	1:A:348:PHE:CD2	2.10	0.85
1:A:722:ARG:NH1	1:A:745:ASP:OD2	2.10	0.85
1:A:347:LYS:HD2	1:A:348:PHE:CE2	2.12	0.85
1:C:722:ARG:NH1	1:C:745:ASP:OD2	2.10	0.84
2:B:552:GLU:CB	2:B:653:PHE:CD2	2.61	0.84
1:C:347:LYS:HD2	1:C:348:PHE:CE2	2.12	0.84
2:D:367:LEU:HD12	2:D:372:LYS:O	1.78	0.84
2:B:367:LEU:HD12	2:B:372:LYS:O	1.78	0.83
2:D:552:GLU:CB	2:D:653:PHE:CD2	2.61	0.83
1:A:347:LYS:CD	1:A:348:PHE:CE2	2.63	0.82
1:C:649:ALA:CB	2:D:650:LEU:HD22	2.10	0.81
2:B:552:GLU:CB	2:B:653:PHE:HE2	1.91	0.81
1:C:827:GLY:O	1:C:831:ILE:N	2.13	0.81
1:C:347:LYS:CD	1:C:348:PHE:CE2	2.63	0.81
1:A:827:GLY:O	1:A:831:ILE:N	2.13	0.81
1:A:649:ALA:CB	2:B:650:LEU:HD22	2.12	0.80
2:B:630:ILE:HD11	1:C:608:TRP:HH2	1.46	0.80
2:D:552:GLU:CB	2:D:653:PHE:HE2	1.91	0.79
1:A:662:GLU:OE1	1:A:662:GLU:HA	1.83	0.77
1:C:662:GLU:HA	1:C:662:GLU:OE1	1.83	0.76
2:B:643:LEU:O	2:B:643:LEU:HD23	1.86	0.75
2:B:650:LEU:HD23	2:B:650:LEU:C	2.12	0.74
2:D:650:LEU:C	2:D:650:LEU:HD23	2.12	0.74
2:D:643:LEU:HD23	2:D:643:LEU:O	1.86	0.74
2:B:133:ILE:HD12	2:B:150:ILE:HD11	1.69	0.72
1:C:663:ARG:CG	1:C:663:ARG:HH11	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ILE:HD11	1:A:679:PHE:HZ	1.54	0.71
2:D:133:ILE:HD12	2:D:150:ILE:HD11	1.69	0.71
1:A:619:ILE:HD11	2:D:632:VAL:HG21	1.72	0.71
1:A:663:ARG:CG	1:A:663:ARG:HH11	2.03	0.71
1:C:664:ILE:HD11	1:C:679:PHE:HZ	1.54	0.70
1:A:347:LYS:HD3	1:A:348:PHE:CE2	2.27	0.70
1:A:647:TYR:OH	2:D:641:ILE:HD12	1.90	0.70
1:A:663:ARG:HH11	1:A:663:ARG:HG3	1.57	0.70
1:A:608:TRP:CH2	2:D:630:ILE:HD11	2.27	0.69
2:B:389:TYR:CE2	2:B:437:GLN:OE1	2.45	0.69
2:D:389:TYR:CE2	2:D:437:GLN:OE1	2.45	0.69
2:D:389:TYR:HE2	2:D:437:GLN:OE1	1.74	0.69
1:C:347:LYS:HD3	1:C:348:PHE:CE2	2.27	0.69
2:B:389:TYR:HE2	2:B:437:GLN:OE1	1.74	0.69
1:C:663:ARG:HH11	1:C:663:ARG:HG3	1.57	0.69
2:B:38:ALA:HB2	2:B:94:ILE:HD13	1.75	0.69
2:D:504:LYS:HB3	2:D:767:GLN:NE2	2.08	0.68
2:D:38:ALA:HB2	2:D:94:ILE:HD13	1.75	0.68
2:B:504:LYS:HB3	2:B:767:GLN:NE2	2.08	0.68
2:B:623:PRO:CB	2:B:628:SER:OG	2.41	0.68
2:B:607:TRP:CZ2	2:B:618:VAL:HG11	2.29	0.68
2:D:607:TRP:CZ2	2:D:618:VAL:HG11	2.28	0.68
2:B:632:VAL:HG21	1:C:619:ILE:HD11	1.75	0.67
1:C:819:LEU:C	1:C:819:LEU:HD13	2.19	0.67
2:D:623:PRO:HB2	2:D:628:SER:CB	2.24	0.67
2:B:566:LEU:HD11	2:B:609:LEU:HB3	1.77	0.67
2:D:269:VAL:HG12	2:D:271:SER:H	1.60	0.66
2:B:623:PRO:HB2	2:B:628:SER:CB	2.24	0.66
2:B:630:ILE:HD11	1:C:608:TRP:CH2	2.30	0.66
2:B:269:VAL:HG12	2:B:271:SER:H	1.61	0.66
1:A:819:LEU:C	1:A:819:LEU:HD13	2.19	0.66
2:D:540:ARG:NH1	2:D:746:CYS:O	2.27	0.66
2:D:566:LEU:HD11	2:D:609:LEU:HB3	1.77	0.66
1:A:647:TYR:CZ	2:D:641:ILE:CD1	2.78	0.66
2:B:540:ARG:NH1	2:B:746:CYS:O	2.27	0.64
2:B:641:ILE:HD12	1:C:647:TYR:OH	1.98	0.64
1:A:125:MET:O	1:A:139:ARG:NH2	2.31	0.64
2:D:650:LEU:HD23	2:D:650:LEU:O	1.98	0.63
1:A:722:ARG:HG2	1:A:722:ARG:HH11	1.64	0.63
1:C:125:MET:O	1:C:139:ARG:NH2	2.31	0.62
2:B:650:LEU:HD23	2:B:650:LEU:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:608:LEU:HB2	2:B:620:VAL:HG11	1.82	0.62
1:C:722:ARG:HG2	1:C:722:ARG:HH11	1.64	0.62
2:D:608:LEU:HB2	2:D:620:VAL:HG11	1.82	0.62
2:D:613:VAL:HG13	2:D:613:VAL:O	2.01	0.61
1:A:357:GLN:HB3	1:A:380:ILE:HG21	1.83	0.61
2:D:623:PRO:CB	2:D:628:SER:OG	2.41	0.61
1:A:680:ILE:O	1:A:727:HIS:HB2	2.01	0.60
2:D:488:LYS:HD3	2:D:490:ILE:HD11	1.83	0.60
2:D:514:THR:HG22	2:D:762:TYR:HE1	1.65	0.60
2:B:536:VAL:HG22	2:B:730:ILE:HG12	1.82	0.60
1:A:682:ALA:HA	1:A:706:MET:HG3	1.84	0.60
1:C:347:LYS:CD	1:C:348:PHE:CD2	2.83	0.60
2:D:607:TRP:HZ2	2:D:618:VAL:HG11	1.67	0.60
2:B:613:VAL:O	2:B:613:VAL:HG13	2.01	0.60
2:B:514:THR:HG22	2:B:762:TYR:HE1	1.65	0.60
2:D:536:VAL:HG22	2:D:730:ILE:HG12	1.82	0.60
2:B:488:LYS:HD3	2:B:490:ILE:HD11	1.83	0.59
2:B:608:LEU:HB2	2:B:620:VAL:CG1	2.32	0.59
2:D:608:LEU:HB2	2:D:620:VAL:CG1	2.33	0.59
2:D:608:LEU:CB	2:D:620:VAL:HG11	2.32	0.59
2:B:608:LEU:CB	2:B:620:VAL:HG11	2.32	0.59
1:C:357:GLN:HB3	1:C:380:ILE:HG21	1.83	0.59
2:B:607:TRP:HZ2	2:B:618:VAL:HG11	1.67	0.59
1:C:682:ALA:HA	1:C:706:MET:HG3	1.84	0.59
2:D:552:GLU:C	2:D:653:PHE:HE2	2.10	0.59
2:B:552:GLU:C	2:B:653:PHE:HE2	2.11	0.59
1:C:680:ILE:O	1:C:727:HIS:HB2	2.01	0.59
2:B:641:ILE:CD1	1:C:647:TYR:CZ	2.85	0.59
1:C:139:ARG:HB2	1:C:345:ASP:HA	1.85	0.58
1:C:608:TRP:O	1:C:611:TRP:N	2.36	0.58
2:B:515:ILE:HG13	2:B:761:GLY:O	2.04	0.58
2:D:242:GLU:HA	2:D:245:ASN:HD21	1.69	0.58
2:B:242:GLU:HA	2:B:245:ASN:HD21	1.69	0.58
2:D:515:ILE:HG13	2:D:761:GLY:O	2.04	0.57
1:A:347:LYS:CD	1:A:348:PHE:CD2	2.83	0.57
2:B:793:GLU:HG2	2:B:797:LEU:HD12	1.87	0.57
2:D:524:ASP:OD2	2:D:773:LYS:HD2	2.04	0.57
2:D:793:GLU:HG2	2:D:797:LEU:HD12	1.87	0.57
2:B:126:ILE:HA	2:B:146:PHE:HD2	1.69	0.57
2:B:524:ASP:OD2	2:B:773:LYS:HD2	2.03	0.56
1:A:608:TRP:O	1:A:611:TRP:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:790:LYS:HG2	1:C:794:ARG:NH2	2.20	0.56
1:A:139:ARG:HB2	1:A:345:ASP:HA	1.85	0.56
1:A:438:GLY:HA3	1:A:478:LEU:HB2	1.88	0.56
2:D:126:ILE:HA	2:D:146:PHE:HD2	1.69	0.56
1:C:438:GLY:HA3	1:C:478:LEU:HB2	1.88	0.56
2:B:514:THR:HG22	2:B:762:TYR:CE1	2.41	0.55
2:D:552:GLU:CB	2:D:653:PHE:HD2	2.16	0.55
1:A:732:ASP:OD2	4:A:901:GLY:N	2.39	0.55
1:A:790:LYS:HG2	1:A:794:ARG:NH2	2.20	0.55
1:C:732:ASP:OD2	4:C:901:GLY:N	2.39	0.55
1:A:487:GLN:HG2	1:A:496:LYS:HE2	1.89	0.54
2:D:514:THR:HG22	2:D:762:TYR:CE1	2.41	0.54
2:B:434:VAL:HG11	2:B:478:LEU:HD22	1.90	0.54
1:A:609:PHE:CD1	1:A:609:PHE:C	2.85	0.54
1:C:487:GLN:HG2	1:C:496:LYS:HE2	1.89	0.54
1:C:609:PHE:CD1	1:C:609:PHE:C	2.85	0.54
2:D:438:LYS:HB3	2:D:480:LEU:HD12	1.90	0.54
2:B:552:GLU:CB	2:B:653:PHE:HD2	2.16	0.54
1:C:221:LEU:HB3	1:C:249:VAL:HG12	1.89	0.53
2:D:82:ILE:HG12	2:D:115:ILE:HD11	1.91	0.53
1:A:309:VAL:HA	2:B:77:ASP:CG	2.32	0.53
1:A:820:VAL:HG13	2:D:565:MET:CE	2.38	0.53
1:A:221:LEU:HB3	1:A:249:VAL:HG12	1.89	0.53
2:B:438:LYS:HB3	2:B:480:LEU:HD12	1.90	0.53
1:C:649:ALA:HB2	2:D:650:LEU:HD22	1.90	0.53
2:B:553:PRO:CG	2:B:646:TYR:HE1	2.21	0.53
1:A:647:TYR:CZ	2:D:641:ILE:HD13	2.44	0.52
1:C:636:TRP:HA	1:C:636:TRP:HE3	1.74	0.52
2:D:553:PRO:CG	2:D:646:TYR:HE1	2.22	0.52
2:B:171:ILE:HD11	2:B:186:ILE:HG21	1.92	0.52
2:D:434:VAL:HG11	2:D:478:LEU:HD22	1.90	0.52
2:B:504:LYS:HB3	2:B:767:GLN:HE22	1.75	0.52
2:B:82:ILE:HG12	2:B:115:ILE:HD11	1.91	0.52
2:D:504:LYS:HB3	2:D:767:GLN:HE22	1.75	0.52
1:A:805:PRO:HB3	2:D:653:PHE:CD1	2.44	0.52
1:C:542:VAL:HG22	1:C:749:THR:CG2	2.40	0.52
1:A:636:TRP:HE3	1:A:636:TRP:HA	1.74	0.51
1:C:636:TRP:HA	1:C:636:TRP:CE3	2.46	0.51
2:D:289:LEU:HD12	2:D:292:ARG:HB2	1.93	0.51
1:C:102:PHE:O	1:C:105:THR:OG1	2.29	0.51
2:D:650:LEU:C	2:D:650:LEU:CD2	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:VAL:HG22	1:A:749:THR:CG2	2.40	0.51
2:D:249:LEU:HD23	2:D:249:LEU:H	1.75	0.51
2:B:289:LEU:HD12	2:B:292:ARG:HB2	1.93	0.51
2:B:123:ILE:HG13	2:B:143:PHE:HD1	1.76	0.51
1:C:510:ALA:O	1:C:763:ARG:NH2	2.44	0.51
1:A:663:ARG:HG3	1:A:663:ARG:NH1	2.25	0.51
2:B:650:LEU:C	2:B:650:LEU:CD2	2.84	0.51
1:A:401:VAL:HG12	1:A:501:MET:HE3	1.92	0.51
1:A:819:LEU:C	1:A:819:LEU:CD1	2.83	0.51
2:B:641:ILE:HD11	1:C:647:TYR:OH	2.08	0.51
2:D:241:PHE:O	2:D:245:ASN:ND2	2.44	0.51
2:D:205:LEU:HB2	2:D:216:ILE:HD12	1.93	0.50
1:A:102:PHE:O	1:A:105:THR:OG1	2.29	0.50
1:A:510:ALA:O	1:A:763:ARG:NH2	2.44	0.50
2:D:123:ILE:HG13	2:D:143:PHE:HD1	1.76	0.50
2:D:414:ALA:HB3	2:D:415:PRO:HD3	1.93	0.50
2:B:205:LEU:HB2	2:B:216:ILE:HD12	1.93	0.50
2:D:171:ILE:HD11	2:D:186:ILE:HG21	1.92	0.50
2:B:241:PHE:O	2:B:245:ASN:ND2	2.44	0.50
1:C:401:VAL:HG12	1:C:501:MET:HE3	1.92	0.50
1:C:819:LEU:C	1:C:819:LEU:CD1	2.83	0.50
2:D:553:PRO:HG3	2:D:646:TYR:CE1	2.47	0.50
2:B:249:LEU:HD23	2:B:249:LEU:H	1.75	0.50
1:A:636:TRP:HA	1:A:636:TRP:CE3	2.46	0.50
2:B:553:PRO:HG3	2:B:646:TYR:CE1	2.46	0.50
1:C:819:LEU:HD13	1:C:819:LEU:O	2.12	0.50
2:D:406:LEU:HD12	2:D:474:PHE:CD2	2.47	0.50
1:C:795:TYR:CD1	1:C:795:TYR:N	2.79	0.50
1:A:795:TYR:CD1	1:A:795:TYR:N	2.79	0.50
1:C:439:PRO:HB3	1:C:444:PRO:HG3	1.94	0.49
2:D:38:ALA:HB3	2:D:97:VAL:HG22	1.94	0.49
2:B:406:LEU:HD12	2:B:474:PHE:CD2	2.47	0.49
2:B:38:ALA:HB3	2:B:97:VAL:HG22	1.94	0.49
1:C:649:ALA:CB	2:D:650:LEU:CD2	2.88	0.49
2:D:101:ASP:OD1	2:D:102:ASP:N	2.42	0.49
2:B:414:ALA:HB3	2:B:415:PRO:HD3	1.93	0.49
1:A:577:LEU:HD23	1:A:632:LEU:HD23	1.95	0.49
1:C:608:TRP:O	1:C:609:PHE:C	2.55	0.49
2:B:625:GLY:O	2:B:629:LYS:HG3	2.13	0.49
1:A:440:ASN:HD21	1:A:447:PRO:HG2	1.78	0.49
1:C:577:LEU:HD23	1:C:632:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:VAL:HG13	2:D:565:MET:HE1	1.94	0.49
1:A:439:PRO:HB3	1:A:444:PRO:HG3	1.95	0.48
2:B:637:PHE:CD1	2:B:637:PHE:C	2.91	0.48
1:C:440:ASN:HD21	1:C:447:PRO:HG2	1.78	0.48
2:D:625:GLY:O	2:D:629:LYS:HG3	2.13	0.48
1:A:819:LEU:HD13	1:A:819:LEU:O	2.12	0.48
2:B:630:ILE:HD13	2:B:630:ILE:N	2.28	0.48
1:A:217:ARG:HB2	1:A:391:GLY:HA2	1.96	0.48
1:C:427:ASN:OD1	1:C:427:ASN:N	2.45	0.48
1:A:608:TRP:NE1	2:D:629:LYS:HD3	2.29	0.48
1:A:647:TYR:OH	2:D:641:ILE:HD11	2.07	0.48
2:B:185:LYS:HA	2:B:185:LYS:HD3	1.67	0.48
2:D:159:ASN:HA	2:D:162:GLU:HG2	1.96	0.48
2:D:630:ILE:HD13	2:D:630:ILE:N	2.28	0.48
2:B:299:ILE:HG12	2:B:342:VAL:HG21	1.96	0.47
1:C:217:ARG:HB2	1:C:391:GLY:HA2	1.96	0.47
2:D:637:PHE:C	2:D:637:PHE:CD1	2.91	0.47
2:B:556:ALA:HA	2:B:559:TRP:HD1	1.79	0.47
1:A:271:LEU:HD23	1:A:274:GLY:HA3	1.96	0.47
1:A:608:TRP:CH2	2:D:630:ILE:CD1	2.96	0.47
1:C:663:ARG:HG3	1:C:663:ARG:NH1	2.25	0.47
2:D:552:GLU:C	2:D:653:PHE:CE2	2.92	0.47
2:D:556:ALA:HA	2:D:559:TRP:HD1	1.79	0.47
1:A:608:TRP:O	1:A:609:PHE:C	2.55	0.47
2:B:159:ASN:HA	2:B:162:GLU:HG2	1.96	0.47
2:B:782:GLN:OE1	1:C:521:ASN:ND2	2.48	0.47
1:C:271:LEU:HD23	1:C:274:GLY:HA3	1.96	0.47
2:B:462:ILE:HG22	2:B:466:LYS:HE3	1.97	0.47
1:C:78:VAL:HG21	1:C:107:VAL:HG22	1.97	0.47
2:D:97:VAL:HB	2:D:123:ILE:HG22	1.97	0.47
1:A:78:VAL:HG21	1:A:107:VAL:HG22	1.97	0.47
2:B:613:VAL:HG23	2:B:639:ALA:HB2	1.97	0.47
2:D:299:ILE:HG12	2:D:342:VAL:HG21	1.96	0.46
2:D:635:TRP:O	2:D:638:PHE:HB3	2.16	0.46
1:C:577:LEU:CD2	1:C:632:LEU:HD23	2.46	0.46
1:A:470:MET:HE3	1:A:771:GLN:HB2	1.98	0.46
2:B:635:TRP:O	2:B:638:PHE:HB3	2.16	0.46
2:D:124:LEU:HD22	2:D:144:PHE:HB2	1.98	0.46
2:D:185:LYS:HA	2:D:185:LYS:HD3	1.68	0.46
2:B:124:LEU:HD22	2:B:144:PHE:HB2	1.98	0.46
1:C:609:PHE:CD1	1:C:609:PHE:O	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:556:ALA:HA	2:D:559:TRP:CD1	2.51	0.46
1:A:577:LEU:CD2	1:A:632:LEU:HD23	2.46	0.46
1:A:609:PHE:CD1	1:A:609:PHE:O	2.69	0.46
2:B:609:LEU:HD13	2:B:635:TRP:CD1	2.52	0.45
2:B:97:VAL:HB	2:B:123:ILE:HG22	1.97	0.45
2:B:556:ALA:HA	2:B:559:TRP:CD1	2.51	0.45
2:D:462:ILE:HG22	2:D:466:LYS:HE3	1.97	0.45
2:D:624:LYS:O	2:D:628:SER:HB3	2.16	0.45
2:B:122:PRO:HG3	2:B:142:MET:SD	2.56	0.45
2:B:653:PHE:CD1	1:C:805:PRO:HB3	2.51	0.45
1:A:517:LEU:HD23	1:A:529:PHE:HE1	1.82	0.45
1:C:517:LEU:HD23	1:C:529:PHE:HE1	1.82	0.45
1:C:400:ILE:HG13	1:C:463:LEU:HD21	1.99	0.45
1:C:470:MET:HE3	1:C:771:GLN:HB2	1.98	0.45
2:D:122:PRO:HG3	2:D:142:MET:SD	2.56	0.45
1:A:400:ILE:HG13	1:A:463:LEU:HD21	1.99	0.45
1:A:749:THR:O	1:A:749:THR:OG1	2.28	0.45
2:D:613:VAL:HG23	2:D:639:ALA:HB2	1.97	0.45
1:A:608:TRP:CE3	1:A:608:TRP:HA	2.52	0.45
1:A:655:LEU:HD13	2:D:649:ASN:OD1	2.17	0.45
2:B:680:PRO:HB2	2:B:705:TYR:OH	2.17	0.45
2:B:641:ILE:HD13	1:C:647:TYR:CZ	2.53	0.44
2:B:624:LYS:O	2:B:628:SER:HB3	2.16	0.44
2:D:637:PHE:CD1	2:D:637:PHE:O	2.70	0.44
2:D:680:PRO:HB2	2:D:705:TYR:OH	2.17	0.44
2:B:565:MET:CE	1:C:820:VAL:HG13	2.47	0.44
2:D:552:GLU:N	2:D:553:PRO:HD2	2.33	0.44
2:B:552:GLU:C	2:B:653:PHE:CE2	2.92	0.44
2:B:637:PHE:CD1	2:B:637:PHE:O	2.70	0.44
2:B:565:MET:HE1	1:C:820:VAL:HG13	2.00	0.44
2:D:609:LEU:HD13	2:D:635:TRP:CD1	2.52	0.44
2:D:678:SER:HB2	2:D:679:PRO:HD2	2.00	0.44
1:C:628:SER:HB2	2:D:836:PHE:HB2	1.98	0.44
1:A:427:ASN:OD1	1:A:427:ASN:N	2.45	0.44
2:B:678:SER:HB2	2:B:679:PRO:HD2	2.00	0.44
2:B:552:GLU:CA	2:B:653:PHE:HE2	2.30	0.44
1:C:608:TRP:HA	1:C:608:TRP:CE3	2.53	0.44
2:D:552:GLU:CA	2:D:653:PHE:HE2	2.30	0.44
2:D:609:LEU:CD1	2:D:635:TRP:CD1	3.01	0.43
2:B:552:GLU:N	2:B:553:PRO:HD2	2.32	0.43
1:C:722:ARG:HH11	1:C:722:ARG:CG	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:TRP:CG	1:A:732:ASP:H	2.37	0.43
1:C:542:VAL:HG22	1:C:749:THR:HG23	2.00	0.43
2:D:138:ASP:HB3	2:D:141:SER:HB2	2.00	0.43
2:D:142:MET:HG2	2:D:336:ASN:HD22	1.84	0.43
2:B:496:GLY:O	2:B:500:GLU:HG2	2.18	0.43
2:B:559:TRP:O	2:B:562:MET:HG3	2.18	0.43
1:C:280:HIS:O	1:C:281:ILE:C	2.60	0.43
2:D:77:ASP:O	2:D:80:SER:OG	2.31	0.43
2:D:559:TRP:O	2:D:562:MET:HG3	2.18	0.43
2:D:496:GLY:O	2:D:500:GLU:HG2	2.18	0.43
2:B:138:ASP:HB3	2:B:141:SER:HB2	2.00	0.43
2:B:609:LEU:CD1	2:B:635:TRP:CD1	3.01	0.43
1:C:749:THR:O	1:C:749:THR:OG1	2.28	0.43
1:A:793:VAL:O	1:A:793:VAL:CG1	2.66	0.43
2:B:142:MET:HG2	2:B:336:ASN:HD22	1.84	0.43
1:A:697:VAL:O	1:A:697:VAL:HG12	2.19	0.43
2:B:705:TYR:O	2:B:708:LYS:HG2	2.19	0.43
2:D:261:LEU:HD23	2:D:261:LEU:H	1.83	0.43
1:A:647:TYR:CE2	2:D:641:ILE:HD13	2.54	0.42
1:A:105:THR:OG1	1:A:106:PRO:HD3	2.20	0.42
1:C:697:VAL:O	1:C:697:VAL:HG12	2.19	0.42
1:A:542:VAL:HG22	1:A:749:THR:HG23	2.00	0.42
1:A:608:TRP:HA	1:A:608:TRP:HE3	1.84	0.42
1:C:685:LYS:HG3	1:C:711:TYR:O	2.19	0.42
2:D:212:GLY:O	2:D:216:ILE:HG12	2.19	0.42
1:A:542:VAL:CG2	1:A:749:THR:CG2	2.97	0.42
1:C:309:VAL:HA	2:D:77:ASP:CG	2.45	0.42
1:C:731:TRP:CG	1:C:732:ASP:H	2.37	0.42
1:A:649:ALA:HB1	2:B:650:LEU:HD22	1.96	0.42
2:D:678:SER:O	2:D:679:PRO:C	2.63	0.42
2:B:101:ASP:OD1	2:B:102:ASP:N	2.42	0.42
2:B:212:GLY:O	2:B:216:ILE:HG12	2.19	0.42
1:C:608:TRP:HA	1:C:608:TRP:HE3	1.84	0.42
1:A:639:PHE:CE2	1:A:643:ILE:HD11	2.55	0.42
2:B:261:LEU:HD23	2:B:261:LEU:H	1.83	0.42
1:C:347:LYS:HG2	1:C:348:PHE:N	2.35	0.42
2:D:620:VAL:HG12	2:D:621:GLN:N	2.35	0.42
1:A:685:LYS:HG3	1:A:711:TYR:O	2.19	0.42
1:C:542:VAL:CG2	1:C:749:THR:CG2	2.97	0.42
2:D:705:TYR:O	2:D:708:LYS:HG2	2.19	0.42
2:B:428:THR:OG1	2:B:429:CYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:553:PRO:CG	2:D:646:TYR:CE1	3.02	0.41
1:A:347:LYS:HG2	1:A:348:PHE:N	2.35	0.41
1:C:614:LEU:HD12	1:C:614:LEU:HA	1.91	0.41
2:B:172:VAL:O	2:B:172:VAL:HG22	2.20	0.41
2:B:553:PRO:HG3	2:B:646:TYR:HE1	1.84	0.41
1:A:647:TYR:CZ	2:D:641:ILE:HD11	2.52	0.41
1:C:793:VAL:O	1:C:793:VAL:CG1	2.66	0.41
2:D:172:VAL:O	2:D:172:VAL:HG22	2.20	0.41
2:B:142:MET:HE3	2:B:336:ASN:HB2	2.02	0.41
2:B:620:VAL:HG12	2:B:621:GLN:N	2.35	0.41
2:D:428:THR:OG1	2:D:429:CYS:N	2.53	0.41
1:C:105:THR:OG1	1:C:106:PRO:HD3	2.20	0.41
1:C:639:PHE:CE2	1:C:643:ILE:HD11	2.55	0.41
1:A:805:PRO:HB3	2:D:653:PHE:CE1	2.56	0.41
1:A:808:LEU:HD12	2:D:554:PHE:HE1	1.85	0.41
2:B:656:GLN:HG2	1:C:803:ASN:CB	2.51	0.41
2:B:695:ILE:HG21	2:B:706:MET:SD	2.61	0.41
1:C:198:ASP:OD1	1:C:198:ASP:N	2.54	0.41
1:C:406:GLU:HB3	1:C:407:PRO:HD3	2.03	0.41
1:A:722:ARG:HH11	1:A:722:ARG:CG	2.30	0.40
2:B:678:SER:O	2:B:679:PRO:C	2.63	0.40
2:D:623:PRO:CG	2:D:628:SER:OG	2.69	0.40
1:A:280:HIS:O	1:A:281:ILE:C	2.60	0.40
2:D:124:LEU:CD2	2:D:144:PHE:HB2	2.52	0.40
2:D:613:VAL:HG23	2:D:639:ALA:CB	2.52	0.40
1:A:443:SER:O	1:A:447:PRO:HD2	2.22	0.40
1:A:820:VAL:HG13	2:D:565:MET:HE2	2.03	0.40
2:B:77:ASP:O	2:B:80:SER:OG	2.31	0.40
1:C:708:LYS:HG3	1:C:709:HIS:CD2	2.57	0.40
1:A:406:GLU:HB3	1:A:407:PRO:HD3	2.03	0.40
2:B:124:LEU:CD2	2:B:144:PHE:HB2	2.52	0.40
2:B:623:PRO:CG	2:B:628:SER:OG	2.69	0.40
2:B:641:ILE:HD11	1:C:647:TYR:CZ	2.55	0.40
2:D:695:ILE:HG21	2:D:706:MET:SD	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	790/847 (93%)	763 (97%)	25 (3%)	2 (0%)	36	64
1	C	790/847 (93%)	763 (97%)	25 (3%)	2 (0%)	36	64
2	B	779/883 (88%)	732 (94%)	47 (6%)	0	100	100
2	D	779/883 (88%)	733 (94%)	46 (6%)	0	100	100
All	All	3138/3460 (91%)	2991 (95%)	143 (5%)	4 (0%)	49	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	663	ARG
1	C	663	ARG
1	A	272	ILE
1	C	272	ILE

5.3.2 Protein sidechains

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	562/728 (77%)	535 (95%)	27 (5%)	23	50
1	C	562/728 (77%)	535 (95%)	27 (5%)	23	50
2	B	562/762 (74%)	531 (94%)	31 (6%)	19	46
2	D	562/762 (74%)	531 (94%)	31 (6%)	19	46
All	All	2248/2980 (75%)	2132 (95%)	116 (5%)	22	48

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	32	VAL
1	A	105	THR
1	A	308	CYS
1	A	425	THR
1	A	427	ASN
1	A	436	CYS
1	A	437	THR
1	A	446	SER
1	A	490	VAL
1	A	512	MET
1	A	602	THR
1	A	631	ILE
1	A	635	VAL
1	A	663	ARG
1	A	664	ILE
1	A	665	THR
1	A	722	ARG
1	A	725	LYS
1	A	730	ILE
1	A	744	CYS
1	A	745	ASP
1	A	756	SER
1	A	795	TYR
1	A	798	CYS
1	A	819	LEU
1	A	828	ILE
2	B	64	VAL
2	B	133	ILE
2	B	137	LYS
2	B	172	VAL
2	B	185	LYS
2	B	272	GLU
2	B	280	VAL
2	B	302	THR
2	B	368	ASN
2	B	437	GLN
2	B	472	VAL
2	B	477	ASP
2	B	485	LYS
2	B	504	LYS
2	B	510	VAL

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Mol	Chain	Res	Type
2	B	513	LEU
2	B	515	ILE
2	B	516	ASN
2	B	527	VAL
2	B	545	VAL
2	B	612	LEU
2	B	613	VAL
2	B	617	SER
2	B	618	VAL
2	B	626	THR
2	B	630	ILE
2	B	642	PHE
2	B	654	MET
2	B	656	GLN
2	B	686	VAL
2	B	808	VAL
1	C	27	VAL
1	C	32	VAL
1	C	105	THR
1	C	308	CYS
1	C	425	THR
1	C	427	ASN
1	C	436	CYS
1	C	437	THR
1	C	446	SER
1	C	490	VAL
1	C	512	MET
1	C	602	THR
1	C	631	ILE
1	C	635	VAL
1	C	663	ARG
1	C	664	ILE
1	C	665	THR
1	C	722	ARG
1	C	725	LYS
1	C	730	ILE
1	C	744	CYS
1	C	745	ASP
1	C	756	SER
1	C	795	TYR
1	C	798	CYS
1	C	819	LEU

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Mol	Chain	Res	Type
1	C	828	ILE
2	D	64	VAL
2	D	133	ILE
2	D	137	LYS
2	D	172	VAL
2	D	185	LYS
2	D	272	GLU
2	D	280	VAL
2	D	302	THR
2	D	368	ASN
2	D	437	GLN
2	D	472	VAL
2	D	477	ASP
2	D	485	LYS
2	D	504	LYS
2	D	510	VAL
2	D	513	LEU
2	D	515	ILE
2	D	516	ASN
2	D	527	VAL
2	D	545	VAL
2	D	612	LEU
2	D	613	VAL
2	D	617	SER
2	D	618	VAL
2	D	626	THR
2	D	630	ILE
2	D	642	PHE
2	D	654	MET
2	D	656	GLN
2	D	686	VAL
2	D	808	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	161	ASN
1	A	357	GLN
1	A	471	GLN
1	A	521	ASN
1	A	705	HIS

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Mol	Chain	Res	Type
1	A	709	HIS
1	A	727	HIS
2	B	152	GLN
2	B	219	GLN
2	B	245	ASN
2	B	336	ASN
2	B	385	GLN
2	B	767	GLN
1	C	47	ASN
1	C	161	ASN
1	C	357	GLN
1	C	453	GLN
1	C	471	GLN
1	C	668	ASN
1	C	705	HIS
1	C	709	HIS
1	C	727	HIS
2	D	152	GLN
2	D	219	GLN
2	D	245	ASN
2	D	336	ASN

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](#)

4 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
3	NAG	E	1	3,2	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	F	1	3,2	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	F	2	3	14,14,15	0.22	0	17,19,21	0.43	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	E	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	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.

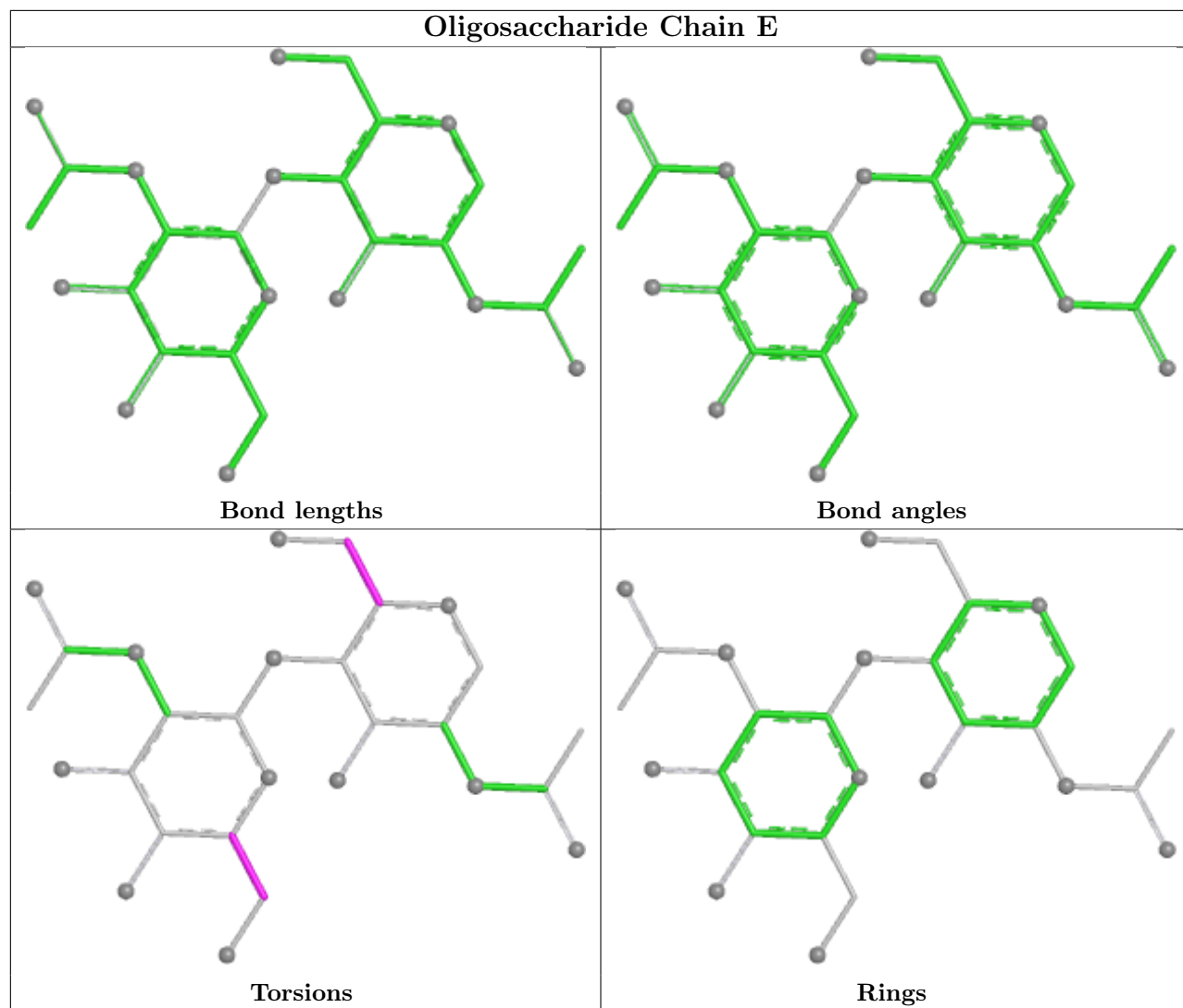
All (8) torsion outliers are listed below:

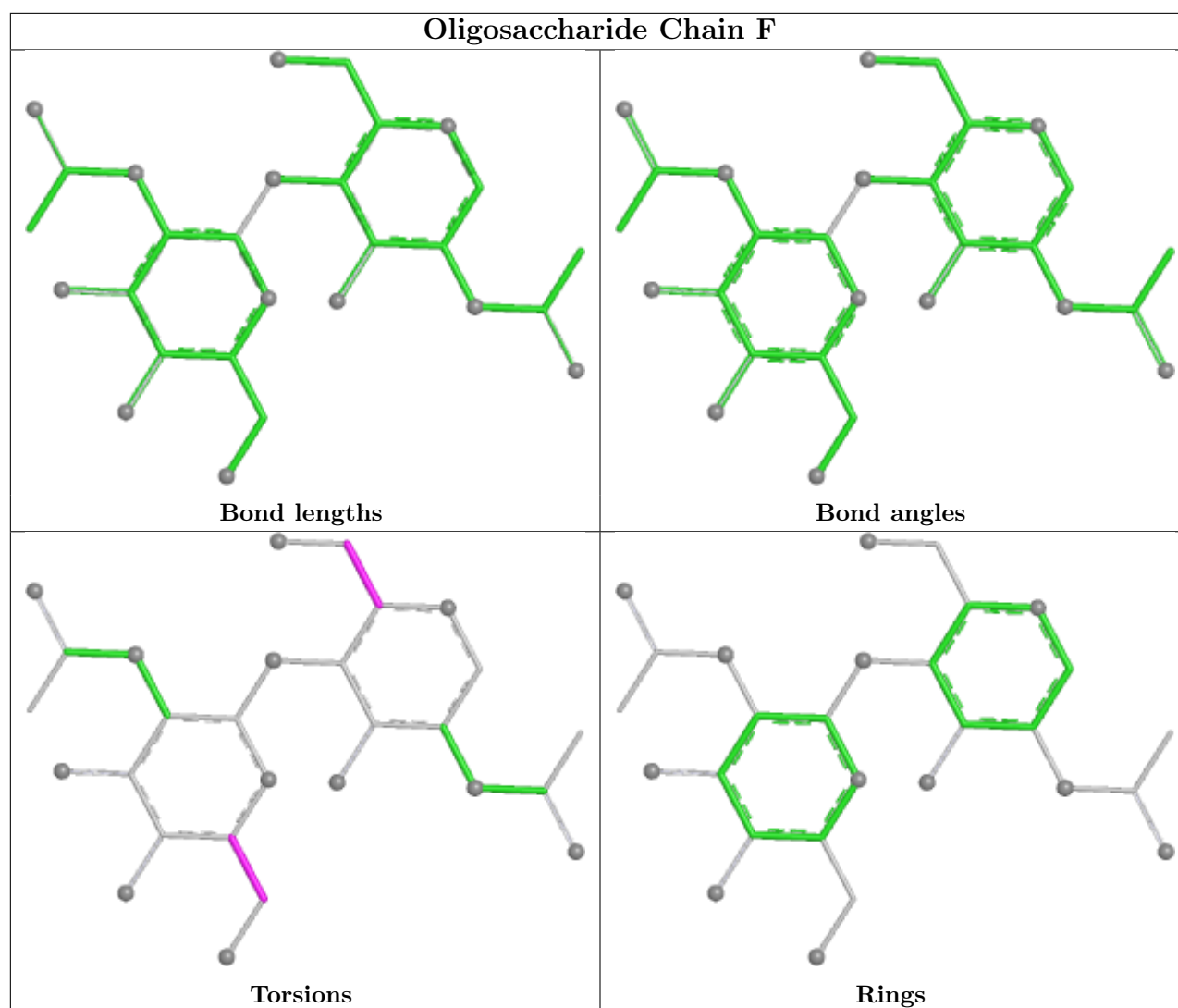
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

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 oligosaccharide.





5.6 Ligand geometry [i](#)

6 ligands 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	$\# Z > 2$
4	GLY	C	901	-	4,4,4	1.14	1 (25%)	3,4,4	1.64	1 (33%)
4	GLY	A	901	-	4,4,4	1.15	1 (25%)	3,4,4	1.63	1 (33%)
5	NAG	D	901	2	14,14,15	0.89	1 (7%)	17,19,21	1.28	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GLU	D	902	-	8,9,9	1.11	1 (12%)	8,11,11	1.20	1 (12%)
5	NAG	B	901	2	14,14,15	0.90	1 (7%)	17,19,21	1.27	1 (5%)
6	GLU	B	902	-	8,9,9	1.11	1 (12%)	8,11,11	1.20	1 (12%)

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
4	GLY	C	901	-	-	0/2/2/2	-
4	GLY	A	901	-	-	0/2/2/2	-
5	NAG	D	901	2	-	1/6/23/26	0/1/1/1
6	GLU	D	902	-	-	0/9/9/9	-
5	NAG	B	901	2	-	1/6/23/26	0/1/1/1
6	GLU	B	902	-	-	0/9/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	NAG	O5-C1	3.18	1.49	1.43
5	D	901	NAG	O5-C1	3.16	1.49	1.43
6	B	902	GLU	OXT-C	-2.23	1.23	1.30
6	D	902	GLU	OXT-C	-2.23	1.23	1.30
4	A	901	GLY	OXT-C	-2.18	1.23	1.30
4	C	901	GLY	OXT-C	-2.16	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	901	NAG	C1-O5-C5	5.04	118.94	112.19
5	B	901	NAG	C1-O5-C5	5.02	118.91	112.19
6	D	902	GLU	OXT-C-O	-2.74	117.87	124.08
6	B	902	GLU	OXT-C-O	-2.71	117.93	124.08
4	C	901	GLY	OXT-C-O	-2.08	117.99	123.33
4	A	901	GLY	OXT-C-O	-2.06	118.03	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

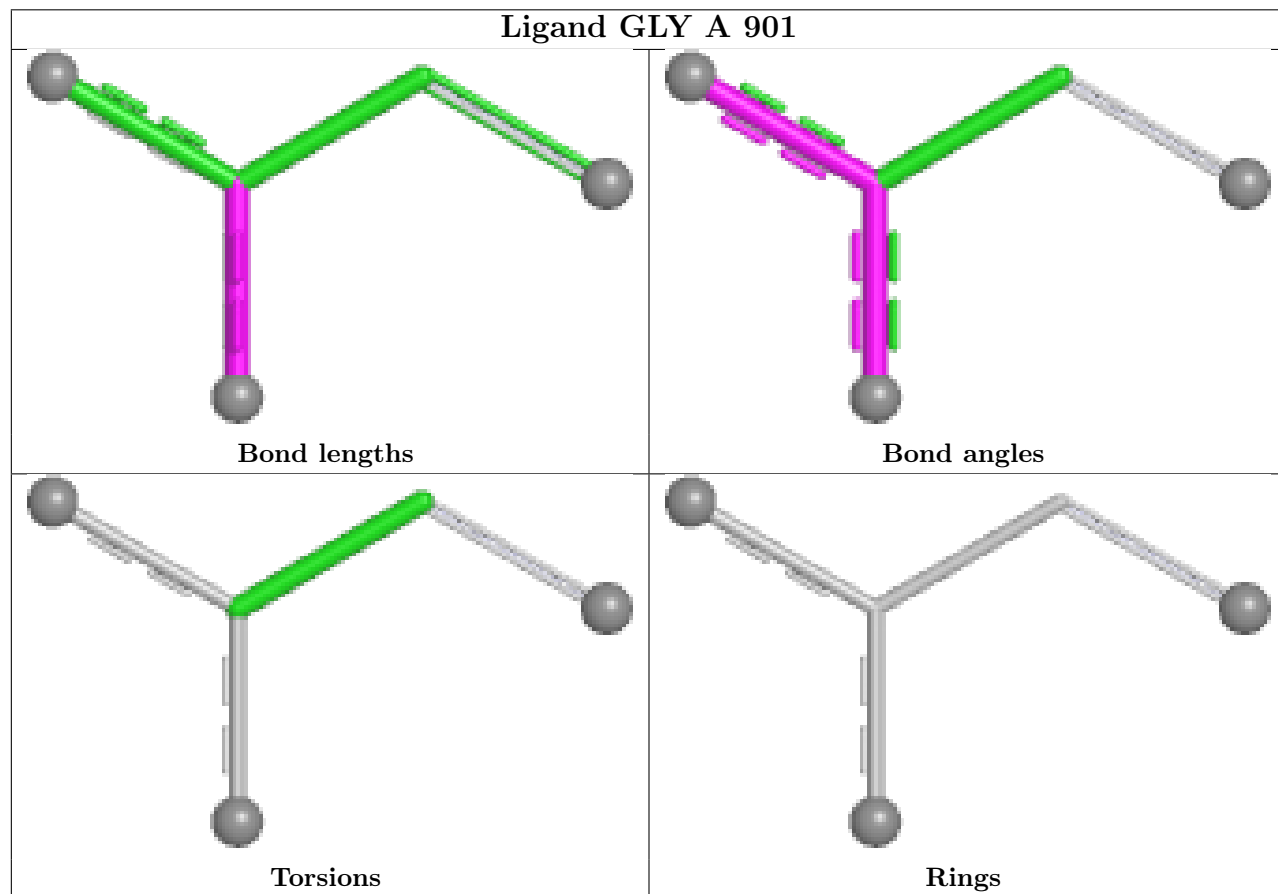
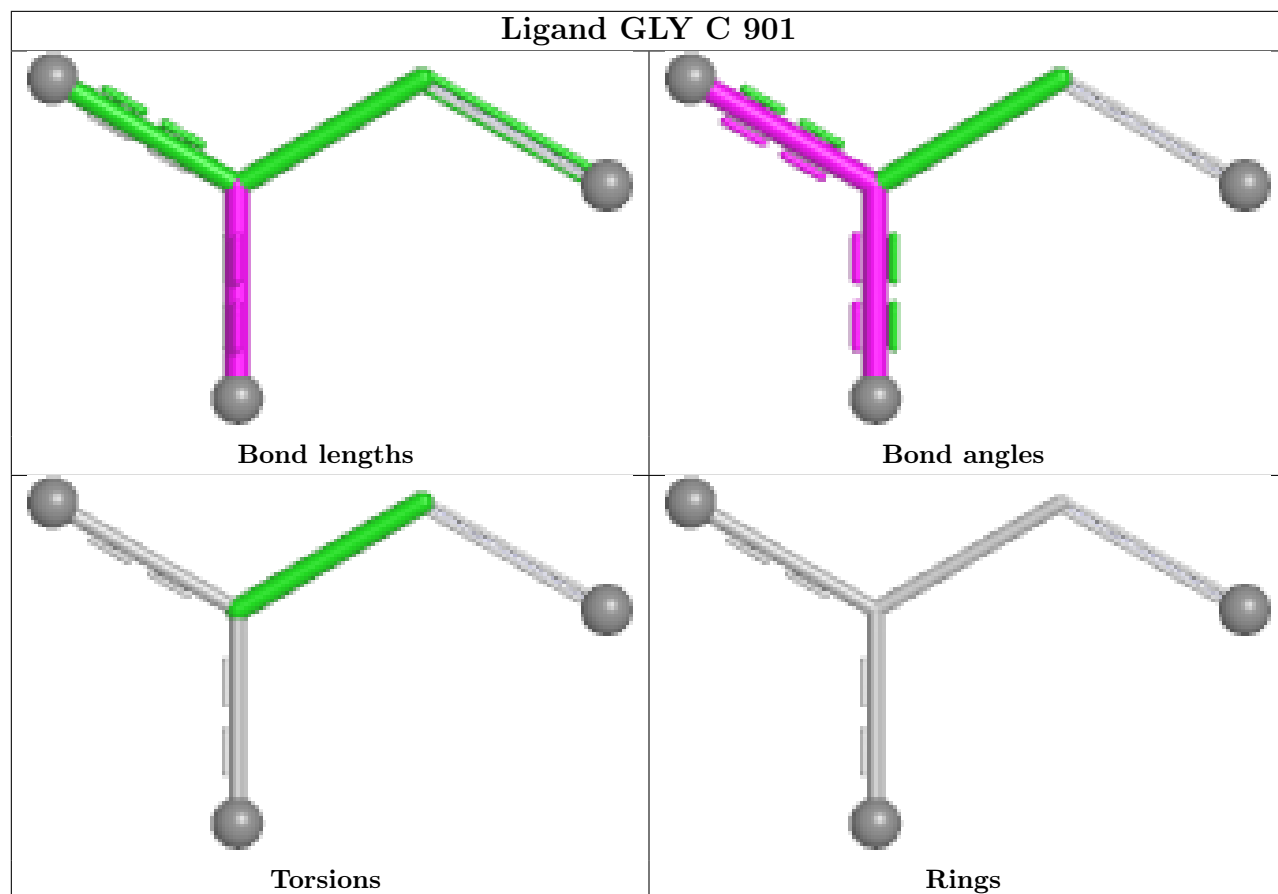
Mol	Chain	Res	Type	Atoms
5	D	901	NAG	O5-C5-C6-O6
5	B	901	NAG	O5-C5-C6-O6

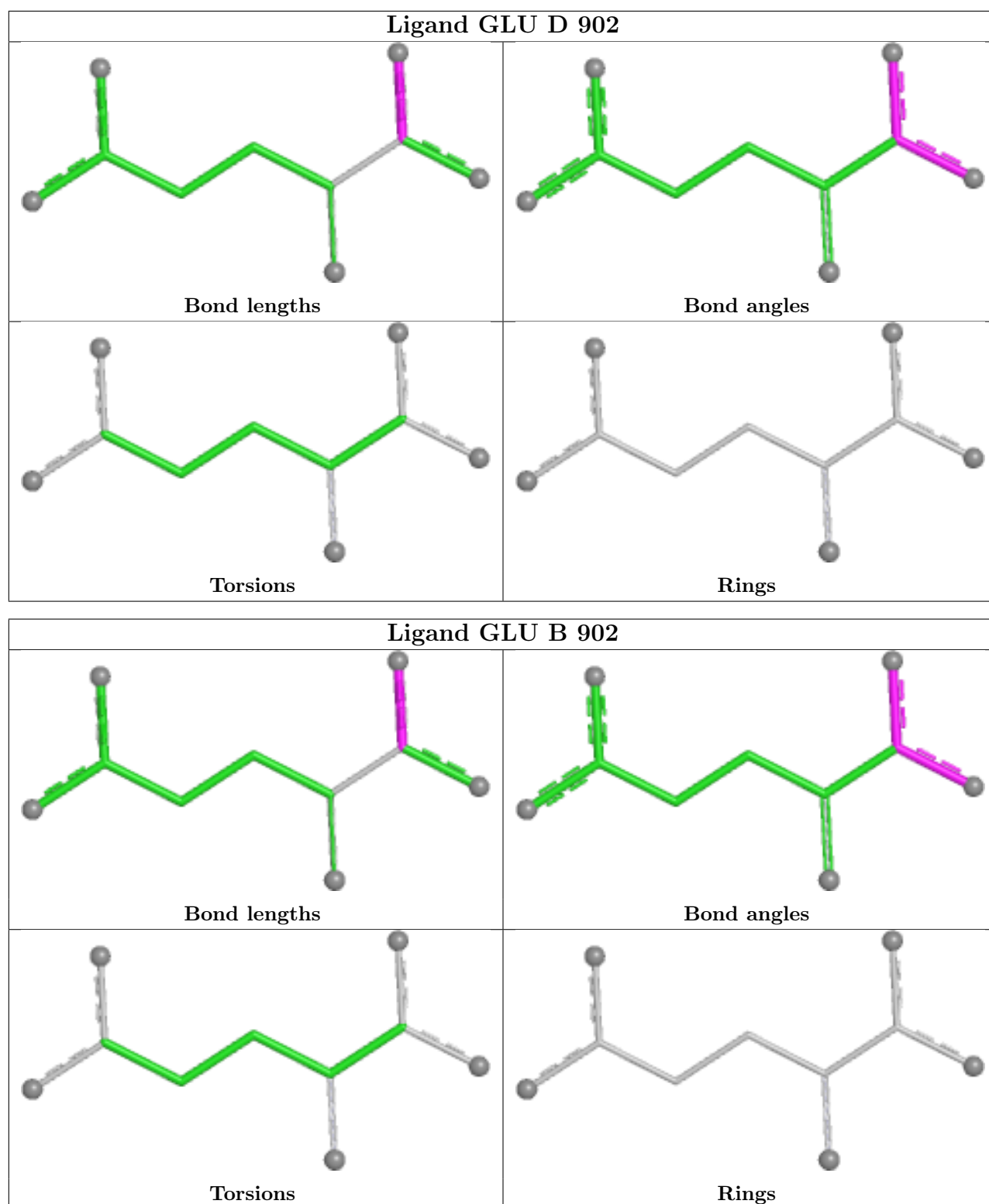
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	901	GLY	1	0
4	A	901	GLY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

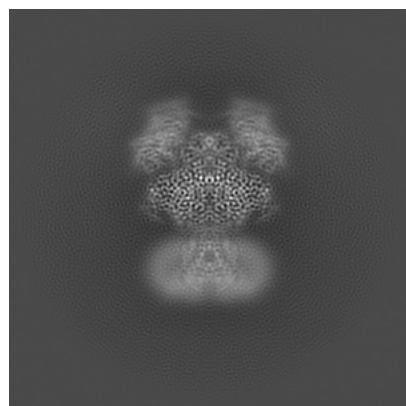
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43780. These allow visual inspection of the internal detail of the map and identification of artifacts.

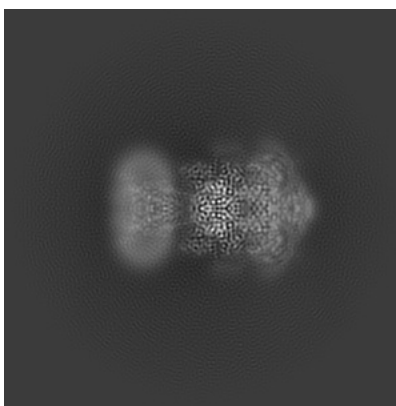
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

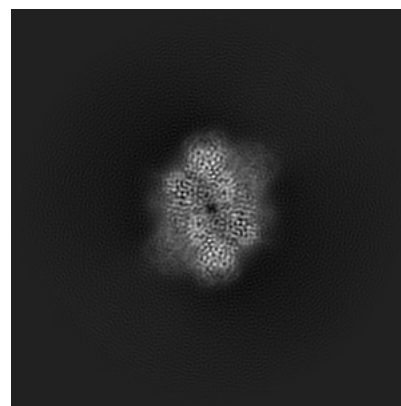
6.1.1 Primary map



X

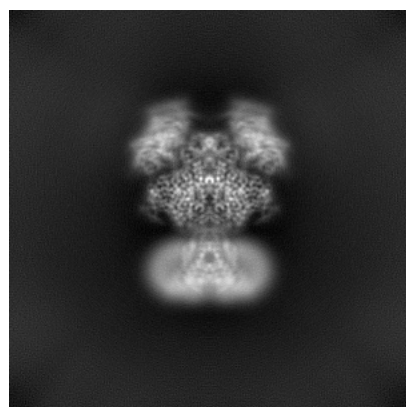


Y

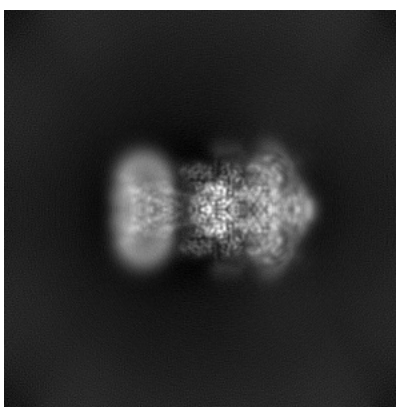


Z

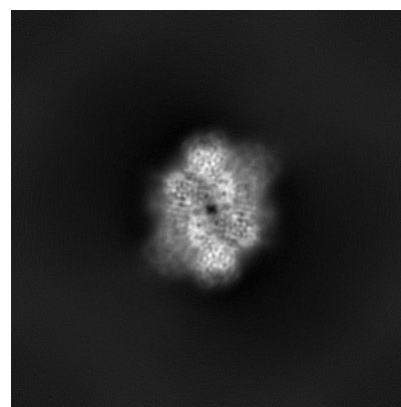
6.1.2 Raw map



X



Y

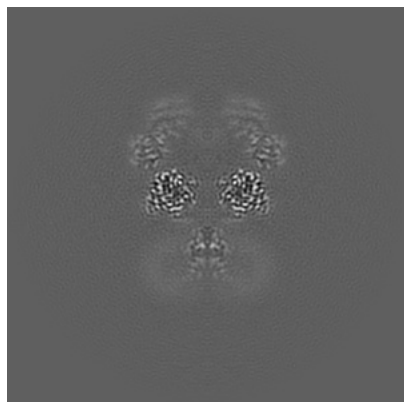


Z

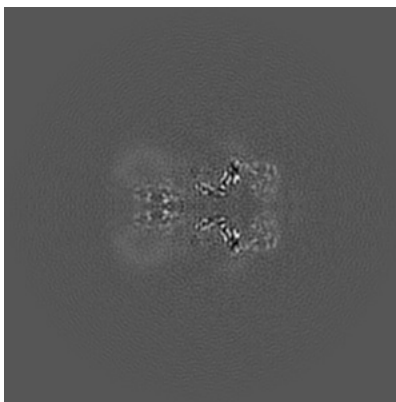
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

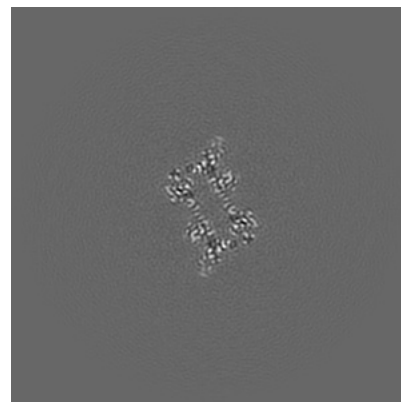
6.2.1 Primary map



X Index: 200

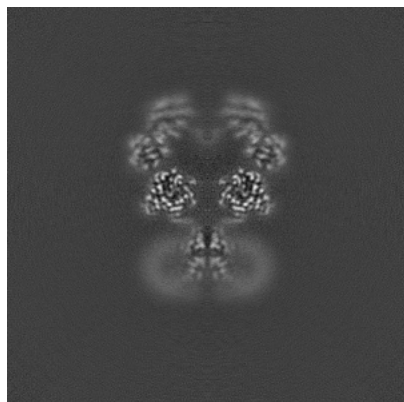


Y Index: 200

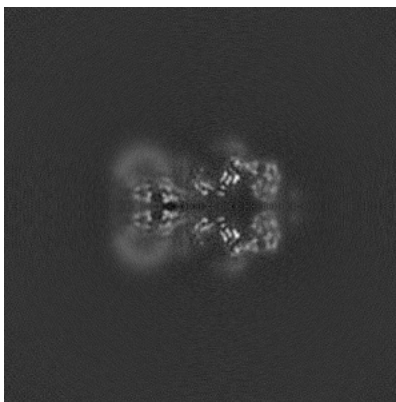


Z Index: 200

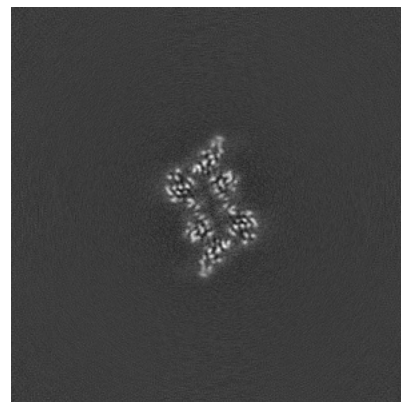
6.2.2 Raw map



X Index: 200



Y Index: 200

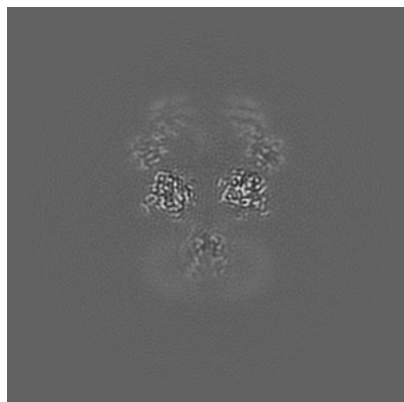


Z Index: 200

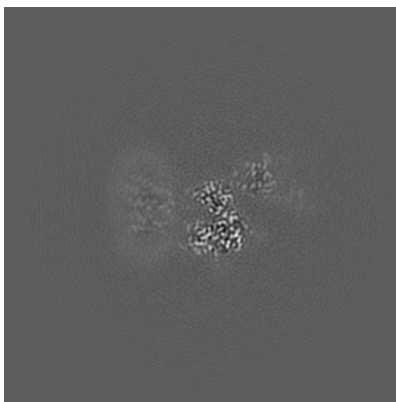
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

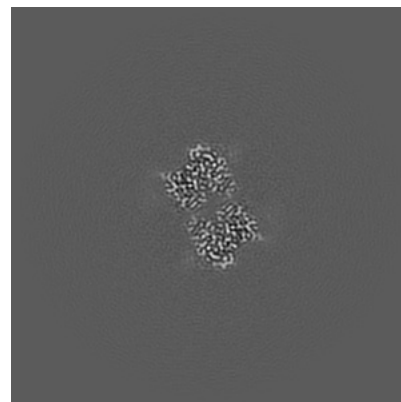
6.3.1 Primary map



X Index: 198

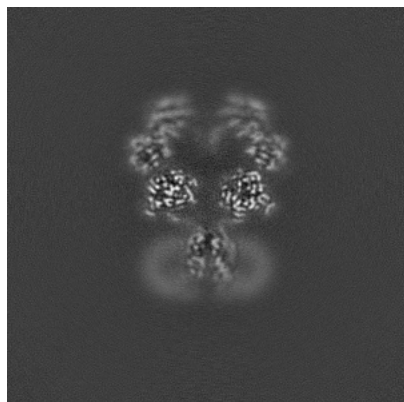


Y Index: 219

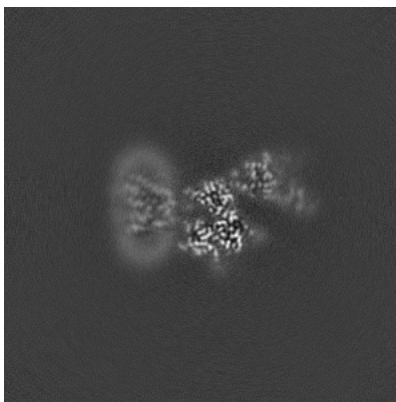


Z Index: 219

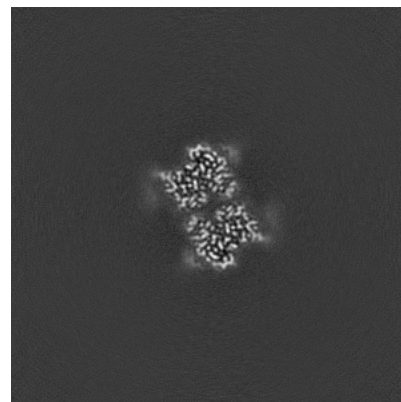
6.3.2 Raw map



X Index: 202



Y Index: 219

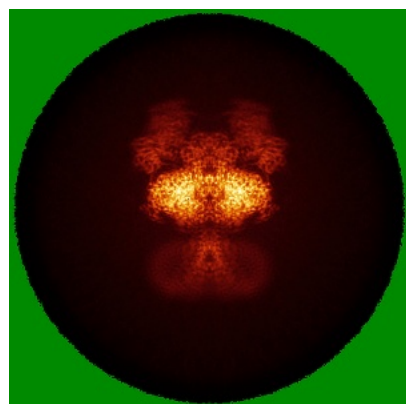


Z Index: 219

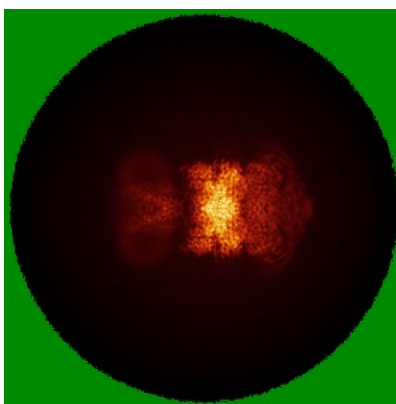
The images above show the largest variance slices of the map in three orthogonal directions.

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

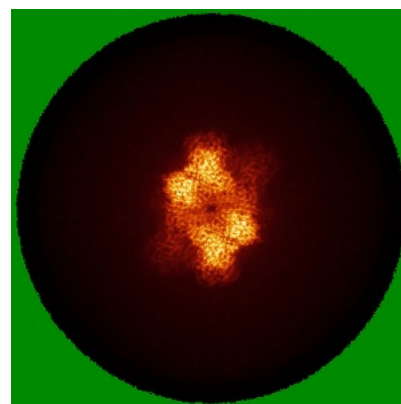
6.4.1 Primary map



X

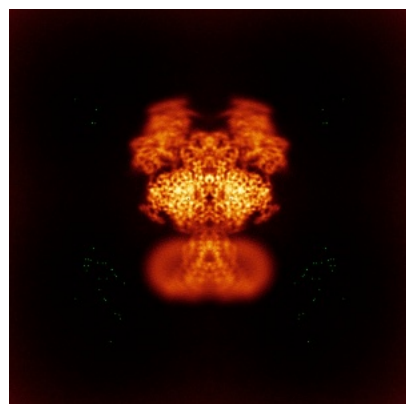


Y

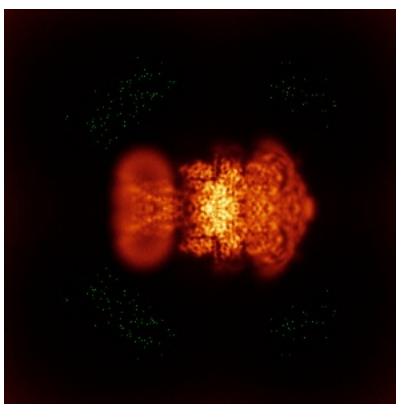


Z

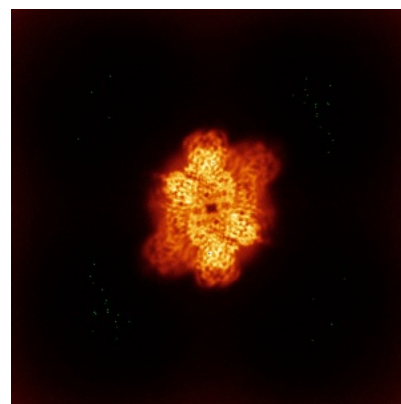
6.4.2 Raw map



X



Y

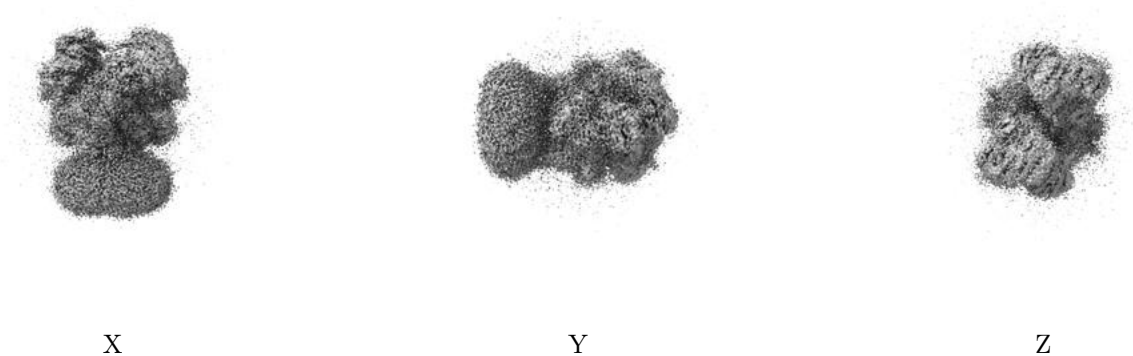


Z

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.

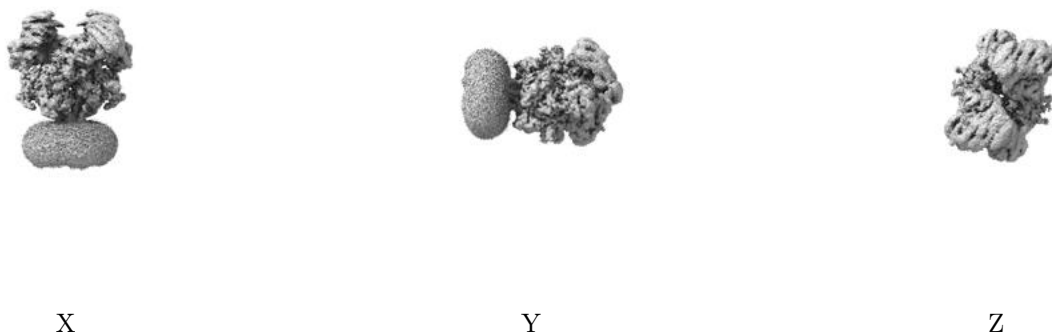
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0704. 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.

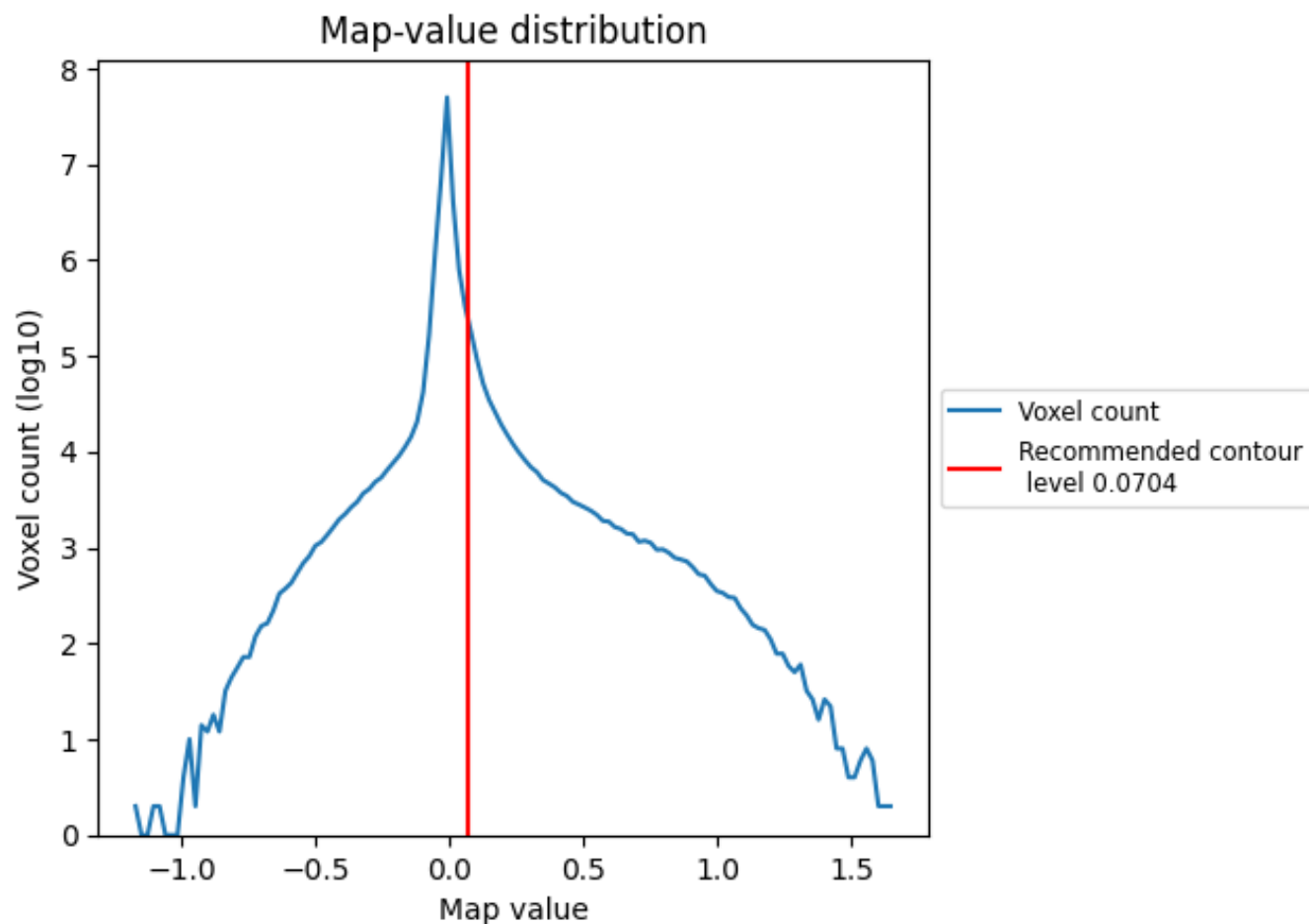
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

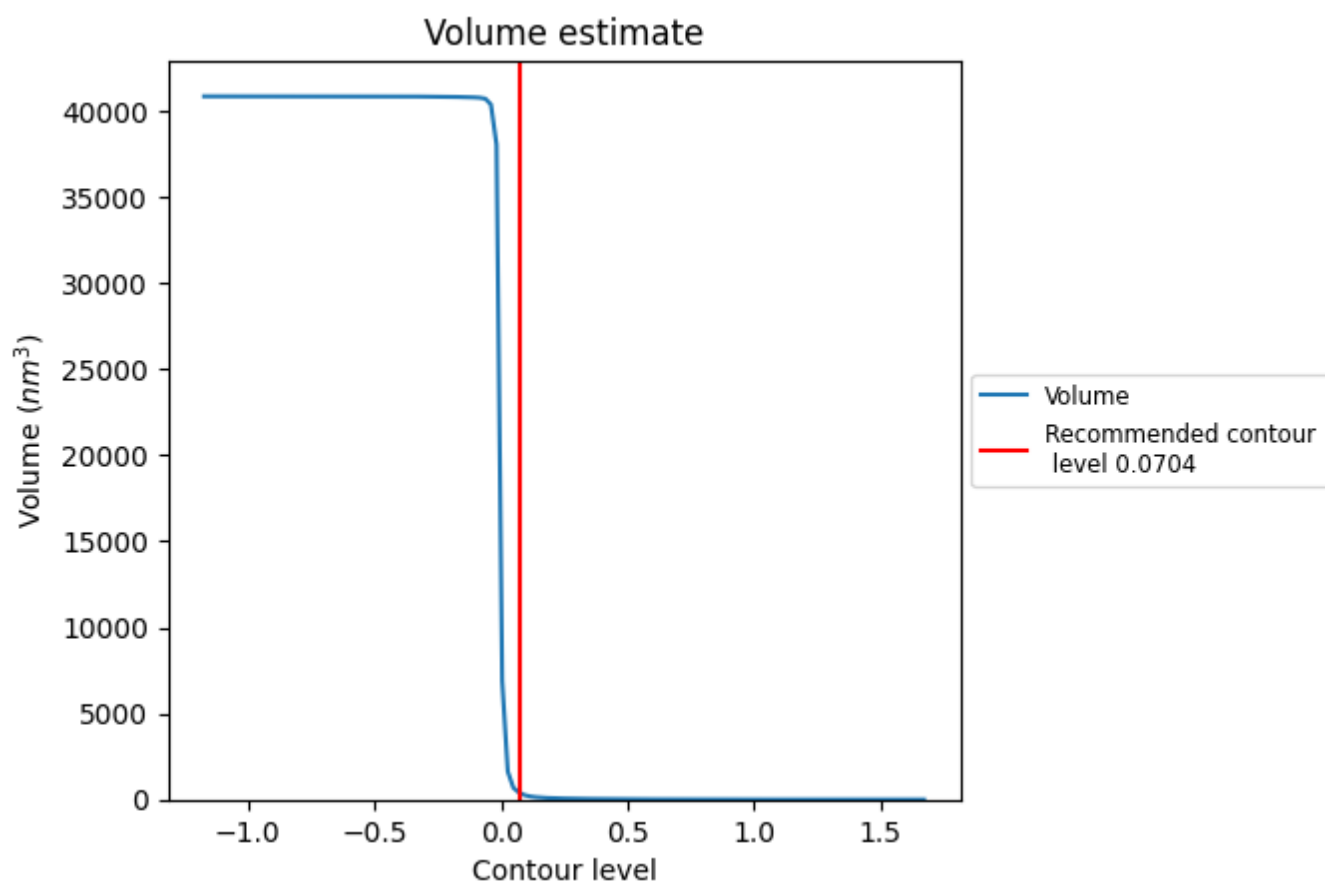
This section contains the results of statistical analysis of the map.

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.

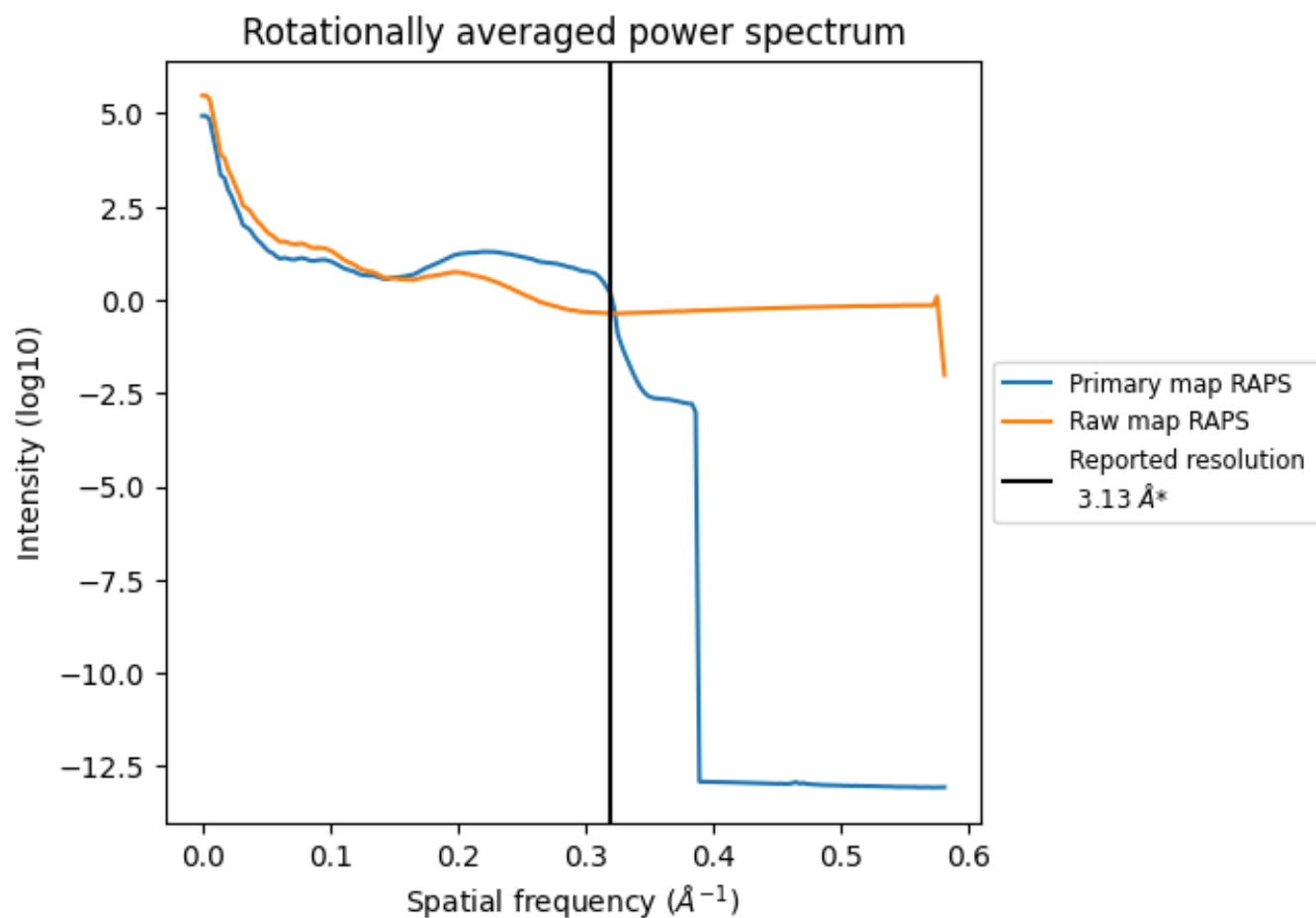
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 411 nm³; this corresponds to an approximate mass of 371 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 ⓘ

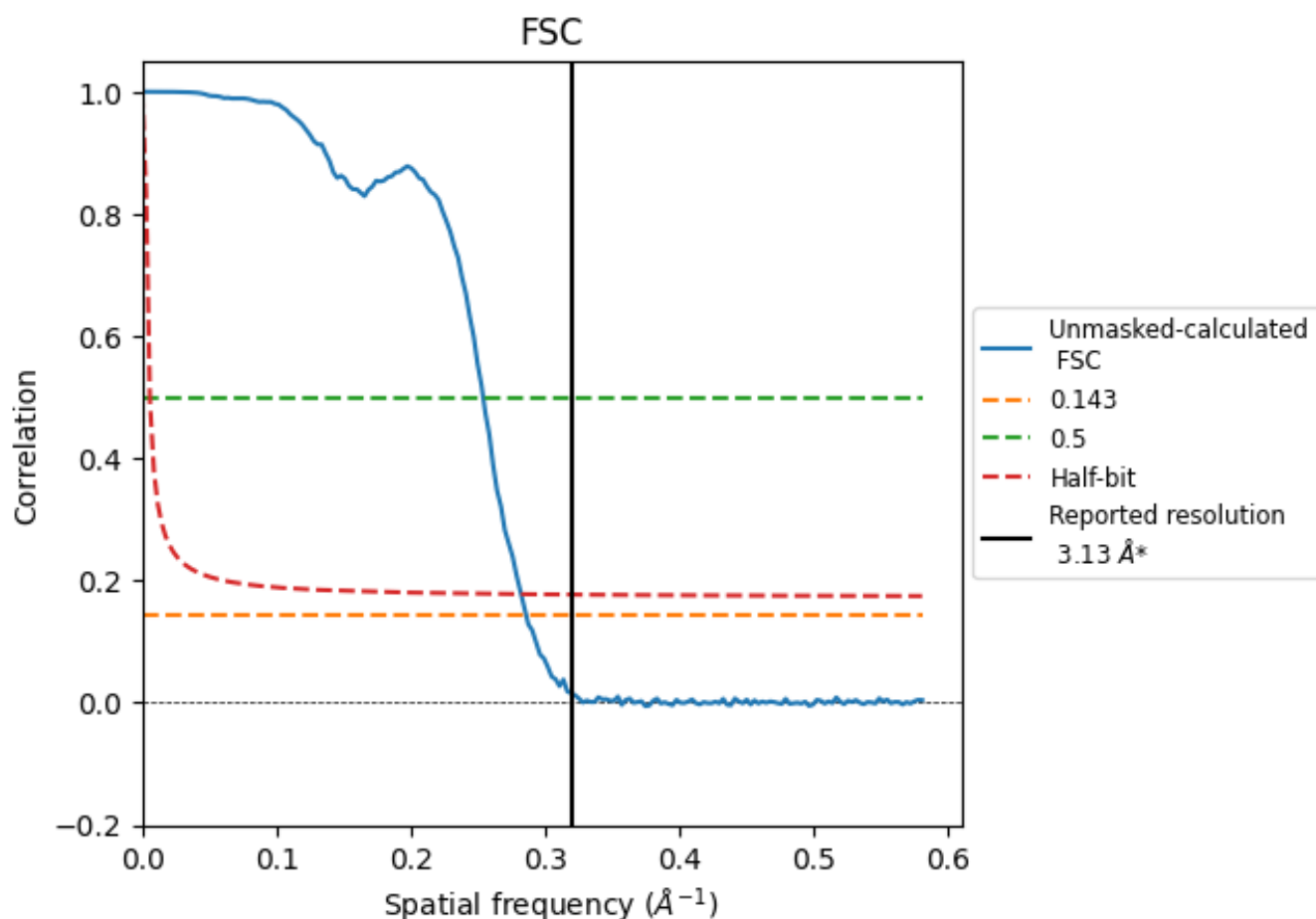


*Reported resolution corresponds to spatial frequency of 0.319 $\text{\AA}^{-1}$

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 $0.319 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

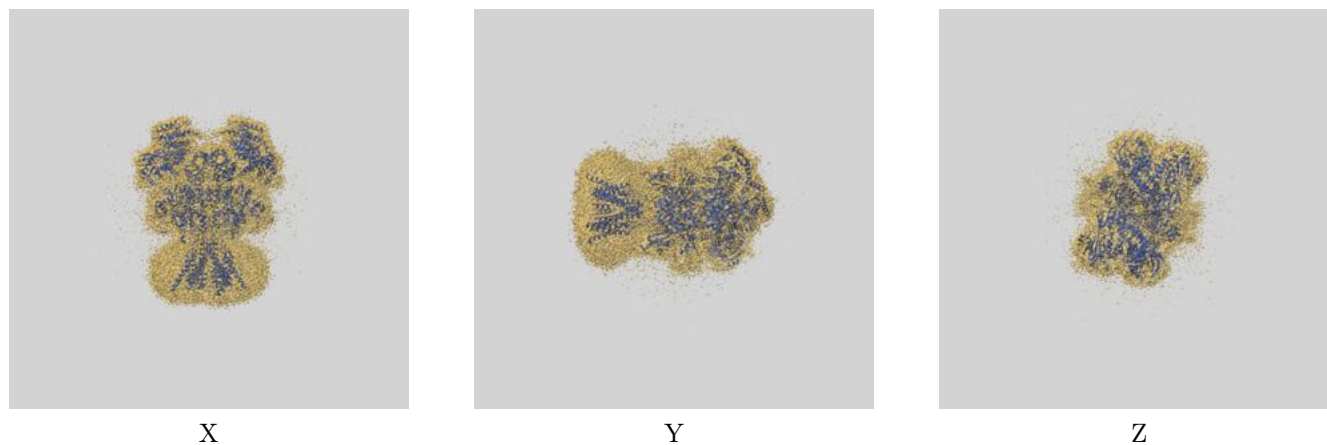
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.50	3.94	3.54

*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 3.50 differs from the reported value 3.13 by more than 10 %

9 Map-model fit [i](#)

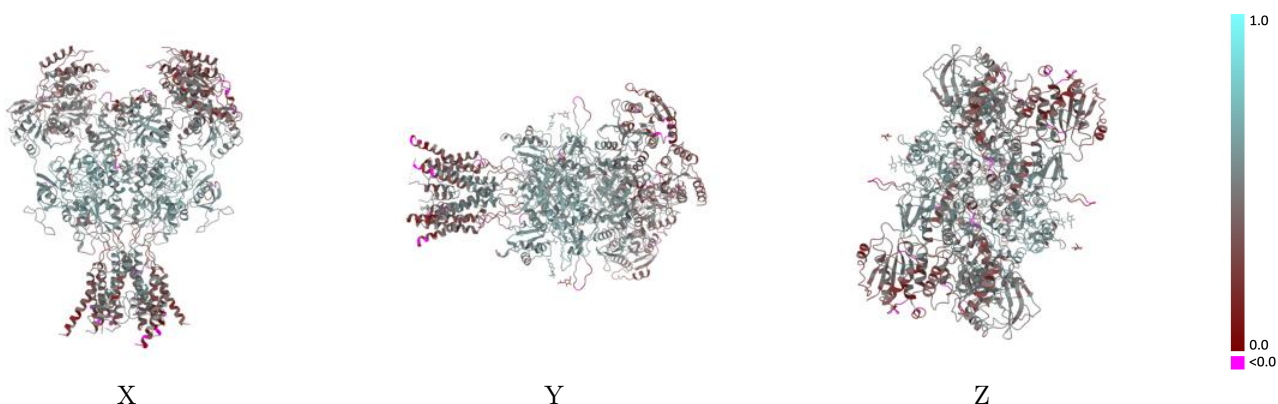
This section contains information regarding the fit between EMDB map EMD-43780 and PDB model 9ARF. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0704 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](#)

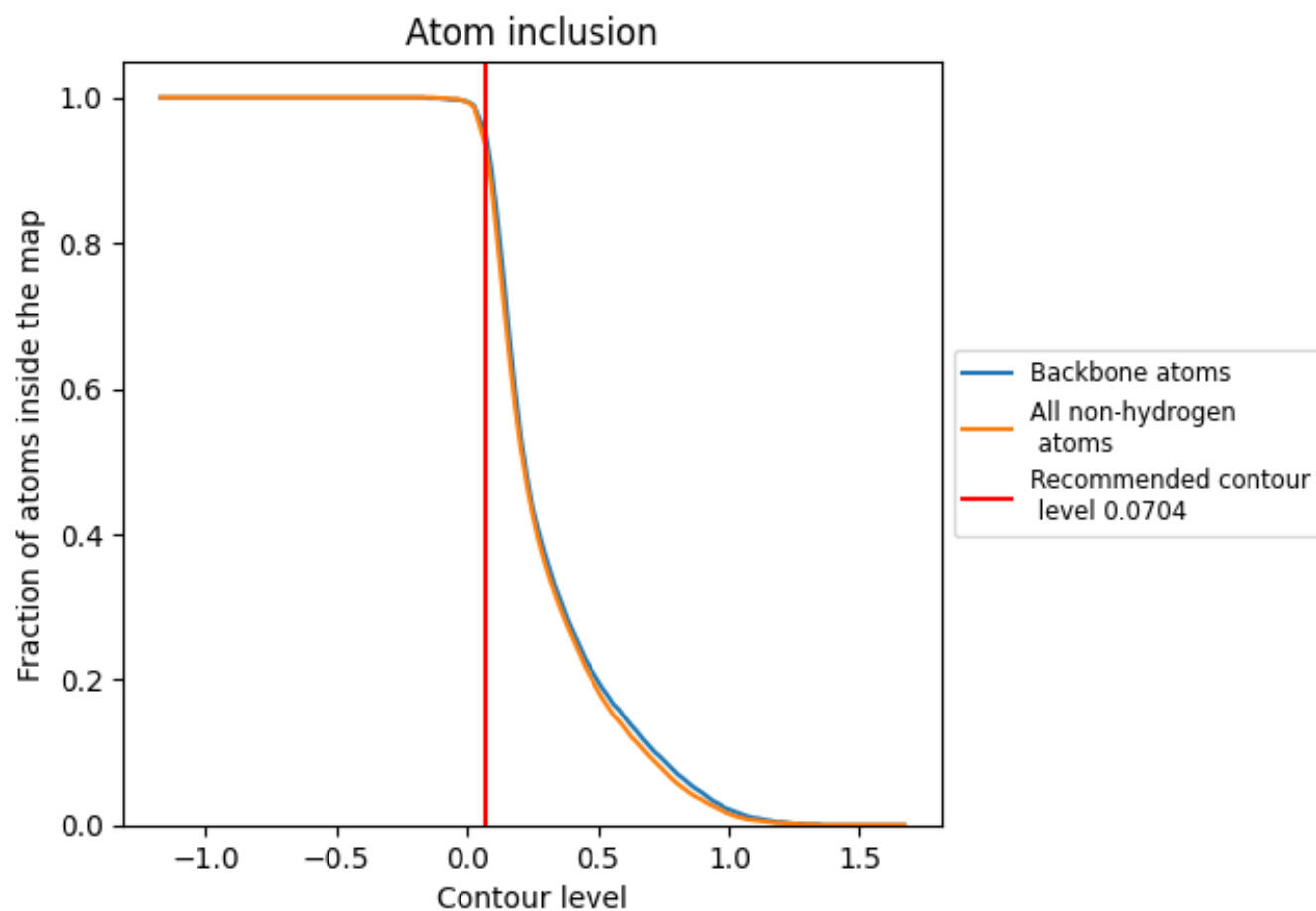


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.0704) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9350	0.4730
A	0.9440	0.4820
B	0.9260	0.4630
C	0.9440	0.4820
D	0.9270	0.4620
E	1.0000	0.5540
F	1.0000	0.5520

1.0

0.0

<0.0