



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:14 PM UTC

PDB ID : 7SAA / pdb_00007saa
EMDB ID : EMD-24946
Title : Glycine and glutamate bound GluN1a-GluN2B NMDA receptors in non-active
1 conformation at 2.97 Angstrom resolution
Authors : Chou, T.-H.; Furukawa, H.
Deposited on : 2021-09-22
Resolution : 2.97 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

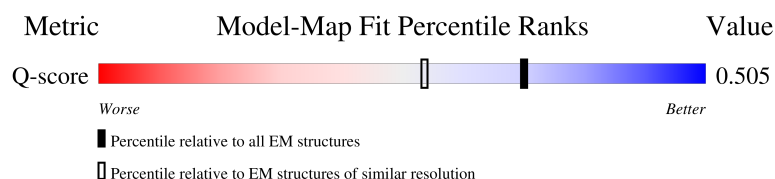
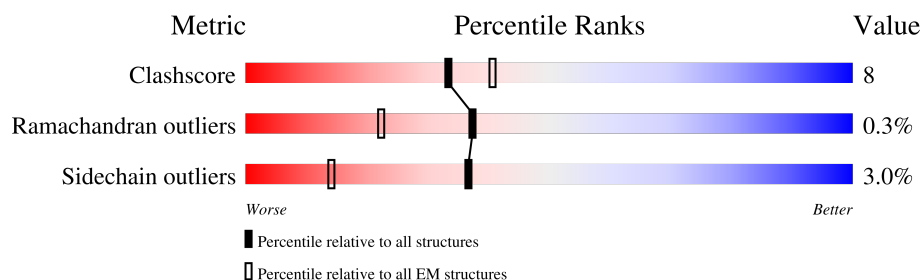
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.97 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	13205 (2.47 - 3.47)

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	 50% 100%
3	G	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23618 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	795	Total	C	N	O	S	0	0
			5937	3789	1011	1106	31		
1	C	795	Total	C	N	O	S	0	0
			5910	3772	1002	1106	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	C	N	O	S	0	0
			5807	3742	947	1084	34		
2	D	785	Total	C	N	O	S	0	0
			5738	3699	935	1071	33		

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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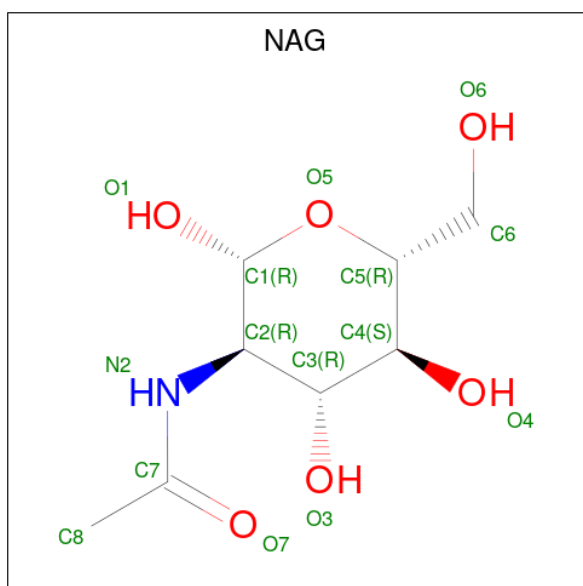
Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	ALA	-	expression tag	UNP Q00960
D	-10	THR	-	expression tag	UNP Q00960
D	-9	GLY	-	expression tag	UNP Q00960
D	-8	TRP	-	expression tag	UNP Q00960
D	-7	SER	-	expression tag	UNP Q00960
D	-6	HIS	-	expression tag	UNP Q00960
D	-5	PRO	-	expression tag	UNP 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		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



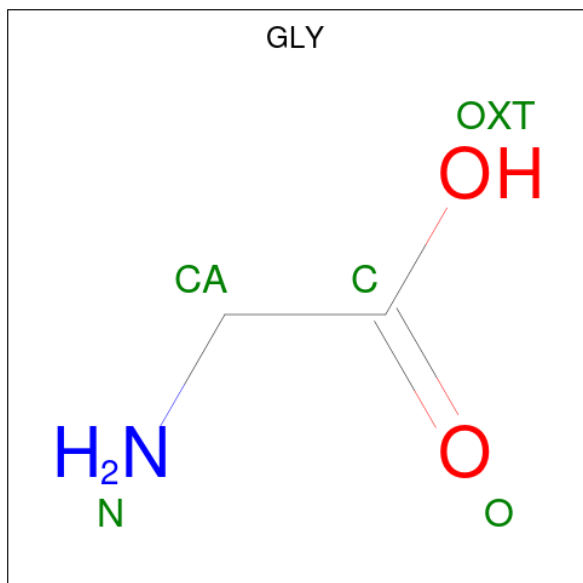
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

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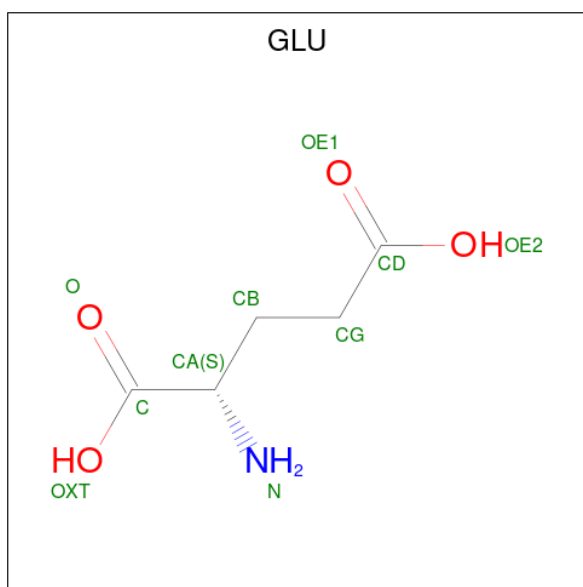
Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$) (labeled as "Ligand of Interest" by depositor).

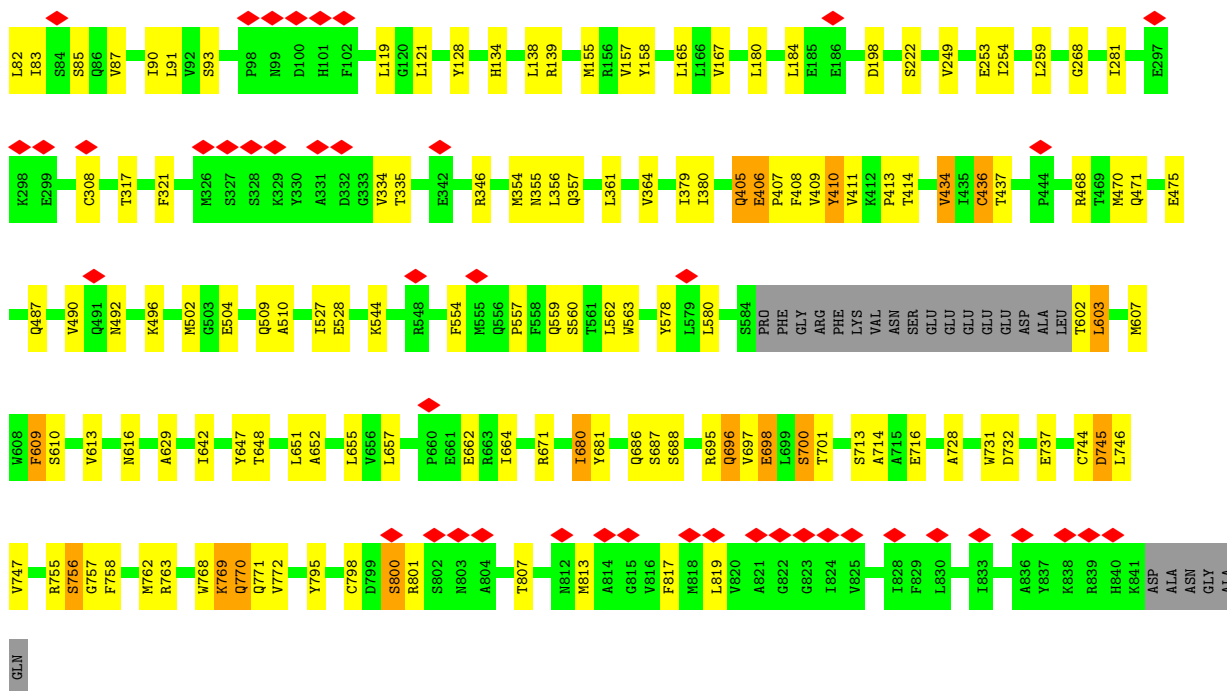


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			5	2	1	2	
5	C	1	Total	C	N	O	0
			5	2	1	2	

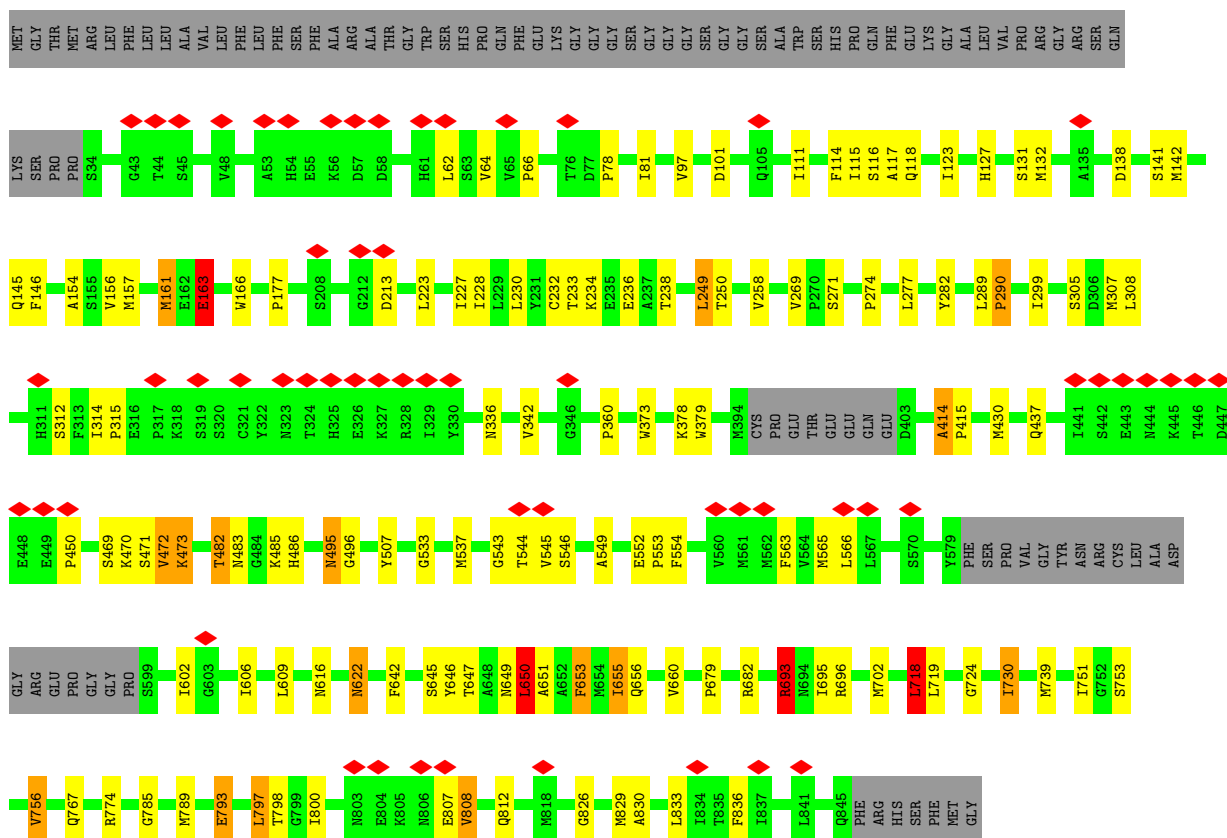
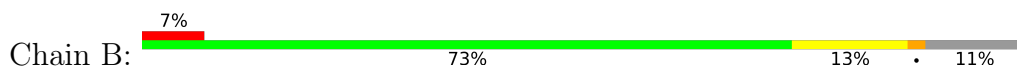
- Molecule 6 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



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

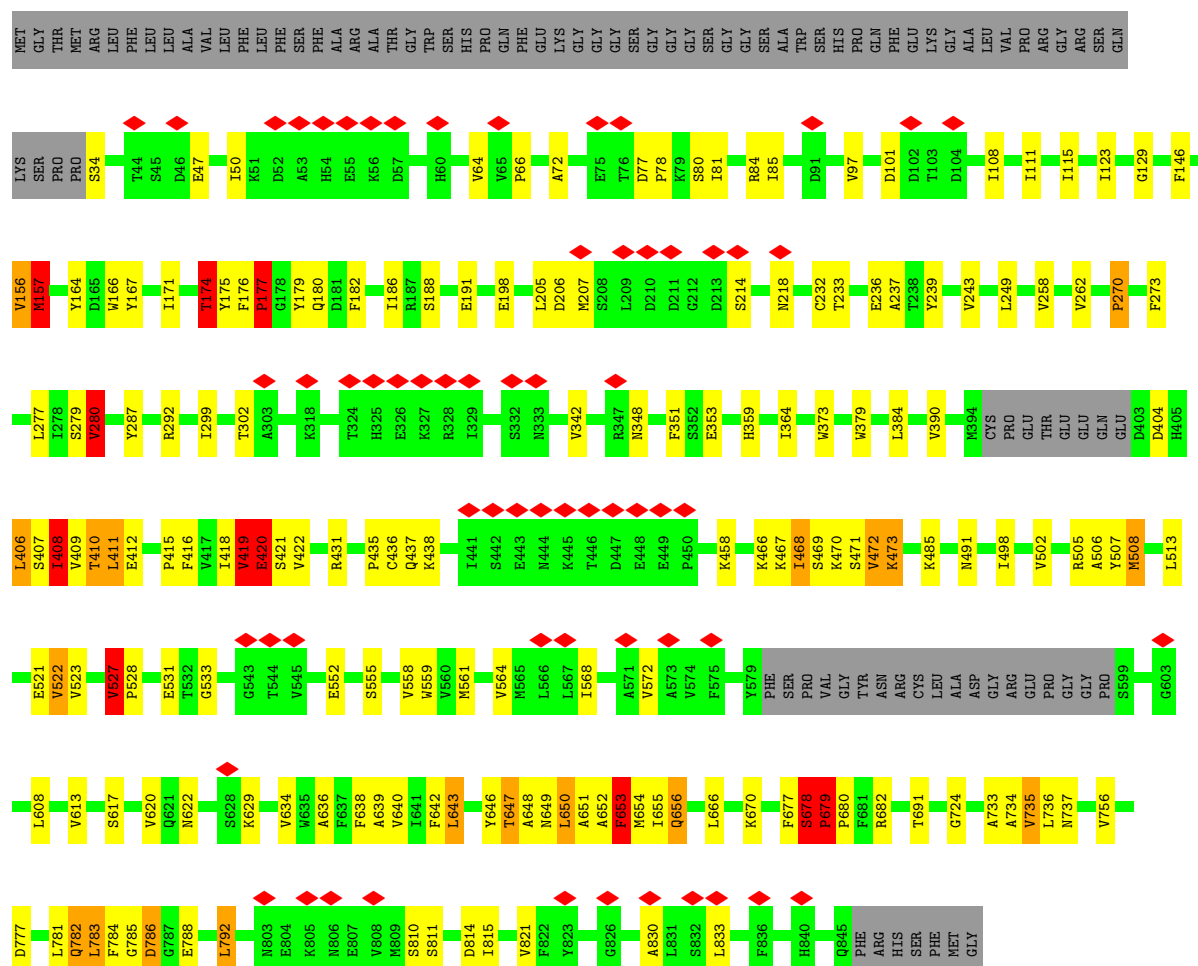


- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain D:  7% 69% 17% 11%

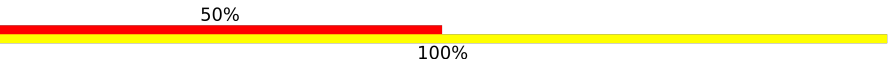


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



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

Chain F:  50% 100%



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

Chain G:

100%

3AG1
3AG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	378892	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	25.478	Depositor
Minimum map value	-13.869	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.620	Depositor
Recommended contour level	2.36	Depositor
Map size ($\text{\AA}$)	342.4, 342.4, 342.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.856, 0.856, 0.856	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.75	34/6063 (0.6%)	0.77	32/8263 (0.4%)
1	C	0.82	39/6034 (0.6%)	0.73	19/8229 (0.2%)
2	B	0.73	29/5928 (0.5%)	0.77	17/8082 (0.2%)
2	D	0.95	56/5857 (1.0%)	0.80	30/7996 (0.4%)
All	All	0.82	158/23882 (0.7%)	0.77	98/32570 (0.3%)

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	D	0	2
All	All	0	4

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	406	GLU	C-O	-15.01	1.10	1.24
1	C	405	GLN	C-O	-14.67	1.07	1.23
2	D	736	LEU	C-O	-12.95	1.08	1.24
2	B	437	GLN	C-O	-12.79	1.07	1.23
2	D	408	ILE	C-O	-12.67	1.11	1.24
1	C	757	GLY	C-O	-12.05	1.11	1.23
1	C	409	VAL	C-O	-11.91	1.12	1.24
1	C	410	TYR	C-O	-11.76	1.09	1.24
1	C	771	GLN	C-O	-11.66	1.10	1.24
2	D	438	LYS	C-O	-11.51	1.08	1.23
1	C	407	PRO	C-O	-11.43	1.10	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	695	ILE	C-O	-11.02	1.11	1.24
2	D	508	MET	C-O	-10.67	1.10	1.23
1	A	689	VAL	C-O	-10.32	1.11	1.24
2	D	782	GLN	C-O	-10.16	1.12	1.24
2	D	469	SER	C-O	-10.03	1.12	1.24
2	D	792	LEU	C-O	-9.88	1.12	1.24
1	A	531	LYS	C-O	-9.59	1.11	1.23
1	C	408	PHE	C-O	-9.58	1.12	1.24
1	A	691	ILE	C-O	-9.54	1.13	1.24
1	A	756	SER	C-O	9.43	1.36	1.24
2	D	781	LEU	C-O	-9.42	1.12	1.24
2	D	734	ALA	C-O	-9.24	1.13	1.24
1	C	758	PHE	C-O	-9.09	1.12	1.24
2	D	468	ILE	C-O	-9.05	1.13	1.24
2	D	523	VAL	C-O	-9.02	1.12	1.23
2	D	735	VAL	C-O	-9.02	1.12	1.24
2	B	774	ARG	C-O	-8.96	1.13	1.24
2	B	485	LYS	C-O	-8.95	1.12	1.24
1	C	737	GLU	C-O	-8.92	1.12	1.24
1	C	437	THR	C-O	-8.73	1.13	1.23
2	D	466	LYS	C-O	-8.52	1.14	1.24
1	C	687	SER	C-O	-8.47	1.14	1.24
2	D	650	LEU	C-O	-8.42	1.14	1.24
1	C	475	GLU	C-O	-8.41	1.14	1.23
1	A	486	THR	C-O	-8.40	1.13	1.23
2	D	418	ILE	C-O	-8.38	1.14	1.24
2	B	693	ARG	C-O	-8.29	1.14	1.24
2	D	531	GLU	C-O	-8.29	1.14	1.23
2	D	784	PHE	C-O	-8.27	1.14	1.24
1	A	690	ASP	C-O	-8.21	1.14	1.24
2	D	513	LEU	C-O	-8.19	1.14	1.24
2	D	783	LEU	C-O	-8.14	1.14	1.24
1	C	713	SER	C-O	-8.04	1.13	1.23
1	A	703	TYR	C-O	-7.96	1.15	1.24
2	D	651	ALA	C-O	-7.95	1.14	1.24
2	D	410	THR	C-O	-7.90	1.14	1.23
2	D	647	THR	C-O	-7.89	1.14	1.24
1	C	714	ALA	C-O	-7.86	1.13	1.24
2	B	486	HIS	C-O	-7.76	1.15	1.24
2	D	470	LYS	C-O	-7.76	1.14	1.24
2	D	522	VAL	C-O	-7.72	1.14	1.24
1	C	747	VAL	C-O	-7.70	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	646	TYR	C-O	-7.70	1.15	1.24
1	C	436	CYS	C-O	-7.60	1.15	1.24
1	A	144	TYR	C-O	-7.58	1.15	1.24
2	B	469	SER	CA-CB	-7.47	1.41	1.53
1	C	405	GLN	CD-NE2	-7.45	1.17	1.33
1	A	694	ARG	C-O	-7.42	1.14	1.24
1	C	413	PRO	C-O	-7.40	1.15	1.23
2	D	167	TYR	C-O	-7.39	1.14	1.24
1	C	768	TRP	C-O	-7.35	1.13	1.23
2	D	471	SER	CA-CB	-7.35	1.44	1.54
1	A	475	GLU	C-O	-7.35	1.15	1.23
2	B	702	MET	C-O	-7.35	1.14	1.24
2	D	406	LEU	C-O	-7.25	1.14	1.23
2	D	411	LEU	C-O	-7.22	1.14	1.23
2	B	483	ASN	C-O	-7.21	1.15	1.24
2	D	527	VAL	C-O	-7.20	1.15	1.24
1	C	770	GLN	C-O	-7.18	1.15	1.24
1	A	705	HIS	C-O	-7.13	1.15	1.24
1	A	741	SER	C-O	-7.08	1.14	1.24
1	A	706	MET	C-O	-7.03	1.16	1.24
1	A	473	THR	C-O	-7.03	1.14	1.23
1	A	704	ARG	C-O	-7.01	1.16	1.24
2	B	651	ALA	C-O	-7.00	1.15	1.24
1	A	710	ASN	C-O	-6.98	1.15	1.23
1	C	434	VAL	C-O	-6.95	1.16	1.23
2	D	786	ASP	C-O	-6.84	1.15	1.24
1	C	405	GLN	CA-C	-6.75	1.44	1.52
2	D	643	LEU	C-O	-6.73	1.16	1.24
1	A	648	THR	C-O	-6.73	1.16	1.24
2	D	648	ALA	C-O	-6.73	1.16	1.24
2	B	496	GLY	C-O	-6.69	1.12	1.23
1	A	695	ARG	C-O	-6.63	1.14	1.24
2	D	157	MET	C-O	-6.62	1.16	1.24
1	A	647	TYR	C-O	-6.61	1.16	1.24
2	D	652	ALA	C-O	-6.60	1.16	1.24
2	D	654	MET	C-O	-6.52	1.15	1.24
2	B	161	MET	C-O	-6.50	1.15	1.24
1	A	757	GLY	C-O	-6.49	1.15	1.23
2	D	280	VAL	C-O	-6.48	1.17	1.24
1	C	755	ARG	C-O	-6.42	1.15	1.23
2	D	409	VAL	C-O	-6.41	1.16	1.24
1	C	686	GLN	C-O	-6.39	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	VAL	C-O	-6.35	1.16	1.23
1	A	688	SER	CA-CB	-6.29	1.42	1.53
2	D	467	LYS	C-O	-6.28	1.16	1.24
2	D	647	THR	CA-C	-6.24	1.44	1.52
2	D	458	LYS	C-O	-6.24	1.16	1.23
2	D	420	GLU	C-O	-6.21	1.16	1.23
2	B	793	GLU	C-O	-6.19	1.16	1.24
2	B	730	ILE	C-O	-6.19	1.17	1.24
1	C	746	LEU	C-O	-6.18	1.16	1.23
1	C	688	SER	CA-CB	-6.18	1.42	1.53
2	B	470	LYS	C-O	-6.15	1.17	1.24
1	C	680	ILE	C-O	-6.14	1.17	1.24
2	B	756	VAL	C-O	-6.11	1.17	1.23
2	B	469	SER	C-O	-6.09	1.16	1.24
1	A	194	VAL	C-O	-6.06	1.17	1.24
1	C	609	PHE	C-O	-6.03	1.17	1.24
1	A	699	LEU	C-O	-6.02	1.16	1.24
2	B	471	SER	CA-CB	-6.02	1.43	1.53
1	C	700	SER	C-O	-6.00	1.17	1.24
1	C	652	ALA	C-O	-5.98	1.17	1.24
1	C	405	GLN	CD-OE1	-5.97	1.12	1.23
2	D	653	PHE	C-O	-5.96	1.17	1.24
2	D	469	SER	CA-CB	-5.92	1.44	1.53
2	B	718	LEU	C-O	-5.83	1.16	1.24
2	D	785	GLY	C-O	-5.81	1.17	1.23
1	C	648	THR	C-O	-5.81	1.17	1.24
1	A	741	SER	CA-CB	-5.80	1.43	1.53
2	D	506	ALA	C-O	-5.80	1.16	1.23
1	C	716	GLU	C-O	-5.78	1.17	1.24
2	D	521	GLU	C-O	-5.66	1.16	1.23
1	C	411	VAL	C-O	-5.65	1.18	1.24
1	C	687	SER	CA-CB	-5.62	1.46	1.53
2	B	378	LYS	C-O	-5.60	1.17	1.23
2	B	473	LYS	C-O	-5.59	1.17	1.24
2	D	437	GLN	C-O	-5.58	1.17	1.23
1	C	769	LYS	C-O	-5.54	1.17	1.24
1	A	646	SER	CA-CB	-5.53	1.44	1.53
1	A	605	SER	C-O	-5.53	1.17	1.24
1	A	688	SER	C-O	-5.50	1.17	1.24
2	D	642	PHE	C-O	-5.50	1.17	1.24
1	A	692	TYR	C-O	-5.47	1.17	1.24
1	A	709	HIS	C-O	-5.46	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	471	SER	C-O	-5.43	1.17	1.24
1	A	142	PRO	C-O	-5.36	1.18	1.24
2	B	797	LEU	C-O	-5.34	1.16	1.24
2	D	507	TYR	C-O	-5.29	1.16	1.23
2	D	649	ASN	CA-C	-5.27	1.46	1.52
2	B	800	ILE	C-O	-5.25	1.18	1.24
2	D	437	GLN	CA-C	-5.24	1.46	1.52
2	B	696	ARG	C-O	-5.22	1.18	1.24
1	C	713	SER	CA-CB	-5.22	1.44	1.53
2	B	647	THR	C-O	-5.19	1.18	1.24
2	D	646	TYR	CA-C	-5.17	1.46	1.52
2	D	419	VAL	C-O	-5.16	1.18	1.24
1	A	707	GLU	C-O	-5.13	1.17	1.24
1	A	645	ALA	C-O	-5.13	1.18	1.24
2	B	495	ASN	C-O	-5.11	1.16	1.23
2	D	505	ARG	C-O	-5.11	1.17	1.24
1	A	608	TRP	C-O	-5.10	1.18	1.24
2	B	163	GLU	C-O	-5.10	1.18	1.24
2	D	473	LYS	C-O	-5.08	1.17	1.24
1	C	756	SER	CA-CB	-5.06	1.45	1.53
2	B	645	SER	CA-CB	-5.02	1.45	1.53

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	406	GLU	N-CA-C	14.46	133.70	113.16
2	B	495	ASN	CB-CA-C	-13.73	83.48	111.22
1	A	690	ASP	CB-CA-C	-13.08	88.62	110.85
1	C	406	GLU	CA-C-O	-12.07	106.63	118.34
1	A	743	LYS	CA-C-N	10.70	135.03	120.38
1	A	743	LYS	C-N-CA	10.70	135.03	120.38
1	C	769	LYS	CB-CA-C	-10.51	94.39	110.88
1	A	755	ARG	CB-CG-CD	-9.91	88.50	111.30
2	D	177	PRO	N-CA-C	9.00	128.36	113.78
2	B	798	THR	CB-CA-C	-8.48	93.86	109.46
2	D	678	SER	CA-C-N	8.36	128.99	120.38
2	D	678	SER	C-N-CA	8.36	128.99	120.38
2	B	437	GLN	CB-CA-C	-8.00	96.59	109.80
1	C	648	THR	CB-CA-C	-7.89	97.44	110.85
1	C	408	PHE	N-CA-C	7.68	119.73	111.36
1	A	610	SER	N-CA-CB	7.63	121.46	110.16
1	C	407	PRO	CA-C-N	7.50	130.94	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	407	PRO	C-N-CA	7.50	130.94	120.29
2	B	800	ILE	N-CA-C	7.49	117.57	110.53
2	D	678	SER	CA-C-O	-7.43	112.70	120.87
2	D	437	GLN	CB-CA-C	-7.34	97.15	109.48
1	C	771	GLN	CB-CG-CD	-7.25	100.28	112.60
2	D	679	PRO	CA-N-CD	-7.21	101.91	112.00
1	C	475	GLU	CB-CG-CD	-7.18	100.40	112.60
1	C	696	GLN	CA-C-N	7.17	133.31	121.54
1	C	696	GLN	C-N-CA	7.17	133.31	121.54
1	A	473	THR	CB-CA-C	7.16	123.43	109.33
1	A	806	ALA	N-CA-C	7.07	120.42	108.90
2	B	793	GLU	CB-CA-C	-7.04	98.89	110.85
1	C	755	ARG	CB-CG-CD	-6.97	95.26	111.30
2	D	191	GLU	CB-CA-C	-6.95	99.04	110.85
1	A	757	GLY	CA-C-N	6.82	132.40	123.00
1	A	757	GLY	C-N-CA	6.82	132.40	123.00
1	A	742	GLN	CB-CG-CD	-6.69	101.23	112.60
2	B	800	ILE	CB-CA-C	-6.68	103.27	112.02
2	D	638	PHE	CB-CA-C	-6.67	100.41	110.88
1	A	756	SER	CA-C-N	6.63	129.65	121.83
1	A	756	SER	C-N-CA	6.63	129.65	121.83
1	A	608	TRP	CB-CA-C	-6.46	100.07	110.79
2	D	467	LYS	CB-CA-C	-6.43	100.11	110.79
1	C	603	LEU	N-CA-C	6.33	120.61	113.01
1	C	408	PHE	CA-C-O	-6.30	113.75	120.42
2	B	774	ARG	CG-CD-NE	-6.29	98.16	112.00
1	C	800	SER	CA-C-N	6.25	133.49	121.54
1	C	800	SER	C-N-CA	6.25	133.49	121.54
2	B	696	ARG	CG-CD-NE	-6.23	98.30	112.00
1	A	705	HIS	CA-C-N	6.12	128.39	120.44
1	A	705	HIS	C-N-CA	6.12	128.39	120.44
2	B	650	LEU	N-CA-C	-6.03	104.71	111.28
1	A	742	GLN	CB-CA-C	-6.02	99.39	109.27
2	B	482	THR	CA-C-N	-5.97	114.76	123.00
2	B	482	THR	C-N-CA	-5.97	114.76	123.00
2	D	642	PHE	CB-CA-C	-5.89	101.64	110.88
2	B	470	LYS	CB-CA-C	-5.81	101.76	110.88
1	C	410	TYR	CA-C-O	-5.80	114.09	120.36
2	D	421	SER	CA-C-N	5.73	129.39	120.34
2	D	421	SER	C-N-CA	5.73	129.39	120.34
1	A	531	LYS	CA-C-N	5.71	125.47	119.76
1	A	531	LYS	C-N-CA	5.71	125.47	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	GLU	CB-CG-CD	-5.67	102.95	112.60
1	A	150	VAL	N-CA-C	-5.67	104.98	110.42
1	A	610	SER	N-CA-C	5.67	117.54	111.36
1	C	406	GLU	CB-CA-C	-5.62	101.32	112.05
2	D	435	PRO	N-CA-C	5.61	119.27	110.80
2	D	174	THR	CA-CB-OG1	-5.59	101.22	109.60
2	D	531	GLU	CB-CA-C	5.58	118.86	109.48
2	B	378	LYS	CB-CA-C	-5.55	98.37	109.35
1	A	609	PHE	CA-C-N	-5.50	112.47	120.29
1	A	609	PHE	C-N-CA	-5.50	112.47	120.29
2	D	527	VAL	CA-C-N	5.50	125.41	119.85
2	D	527	VAL	C-N-CA	5.50	125.41	119.85
2	B	471	SER	N-CA-C	5.48	117.33	111.36
1	A	696	GLN	CB-CA-C	-5.47	100.26	109.72
1	A	695	ARG	CB-CG-CD	5.43	123.80	111.30
2	B	653	PHE	CB-CA-C	-5.36	102.46	110.88
2	D	420	GLU	CB-CA-C	-5.29	99.08	110.45
2	D	270	PRO	CA-N-CD	-5.27	104.63	112.00
2	D	786	ASP	CB-CA-C	-5.26	100.56	110.67
2	B	739	MET	CB-CA-C	-5.25	102.07	110.79
2	B	696	ARG	CA-C-O	-5.24	115.00	120.55
1	A	648	THR	CB-CA-C	-5.22	102.12	110.79
1	A	755	ARG	CG-CD-NE	-5.21	100.53	112.00
2	D	156	VAL	CA-C-N	5.20	127.68	120.29
2	D	156	VAL	C-N-CA	5.20	127.68	120.29
2	D	472	VAL	N-CA-C	-5.17	107.72	112.83
2	D	410	THR	CA-CB-CG2	5.14	119.24	110.50
2	D	680	PRO	CA-C-N	5.14	128.15	120.90
2	D	680	PRO	C-N-CA	5.14	128.15	120.90
2	D	679	PRO	N-CD-CG	-5.14	95.49	103.20
1	A	486	THR	N-CA-CB	5.14	119.68	111.56
2	D	638	PHE	N-CA-C	-5.11	105.60	111.07
2	D	177	PRO	CB-CA-C	-5.10	104.58	113.20
1	A	531	LYS	O-C-N	-5.10	115.72	121.43
1	C	737	GLU	CB-CA-C	5.10	120.46	110.67
1	A	696	GLN	CA-C-O	-5.09	114.83	120.38
2	D	420	GLU	CB-CG-CD	-5.08	103.96	112.60
1	A	757	GLY	CA-C-O	-5.06	115.37	122.36
1	A	650	ASN	CB-CA-C	-5.02	102.96	110.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	706	MET	Mainchain
1	C	405	GLN	Mainchain
2	D	678	SER	Mainchain
2	D	783	LEU	Mainchain

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	5937	0	5691	106	0
1	C	5910	0	5640	91	0
2	B	5807	0	5536	105	0
2	D	5738	0	5415	111	0
3	E	28	0	25	0	0
3	F	28	0	25	1	0
3	G	28	0	25	0	0
4	A	42	0	39	0	0
4	B	14	0	13	0	0
4	C	28	0	26	0	0
4	D	28	0	26	1	0
5	A	5	0	2	0	0
5	C	5	0	2	0	0
6	B	10	0	5	0	0
6	D	10	0	5	1	0
All	All	23618	0	22475	382	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 (382) 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:B:544:THR:HG22	2:B:808:VAL:CG2	1.16	1.56
1:C:554:PHE:HE2	1:C:819:LEU:CD1	1.16	1.55
1:C:554:PHE:CE2	1:C:819:LEU:CD1	2.01	1.43
2:D:552:GLU:CB	2:D:653:PHE:HE2	1.37	1.38
2:B:544:THR:CG2	2:B:808:VAL:CG2	2.05	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:744:CYS:SG	1:C:798:CYS:SG	1.42	1.34
2:D:552:GLU:CB	2:D:653:PHE:CE2	2.11	1.34
1:C:554:PHE:CE2	1:C:819:LEU:HD11	1.58	1.30
1:A:115:ARG:NH2	1:A:135:LEU:HD13	1.46	1.28
1:A:115:ARG:NH2	1:A:135:LEU:CD1	2.01	1.23
1:A:695:ARG:NH2	2:D:782:GLN:OE1	1.72	1.21
1:A:610:SER:OG	1:A:636:TRP:NE1	1.74	1.20
2:B:544:THR:CG2	2:B:808:VAL:HG23	1.71	1.17
2:B:544:THR:CG2	2:B:808:VAL:HG21	1.71	1.12
2:B:544:THR:HG22	2:B:808:VAL:HG23	1.20	1.08
1:A:115:ARG:HH22	1:A:135:LEU:CD1	1.65	1.07
2:D:176:PHE:CD1	2:D:177:PRO:HD2	1.91	1.05
1:C:578:TYR:CB	1:C:603:LEU:HD21	1.87	1.03
2:B:789:MET:O	2:B:793:GLU:HG2	1.62	0.98
1:C:554:PHE:CE2	1:C:819:LEU:HD12	1.99	0.97
2:B:693:ARG:HB2	2:B:693:ARG:NH2	1.80	0.97
1:C:744:CYS:SG	1:C:798:CYS:CB	2.53	0.96
1:C:544:LYS:HB2	1:C:745:ASP:O	1.66	0.95
1:A:115:ARG:HH21	1:A:135:LEU:HD13	1.32	0.93
2:B:693:ARG:HB2	2:B:693:ARG:HH21	1.33	0.92
2:D:176:PHE:CD1	2:D:177:PRO:CD	2.53	0.90
1:C:554:PHE:HE2	1:C:819:LEU:HD11	0.75	0.90
2:B:250:THR:CG2	2:B:274:PRO:HB3	2.03	0.89
2:D:176:PHE:CG	2:D:177:PRO:HD2	2.07	0.89
2:D:656:GLN:HE21	2:D:656:GLN:HA	1.36	0.89
1:C:745:ASP:OD1	1:C:745:ASP:N	2.06	0.85
1:A:745:ASP:OD1	1:A:745:ASP:N	2.09	0.83
1:A:656:VAL:CG2	2:B:655:ILE:HD11	2.09	0.83
1:A:657:LEU:HD22	2:B:807:GLU:CB	2.09	0.83
1:A:115:ARG:NH2	1:A:135:LEU:HD12	1.92	0.82
2:D:650:LEU:HD12	2:D:650:LEU:O	1.79	0.82
2:B:552:GLU:CB	2:B:653:PHE:CE2	2.63	0.81
2:B:250:THR:HG22	2:B:274:PRO:HB3	1.59	0.81
1:C:554:PHE:CZ	1:C:819:LEU:HD12	2.17	0.79
1:A:556:GLN:HA	1:A:556:GLN:HE21	1.47	0.79
2:B:544:THR:HG22	2:B:808:VAL:HG21	0.79	0.79
2:B:250:THR:HG23	2:B:274:PRO:CG	2.12	0.78
1:A:610:SER:OG	1:A:636:TRP:CE2	2.36	0.77
2:B:250:THR:CG2	2:B:274:PRO:HG3	2.13	0.77
2:B:250:THR:CG2	2:B:274:PRO:CG	2.62	0.77
1:C:554:PHE:CZ	1:C:819:LEU:CD1	2.68	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:LEU:HD11	2:D:634:VAL:CG2	2.14	0.77
1:C:406:GLU:OE2	1:C:410:TYR:CE2	2.37	0.77
1:C:698:GLU:O	1:C:698:GLU:HG2	1.85	0.76
1:C:554:PHE:CE2	1:C:819:LEU:HD13	2.20	0.76
2:D:527:VAL:HG13	2:D:777:ASP:HB2	1.66	0.76
1:C:528:GLU:HG2	1:C:769:LYS:HD2	1.66	0.76
2:B:250:THR:HG21	2:B:274:PRO:HG3	1.66	0.75
2:D:174:THR:HB	2:D:232:CYS:SG	2.27	0.75
2:B:552:GLU:CB	2:B:653:PHE:HE2	1.98	0.74
1:A:656:VAL:HG21	2:B:655:ILE:HD11	1.69	0.74
2:B:142:MET:HE1	2:B:336:ASN:HB2	1.67	0.74
2:D:179:TYR:CD2	2:D:180:GLN:N	2.55	0.74
1:A:610:SER:HG	1:A:636:TRP:NE1	1.83	0.74
2:B:543:GLY:O	2:B:808:VAL:HG11	1.88	0.74
1:A:153:GLU:HA	1:A:153:GLU:OE1	1.88	0.73
2:D:299:ILE:HG22	2:D:342:VAL:HG11	1.70	0.73
1:A:578:TYR:CB	1:A:603:LEU:CD2	2.67	0.73
1:A:819:LEU:HD12	1:A:819:LEU:C	2.14	0.73
1:A:608:TRP:CE3	1:A:608:TRP:HA	2.22	0.72
1:A:695:ARG:O	1:A:695:ARG:HG2	1.87	0.72
1:C:544:LYS:CB	1:C:745:ASP:O	2.36	0.72
2:D:179:TYR:CG	2:D:180:GLN:N	2.58	0.72
2:B:544:THR:HG21	2:B:808:VAL:HG23	1.69	0.71
2:B:250:THR:CG2	2:B:274:PRO:CB	2.68	0.71
2:B:163:GLU:OE2	2:B:163:GLU:HA	1.91	0.71
2:B:249:LEU:HD12	2:B:249:LEU:O	1.91	0.70
1:C:662:GLU:HB3	1:C:671:ARG:HH22	1.56	0.70
2:B:289:LEU:C	2:B:289:LEU:HD23	2.16	0.70
1:C:762:MET:HE1	1:C:769:LYS:HA	1.73	0.69
2:D:176:PHE:CE1	2:D:177:PRO:HD2	2.28	0.68
1:A:608:TRP:HA	1:A:608:TRP:HE3	1.58	0.68
1:A:425:THR:OG1	1:A:429:ASP:OD1	2.12	0.68
2:D:412:GLU:HG3	2:D:419:VAL:HG13	1.75	0.68
1:A:739:GLU:OE1	1:A:743:LYS:NZ	2.27	0.68
2:B:785:GLY:O	1:C:695:ARG:NH2	2.27	0.67
1:A:578:TYR:CB	1:A:603:LEU:HD21	2.24	0.67
1:A:125:MET:O	1:A:139:ARG:NH2	2.26	0.67
1:C:128:TYR:HB2	1:C:139:ARG:HH21	1.60	0.66
1:A:167:VAL:HG12	1:A:222:SER:HB3	1.78	0.66
1:A:71:ALA:HB1	1:A:106:PRO:HG3	1.77	0.66
2:B:289:LEU:HD23	2:B:289:LEU:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:656:GLN:HE21	2:D:656:GLN:CA	2.00	0.66
2:D:643:LEU:O	2:D:643:LEU:HD12	1.95	0.65
1:A:578:TYR:CB	1:A:603:LEU:HD22	2.26	0.65
1:C:502:MET:HE1	1:C:527:ILE:HG12	1.78	0.65
2:B:546:SER:HB3	2:B:549:ALA:HB2	1.78	0.65
2:D:175:TYR:CD2	2:D:206:ASP:HA	2.32	0.65
2:D:552:GLU:CB	2:D:653:PHE:CD2	2.76	0.65
1:A:354:MET:HE3	1:A:361:LEU:HB3	1.79	0.65
2:B:554:PHE:HE2	2:B:642:PHE:CE1	2.14	0.65
2:B:64:VAL:HG23	2:B:66:PRO:HD3	1.79	0.64
1:C:28:ASN:ND2	1:C:85:SER:O	2.29	0.64
2:D:407:SER:C	2:D:408:ILE:HG12	2.21	0.64
1:A:556:GLN:HB2	1:A:557:PRO:HD3	1.79	0.64
1:C:30:GLY:H	1:C:87:VAL:HG13	1.62	0.64
1:C:354:MET:HE2	1:C:361:LEU:HB3	1.79	0.64
2:D:72:ALA:O	2:D:84:ARG:NH2	2.31	0.64
1:A:177:GLN:O	1:A:181:GLU:HG3	1.98	0.64
1:C:554:PHE:HE2	1:C:819:LEU:HD13	1.45	0.64
2:D:412:GLU:HG3	2:D:419:VAL:CG1	2.28	0.64
1:A:522:GLU:N	1:A:522:GLU:OE1	2.31	0.63
2:D:157:MET:CE	2:D:182:PHE:HZ	2.12	0.63
1:C:254:ILE:HD11	1:C:268:GLY:HA3	1.81	0.62
1:A:487:GLN:HG2	1:A:496:LYS:HG2	1.81	0.62
2:B:414:ALA:HB1	2:B:415:PRO:HD2	1.81	0.62
2:D:176:PHE:CD1	2:D:177:PRO:HD3	2.33	0.62
2:D:176:PHE:CG	2:D:177:PRO:CD	2.79	0.62
2:D:655:ILE:HG22	2:D:655:ILE:O	1.99	0.61
2:D:420:GLU:O	2:D:420:GLU:HG2	2.00	0.61
2:D:650:LEU:HD12	2:D:650:LEU:C	2.23	0.61
1:A:510:ALA:O	1:A:763:ARG:NH2	2.33	0.61
2:B:97:VAL:HB	2:B:123:ILE:HG22	1.81	0.61
1:C:259:LEU:HD11	1:C:361:LEU:HD11	1.83	0.60
2:D:101:ASP:OD1	2:D:129:GLY:N	2.32	0.60
1:A:559:GLN:NE2	2:B:812:GLN:OE1	2.35	0.60
2:B:649:ASN:OD1	1:C:655:LEU:HD13	2.01	0.60
2:D:407:SER:O	2:D:408:ILE:HG12	2.01	0.60
1:C:544:LYS:N	1:C:745:ASP:O	2.33	0.60
1:A:619:ILE:HD11	2:D:629:LYS:HG2	1.84	0.60
2:D:34:SER:N	2:D:64:VAL:O	2.35	0.60
2:D:157:MET:HE2	2:D:182:PHE:HZ	1.67	0.60
2:B:250:THR:HG23	2:B:274:PRO:CB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:616:ASN:ND2	1:C:616:ASN:O	2.35	0.59
2:B:655:ILE:HG22	2:B:656:GLN:HG3	1.84	0.59
1:C:364:VAL:HG11	1:C:379:ILE:HG13	1.82	0.59
2:D:78:PRO:HA	2:D:81:ILE:HD12	1.83	0.59
2:B:554:PHE:O	1:C:807:THR:CG2	2.50	0.59
2:B:622:ASN:H	2:B:622:ASN:ND2	2.00	0.59
2:D:678:SER:HB2	2:D:679:PRO:HD2	1.84	0.59
1:C:651:LEU:HD23	1:C:651:LEU:O	2.03	0.59
1:A:512:MET:HG3	1:A:762:MET:HE3	1.85	0.59
2:B:250:THR:HG22	2:B:250:THR:O	2.03	0.59
2:B:554:PHE:CE2	2:B:642:PHE:CE1	2.91	0.58
1:A:642:ILE:CD1	2:B:646:TYR:OH	2.51	0.58
2:B:138:ASP:HB3	2:B:141:SER:HB2	1.86	0.58
1:A:139:ARG:HB2	1:A:345:ASP:HA	1.86	0.58
1:C:167:VAL:HG12	1:C:222:SER:HB3	1.86	0.58
2:D:682:ARG:NH2	2:D:724:GLY:O	2.37	0.58
1:C:82:LEU:HD12	1:C:87:VAL:H	1.69	0.58
1:A:807:THR:OG1	2:D:552:GLU:O	2.23	0.57
2:B:826:GLY:HA2	2:B:829:MET:HE2	1.87	0.57
2:D:348:ASN:HD22	2:D:359:HIS:CD2	2.23	0.57
1:C:559:GLN:HB3	1:C:562:LEU:HD23	1.86	0.57
1:A:147:GLN:O	1:A:147:GLN:HG3	2.04	0.57
1:A:618:GLY:O	2:D:622:ASN:ND2	2.37	0.57
1:A:88:TYR:OH	1:A:303:ASP:OD1	2.23	0.56
2:D:77:ASP:O	2:D:80:SER:OG	2.23	0.56
2:B:553:PRO:O	2:B:554:PHE:HB2	2.04	0.56
1:C:487:GLN:HG2	1:C:496:LYS:HG2	1.86	0.56
2:D:175:TYR:CD2	2:D:205:LEU:O	2.59	0.56
2:D:558:VAL:HA	2:D:561:MET:HG2	1.87	0.56
2:B:223:LEU:HD23	2:B:228:ILE:HD12	1.86	0.56
2:B:650:LEU:HD23	2:B:650:LEU:O	2.06	0.56
1:C:157:VAL:HG13	1:C:158:TYR:HD1	1.70	0.55
1:C:762:MET:CE	1:C:769:LYS:HA	2.37	0.55
2:D:608:LEU:HA	2:D:620:VAL:HG11	1.88	0.55
1:A:313:ASN:OD1	1:A:314:ILE:N	2.40	0.55
1:A:559:GLN:HB2	2:B:812:GLN:HB3	1.88	0.55
1:A:101:HIS:O	1:A:128:TYR:OH	2.25	0.55
2:D:207:MET:HE1	2:D:236:GLU:HB3	1.88	0.55
1:C:334:VAL:HG13	1:C:335:THR:HG23	1.89	0.55
1:A:140:THR:O	1:A:346:ARG:NH1	2.39	0.55
1:A:647:TYR:CD1	1:A:647:TYR:C	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HG11	1:A:269:LEU:HD21	1.90	0.54
1:A:113:PHE:CD1	1:A:113:PHE:C	2.84	0.54
2:B:299:ILE:HG23	2:B:342:VAL:HG21	1.87	0.54
2:D:97:VAL:HB	2:D:123:ILE:HG12	1.90	0.54
2:D:64:VAL:HG23	2:D:66:PRO:HD3	1.89	0.54
1:C:651:LEU:HD23	1:C:651:LEU:C	2.33	0.54
2:D:233:THR:O	2:D:237:ALA:N	2.34	0.54
1:A:446:SER:HB2	1:A:447:PRO:HD3	1.90	0.54
2:D:670:LYS:HG2	2:D:677:PHE:CE2	2.43	0.54
2:B:277:LEU:HD23	2:B:373:TRP:HH2	1.74	0.53
2:B:793:GLU:OE1	2:B:797:LEU:HD12	2.08	0.53
1:C:32:VAL:N	1:C:91:LEU:O	2.36	0.53
2:D:179:TYR:CD2	2:D:179:TYR:C	2.85	0.53
1:C:609:PHE:CD1	1:C:609:PHE:C	2.85	0.53
1:A:93:SER:HB3	1:A:121:LEU:HD12	1.90	0.52
2:D:175:TYR:HD2	2:D:206:ASP:HA	1.75	0.52
1:C:165:LEU:HD22	1:C:180:LEU:HD23	1.90	0.52
2:B:111:ILE:O	2:B:115:ILE:HD12	2.10	0.52
2:D:78:PRO:HB3	2:D:111:ILE:HD13	1.91	0.52
2:D:636:ALA:O	2:D:640:VAL:HG23	2.10	0.52
1:A:809:THR:OG1	1:A:811:GLU:OE1	2.22	0.52
1:C:580:LEU:HG	1:C:629:ALA:HB2	1.90	0.52
2:B:269:VAL:HG12	2:B:271:SER:H	1.73	0.52
1:C:79:CYS:HA	1:C:82:LEU:HB3	1.91	0.51
2:D:647:THR:O	2:D:647:THR:HG22	2.10	0.51
1:A:707:GLU:O	1:A:707:GLU:HG3	2.08	0.51
1:A:656:VAL:CG2	2:B:655:ILE:CD1	2.87	0.51
1:A:604:SER:O	1:A:605:SER:C	2.52	0.51
2:B:789:MET:O	2:B:793:GLU:CG	2.47	0.51
2:D:643:LEU:HD12	2:D:643:LEU:C	2.33	0.51
1:C:74:MET:O	1:C:78:VAL:HG23	2.10	0.51
1:A:400:ILE:HB	1:A:476:VAL:HG12	1.92	0.51
1:A:545:GLU:N	1:A:545:GLU:OE1	2.43	0.51
1:C:470:MET:HE1	1:C:772:VAL:HG22	1.92	0.51
1:A:613:VAL:O	1:A:613:VAL:HG12	2.11	0.51
1:A:27:VAL:HG21	1:A:296:LEU:HD11	1.93	0.51
1:C:490:VAL:HG23	1:C:492:ASN:H	1.77	0.50
1:A:132:SER:HB2	2:B:177:PRO:HG3	1.94	0.50
1:C:308:CYS:O	2:D:77:ASP:HB3	2.12	0.50
1:C:651:LEU:C	1:C:651:LEU:CD2	2.84	0.50
2:B:533:GLY:HA3	2:B:756:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:545:VAL:HG11	2:B:660:VAL:HG23	1.94	0.50
1:C:93:SER:HB2	1:C:121:LEU:HD12	1.94	0.50
2:D:249:LEU:HD23	2:D:249:LEU:O	2.12	0.50
1:C:357:GLN:HG2	1:C:380:ILE:HG12	1.93	0.50
2:D:733:ALA:O	2:D:737:ASN:ND2	2.37	0.50
2:B:682:ARG:NH2	2:B:724:GLY:O	2.44	0.49
1:C:46:VAL:HG11	1:C:62:ALA:HB2	1.93	0.49
1:A:704:ARG:HD3	2:B:430:MET:HE3	1.94	0.49
2:D:691:THR:OG1	6:D:903:GLU:OE2	2.26	0.49
2:B:308:LEU:HD13	2:B:314:ILE:HB	1.95	0.49
1:C:560:SER:HA	1:C:563:TRP:HD1	1.78	0.49
2:D:270:PRO:HG2	2:D:273:PHE:CE2	2.48	0.49
1:C:35:THR:HG22	1:C:37:LYS:H	1.76	0.49
1:C:813:MET:O	1:C:817:PHE:N	2.45	0.49
2:B:563:PHE:HA	2:B:566:LEU:HD13	1.94	0.48
1:A:88:TYR:CE1	1:A:304:PRO:HD2	2.48	0.48
2:B:213:ASP:OD1	2:B:213:ASP:N	2.44	0.48
2:B:565:MET:HE1	1:C:817:PHE:HB3	1.95	0.48
1:A:657:LEU:CD2	2:B:807:GLU:CB	2.86	0.48
2:D:422:VAL:HG23	2:D:422:VAL:O	2.12	0.48
1:C:504:GLU:HG3	1:C:509:GLN:HB2	1.95	0.48
2:D:214:SER:O	2:D:218:ASN:ND2	2.46	0.48
2:D:407:SER:C	2:D:408:ILE:CG1	2.85	0.48
1:A:95:PRO:HG3	1:A:103:THR:HG21	1.96	0.48
1:A:253:GLU:OE1	1:A:253:GLU:N	2.41	0.48
2:B:289:LEU:C	2:B:289:LEU:CD2	2.85	0.48
1:A:819:LEU:HD11	2:D:634:VAL:HG22	1.93	0.47
1:C:406:GLU:OE2	1:C:410:TYR:HE2	1.92	0.47
1:A:35:THR:HG22	1:A:38:HIS:H	1.79	0.47
1:A:150:VAL:HG11	1:A:269:LEU:CD2	2.44	0.47
2:B:307:MET:HE1	2:B:315:PRO:HD3	1.95	0.47
1:C:770:GLN:O	1:C:770:GLN:HG3	2.14	0.47
2:D:258:VAL:HB	2:D:262:VAL:HG21	1.96	0.47
1:C:77:SER:HA	1:C:80:GLU:HB2	1.96	0.47
1:A:388:LYS:HE2	1:A:388:LYS:HB3	1.48	0.47
2:B:101:ASP:O	2:B:127:HIS:ND1	2.47	0.47
1:C:128:TYR:HA	1:C:134:HIS:ND1	2.30	0.47
2:D:47:GLU:HA	2:D:50:ILE:HD12	1.96	0.47
2:D:555:SER:O	2:D:558:VAL:HG22	2.15	0.47
2:B:154:ALA:HA	2:B:157:MET:HG2	1.97	0.47
2:D:815:ILE:H	2:D:815:ILE:HD12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:287:TYR:CE2	2:D:292:ARG:HG2	2.50	0.47
2:B:650:LEU:C	2:B:650:LEU:CD2	2.88	0.47
1:A:119:LEU:HD23	1:A:284:ALA:HB1	1.97	0.46
2:B:117:ALA:HA	2:B:141:SER:HA	1.97	0.46
2:D:353:GLU:CD	2:D:353:GLU:H	2.23	0.46
1:A:481:ASP:OD1	1:A:481:ASP:N	2.43	0.46
1:A:559:GLN:N	2:B:812:GLN:O	2.47	0.46
2:D:85:ILE:HD13	2:D:115:ILE:HG21	1.97	0.46
2:B:161:MET:HE2	2:B:166:TRP:O	2.15	0.46
2:B:312:SER:O	2:B:312:SER:OG	2.31	0.46
2:D:473:LYS:HB2	2:D:473:LYS:HE2	1.61	0.46
1:C:557:PRO:HG2	1:C:647:TYR:HE1	1.81	0.46
2:B:116:SER:HB3	2:B:142:MET:O	2.15	0.46
2:B:233:THR:HG22	2:B:234:LYS:H	1.81	0.46
2:B:793:GLU:HG2	2:B:793:GLU:H	1.58	0.46
2:D:146:PHE:HE1	2:D:351:PHE:HZ	1.63	0.46
2:D:277:LEU:HD23	2:D:373:TRP:HH2	1.81	0.46
1:C:795:TYR:O	1:C:795:TYR:CD2	2.69	0.45
2:D:491:ASN:ND2	4:D:901:NAG:O7	2.48	0.45
1:A:103:THR:OG1	1:A:104:PRO:HD3	2.17	0.45
1:A:105:THR:OG1	1:A:106:PRO:HD3	2.16	0.45
2:D:830:ALA:O	2:D:833:LEU:HG	2.17	0.45
2:B:166:TRP:HB3	2:B:227:ILE:HG13	1.97	0.45
2:D:411:LEU:HD22	2:D:485:LYS:O	2.17	0.45
1:A:90:ILE:HB	1:A:118:VAL:HG22	1.97	0.45
2:D:280:VAL:O	2:D:280:VAL:HG22	2.17	0.45
1:A:126:SER:OG	1:A:172:GLU:OE2	2.28	0.45
2:B:78:PRO:HA	2:B:81:ILE:HD12	1.99	0.45
1:A:46:VAL:HG11	1:A:62:ALA:HB2	1.98	0.44
2:D:175:TYR:CE2	2:D:206:ASP:HA	2.51	0.44
2:B:230:LEU:HB3	2:B:258:VAL:HG12	2.00	0.44
2:D:164:TYR:O	2:D:166:TRP:N	2.50	0.44
2:D:302:THR:HG21	2:D:342:VAL:HG13	1.99	0.44
1:C:613:VAL:HG13	2:D:617:SER:HB3	1.99	0.44
2:D:786:ASP:HB2	2:D:788:GLU:OE1	2.17	0.44
1:C:198:ASP:OD1	1:C:198:ASP:N	2.49	0.44
1:C:355:ASN:OD1	1:C:356:LEU:N	2.43	0.44
1:A:812:ASN:OD1	1:A:813:MET:N	2.51	0.44
1:C:87:VAL:HG11	1:C:90:ILE:HG13	1.98	0.44
1:A:197:PHE:HB3	1:A:207:LEU:HD22	2.00	0.44
1:C:66:THR:OG1	1:C:67:HIS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:VAL:HG22	2:B:379:TRP:CE2	2.53	0.44
2:D:364:ILE:HD11	2:D:384:LEU:HD11	1.99	0.44
3:F:1:NAG:O6	3:F:2:NAG:N2	2.49	0.44
1:C:557:PRO:HG2	1:C:647:TYR:CE1	2.53	0.43
1:A:541:LEU:HB2	1:A:736:LEU:HD13	2.01	0.43
2:D:198:GLU:OE2	2:D:431:ARG:NH1	2.52	0.43
1:C:468:ARG:O	1:C:471:GLN:NE2	2.51	0.43
2:D:156:VAL:HG22	2:D:379:TRP:CE2	2.53	0.43
2:D:561:MET:HA	2:D:564:VAL:HG22	2.01	0.43
2:D:568:ILE:O	2:D:572:VAL:HG23	2.19	0.43
1:A:177:GLN:NE2	1:A:181:GLU:OE2	2.47	0.43
2:D:533:GLY:HA3	2:D:756:VAL:HG13	2.00	0.43
1:A:78:VAL:HG21	1:A:107:VAL:HG22	2.01	0.43
1:C:657:LEU:HD21	2:D:655:ILE:HG23	2.00	0.43
1:C:681:TYR:HB3	1:C:728:ALA:HB3	1.99	0.43
2:B:97:VAL:O	2:B:123:ILE:HA	2.19	0.43
2:D:175:TYR:CE2	2:D:206:ASP:CB	3.02	0.43
2:D:404:ASP:OD1	2:D:404:ASP:N	2.50	0.43
1:A:443:SER:O	1:A:447:PRO:HD2	2.19	0.43
1:A:731:TRP:CG	1:A:732:ASP:H	2.37	0.43
2:B:289:LEU:HB3	2:B:290:PRO:HD3	2.00	0.43
2:B:132:MET:O	2:B:145:GLN:NE2	2.32	0.42
2:D:176:PHE:CD2	2:D:177:PRO:HD2	2.51	0.42
2:D:239:TYR:O	2:D:243:VAL:HG23	2.19	0.42
1:A:656:VAL:HG21	2:B:655:ILE:CD1	2.45	0.42
2:D:108:ILE:HD12	2:D:108:ILE:H	1.84	0.42
1:A:155:MET:HE2	1:A:155:MET:HB3	1.76	0.42
1:A:556:GLN:HA	1:A:556:GLN:NE2	2.24	0.42
1:A:694:ARG:NH1	1:A:703:TYR:OH	2.50	0.42
1:A:819:LEU:CD1	2:D:634:VAL:CG2	2.91	0.42
2:B:537:MET:HE1	2:B:718:LEU:HD21	2.01	0.42
1:C:33:LEU:HD11	1:C:281:ILE:HD11	2.02	0.42
1:C:642:ILE:HG21	2:D:821:VAL:HG11	2.02	0.42
2:B:472:VAL:HG23	2:B:472:VAL:O	2.19	0.42
2:B:830:ALA:O	2:B:833:LEU:HG	2.19	0.42
2:B:131:SER:OG	2:B:146:PHE:O	2.37	0.42
2:D:175:TYR:CE2	2:D:206:ASP:CA	3.03	0.42
2:D:555:SER:O	2:D:559:TRP:HD1	2.03	0.42
2:B:282:TYR:HE1	2:B:360:PRO:HB3	1.84	0.42
2:D:415:PRO:HG2	2:D:416:PHE:CD2	2.54	0.42
1:C:155:MET:HE1	1:C:184:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:TRP:CG	1:C:732:ASP:H	2.37	0.42
2:D:666:LEU:HD12	2:D:666:LEU:HA	1.75	0.42
2:D:810:SER:OG	2:D:811:SER:N	2.53	0.42
1:A:325:LEU:O	1:A:328:SER:OG	2.37	0.42
1:A:681:TYR:HB3	1:A:728:ALA:HB3	2.00	0.42
1:C:510:ALA:O	1:C:763:ARG:NH2	2.52	0.41
2:D:174:THR:HG21	2:D:236:GLU:OE1	2.20	0.41
1:A:608:TRP:CE3	1:A:608:TRP:CA	2.99	0.41
2:B:234:LYS:O	2:B:238:THR:HG23	2.19	0.41
2:B:250:THR:HG23	2:B:274:PRO:HB3	1.90	0.41
2:D:498:ILE:O	2:D:502:VAL:HG23	2.20	0.41
2:D:613:VAL:HA	2:D:639:ALA:HB1	2.02	0.41
1:A:552:ASP:O	1:A:556:GLN:HG2	2.21	0.41
1:C:335:THR:O	1:C:346:ARG:NH2	2.51	0.41
1:C:562:LEU:HD21	2:D:814:ASP:HA	2.02	0.41
1:A:531:LYS:HA	1:A:532:PRO:HD3	1.88	0.41
1:A:789:ASP:HB3	1:A:794:ARG:HE	1.86	0.41
1:C:83:ILE:HD11	1:C:308:CYS:HB3	2.01	0.41
1:C:436:CYS:O	1:C:436:CYS:SG	2.77	0.41
1:A:628:SER:CB	2:B:836:PHE:HB2	2.50	0.41
2:B:62:LEU:HD12	2:B:305:SER:OG	2.20	0.41
2:B:114:PHE:O	2:B:118:GLN:HG3	2.20	0.41
1:C:91:LEU:HD12	1:C:121:LEU:HD21	2.03	0.41
1:C:578:TYR:CA	1:C:603:LEU:HD21	2.48	0.41
2:D:171:ILE:HD11	2:D:186:ILE:HG21	2.01	0.41
2:D:527:VAL:HA	2:D:528:PRO:HD3	1.91	0.41
2:D:656:GLN:CA	2:D:656:GLN:NE2	2.72	0.41
2:B:232:CYS:HB3	2:B:236:GLU:HG2	2.02	0.41
2:B:507:TYR:HA	2:B:767:GLN:HG3	2.03	0.41
2:B:566:LEU:HA	2:B:609:LEU:HD21	2.02	0.41
1:C:317:THR:HB	1:C:321:PHE:CE1	2.55	0.41
1:C:406:GLU:O	1:C:406:GLU:CG	2.65	0.41
1:A:541:LEU:HD22	1:A:736:LEU:HD22	2.03	0.41
1:A:609:PHE:CD1	1:A:609:PHE:C	2.97	0.41
2:B:314:ILE:HA	2:B:315:PRO:HD3	1.93	0.41
1:C:119:LEU:HD13	1:C:138:LEU:HB2	2.03	0.41
1:A:628:SER:HB2	2:B:836:PHE:HB2	2.03	0.41
2:B:719:LEU:HD23	2:B:719:LEU:HA	1.95	0.41
1:C:249:VAL:HB	1:C:253:GLU:HB2	2.02	0.41
2:D:678:SER:CB	2:D:679:PRO:HD2	2.50	0.41
1:A:584:SER:HB2	2:B:836:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:602:ILE:O	2:B:606:ILE:HD12	2.21	0.40
2:D:527:VAL:CG1	2:D:777:ASP:HB2	2.45	0.40
1:A:152:PHE:HE1	1:A:187:ARG:NH2	2.19	0.40
1:A:31:ALA:HA	1:A:91:LEU:H	1.86	0.40
1:A:260:ARG:NH2	1:A:261:TYR:OH	2.55	0.40
1:A:639:PHE:O	1:A:642:ILE:HG22	2.20	0.40
1:C:254:ILE:O	1:C:259:LEU:HB2	2.21	0.40
1:A:403:ILE:HB	1:A:501:MET:SD	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	789/847 (93%)	751 (95%)	37 (5%)	1 (0%)	48	78
1	C	789/847 (93%)	758 (96%)	29 (4%)	2 (0%)	36	67
2	B	779/883 (88%)	726 (93%)	49 (6%)	4 (0%)	24	58
2	D	779/883 (88%)	741 (95%)	37 (5%)	1 (0%)	48	78
All	All	3136/3460 (91%)	2976 (95%)	152 (5%)	8 (0%)	37	67

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	450	PRO
2	B	679	PRO
2	D	679	PRO
2	B	414	ALA
1	A	446	SER
1	C	801	ARG
2	B	473	LYS

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Mol	Chain	Res	Type
1	C	664	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	606/728 (83%)	586 (97%)	20 (3%)	33	65
1	C	599/728 (82%)	585 (98%)	14 (2%)	44	72
2	B	592/762 (78%)	577 (98%)	15 (2%)	42	71
2	D	574/762 (75%)	552 (96%)	22 (4%)	29	61
All	All	2371/2980 (80%)	2300 (97%)	71 (3%)	37	67

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	146	HIS
1	A	153	GLU
1	A	388	LYS
1	A	434	VAL
1	A	473	THR
1	A	556	GLN
1	A	603	LEU
1	A	607	MET
1	A	608	TRP
1	A	610	SER
1	A	647	TYR
1	A	697	VAL
1	A	698	GLU
1	A	706	MET
1	A	708	LYS
1	A	745	ASP
1	A	756	SER
1	A	807	THR
1	A	819	LEU

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Mol	Chain	Res	Type
2	B	163	GLU
2	B	249	LEU
2	B	290	PRO
2	B	472	VAL
2	B	482	THR
2	B	495	ASN
2	B	622	ASN
2	B	650	LEU
2	B	655	ILE
2	B	693	ARG
2	B	718	LEU
2	B	730	ILE
2	B	751	ILE
2	B	753	SER
2	B	808	VAL
1	C	414	THR
1	C	434	VAL
1	C	602	THR
1	C	607	MET
1	C	610	SER
1	C	680	ILE
1	C	696	GLN
1	C	697	VAL
1	C	698	GLU
1	C	700	SER
1	C	701	THR
1	C	745	ASP
1	C	756	SER
1	C	800	SER
2	D	157	MET
2	D	174	THR
2	D	177	PRO
2	D	188	SER
2	D	279	SER
2	D	280	VAL
2	D	390	VAL
2	D	406	LEU
2	D	408	ILE
2	D	410	THR
2	D	419	VAL
2	D	420	GLU
2	D	436	CYS

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Mol	Chain	Res	Type
2	D	468	ILE
2	D	472	VAL
2	D	508	MET
2	D	522	VAL
2	D	527	VAL
2	D	653	PHE
2	D	656	GLN
2	D	735	VAL
2	D	792	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	556	GLN
1	A	668	ASN
1	A	742	GLN
2	B	152	GLN
2	B	180	GLN
2	B	437	GLN
2	B	495	ASN
2	B	615	ASN
2	B	616	ASN
2	B	622	ASN
2	B	817	ASN
1	C	350	GLN
1	C	405	GLN
1	C	471	GLN
1	C	521	ASN
1	C	696	GLN
1	C	709	HIS
1	C	770	GLN
2	D	153	GLN
2	D	348	ASN
2	D	656	GLN
2	D	711	GLN
2	D	817	ASN

5.3.3 RNA ⓘ

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	$\# Z > 2$
3	NAG	E	1	3,2	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	E	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	F	1	3,1	14,14,15	0.35	0	17,19,21	0.60	0
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	G	1	3,2	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	G	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	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

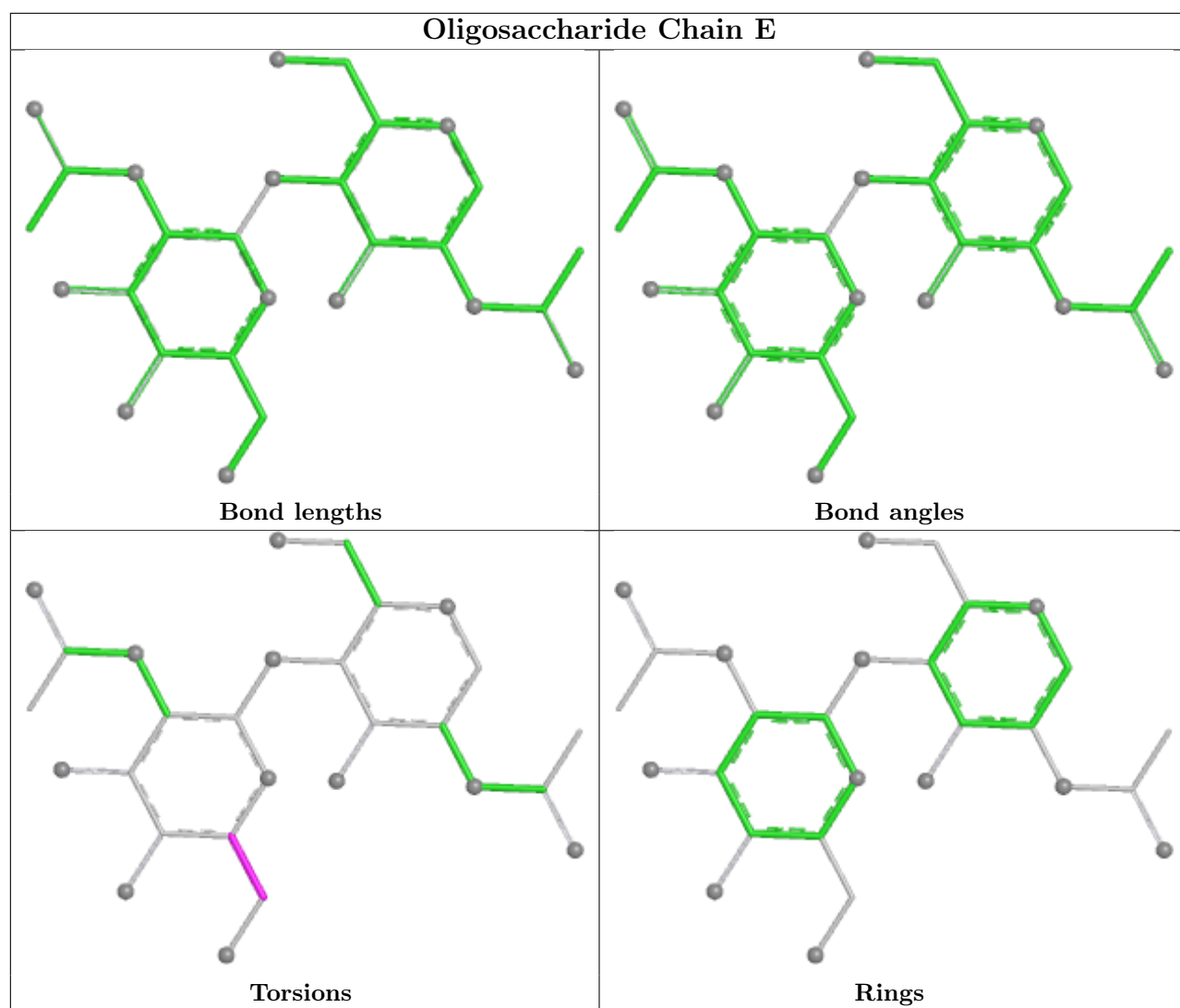
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7
3	F	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6

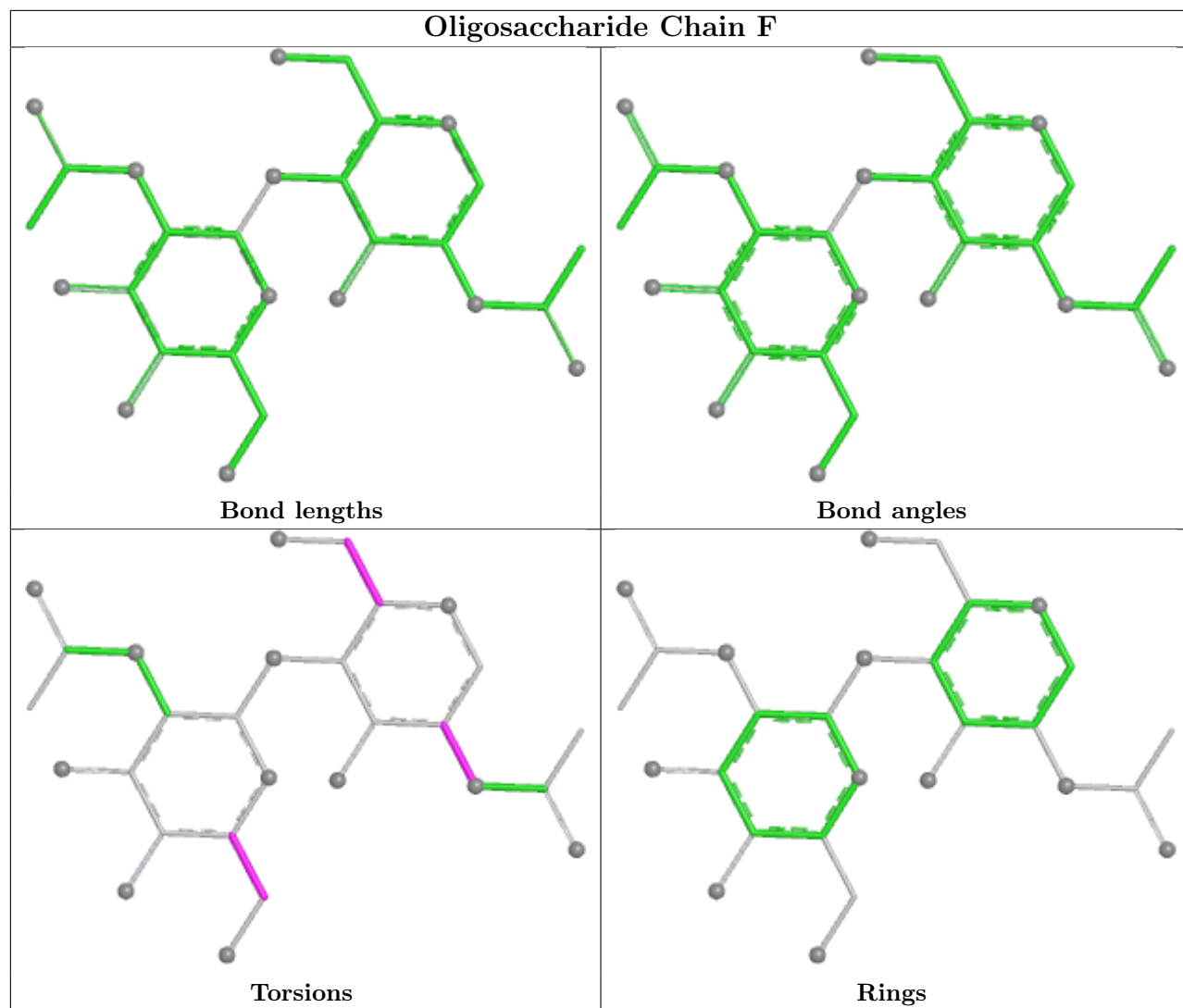
There are no ring outliers.

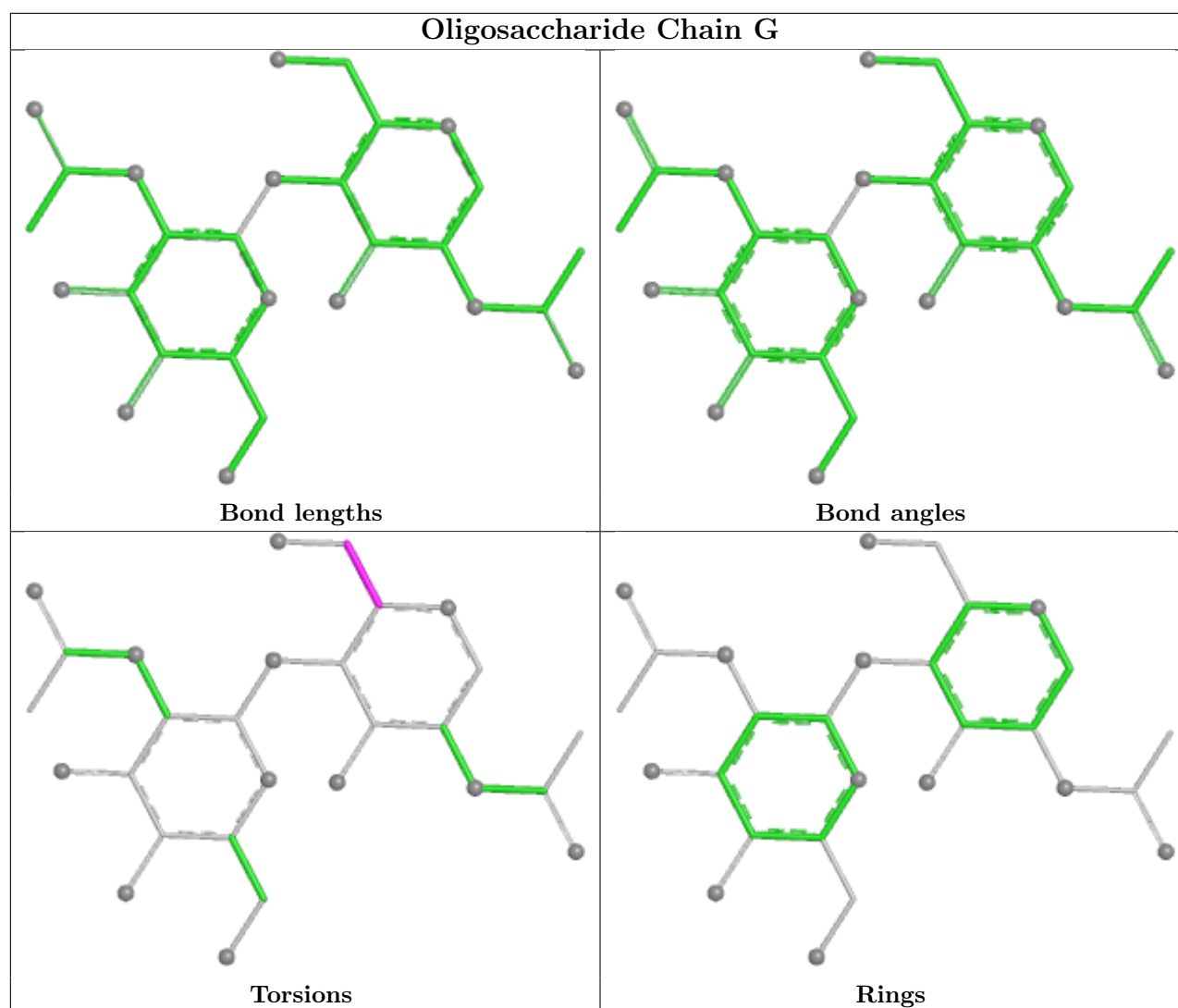
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	1	0
3	F	1	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](#)

12 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	NAG	B	901	2	14,14,15	0.94	1 (7%)	17,19,21	1.21	1 (5%)
4	NAG	A	902	-	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	D	901	-	14,14,15	0.43	0	17,19,21	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	902	-	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	D	902	-	14,14,15	0.21	0	17,19,21	0.44	0
5	GLY	A	904	-	4,4,4	1.16	1 (25%)	3,4,4	1.63	1 (33%)
6	GLU	D	903	-	8,9,9	2.36	3 (37%)	8,11,11	1.61	2 (25%)
5	GLY	C	903	-	4,4,4	1.17	1 (25%)	3,4,4	1.61	1 (33%)
6	GLU	B	902	-	8,9,9	1.10	1 (12%)	8,11,11	1.18	1 (12%)
4	NAG	C	901	-	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	A	901	-	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	A	903	1	14,14,15	0.38	0	17,19,21	0.65	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
4	NAG	B	901	2	-	1/6/23/26	0/1/1/1
4	NAG	A	902	-	-	2/6/23/26	0/1/1/1
4	NAG	D	901	-	-	0/6/23/26	0/1/1/1
4	NAG	C	902	-	-	0/6/23/26	0/1/1/1
4	NAG	D	902	-	-	2/6/23/26	0/1/1/1
5	GLY	A	904	-	-	0/2/2/2	-
6	GLU	D	903	-	-	1/9/9/9	-
5	GLY	C	903	-	-	0/2/2/2	-
6	GLU	B	902	-	-	0/9/9/9	-
4	NAG	C	901	-	-	2/6/23/26	0/1/1/1
4	NAG	A	901	-	-	1/6/23/26	0/1/1/1
4	NAG	A	903	1	-	3/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	903	GLU	OXT-C	-5.06	1.14	1.30
4	B	901	NAG	O5-C1	3.22	1.49	1.43
6	D	903	GLU	OE2-CD	-3.10	1.20	1.30
6	D	903	GLU	OE1-CD	-2.32	1.14	1.22
6	B	902	GLU	OXT-C	-2.26	1.23	1.30
5	C	903	GLY	OXT-C	-2.22	1.23	1.30
5	A	904	GLY	OXT-C	-2.21	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	NAG	C1-O5-C5	4.74	118.53	112.19
4	D	901	NAG	C1-O5-C5	3.00	116.21	112.19
6	D	903	GLU	OE2-CD-CG	2.82	122.92	114.00
6	B	902	GLU	OXT-C-O	-2.66	118.04	124.08
6	D	903	GLU	OE1-CD-CG	-2.62	114.80	123.09
5	A	904	GLY	OXT-C-O	-2.07	118.01	123.33
5	C	903	GLY	OXT-C-O	-2.05	118.06	123.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	902	NAG	O5-C5-C6-O6
4	D	902	NAG	C4-C5-C6-O6
4	C	901	NAG	O5-C5-C6-O6
4	A	902	NAG	O5-C5-C6-O6
4	C	901	NAG	C4-C5-C6-O6
4	A	902	NAG	C4-C5-C6-O6
4	A	903	NAG	O5-C5-C6-O6
4	A	903	NAG	C1-C2-N2-C7
4	A	901	NAG	C4-C5-C6-O6
4	B	901	NAG	O5-C5-C6-O6
4	A	903	NAG	C3-C2-N2-C7
6	D	903	GLU	OE2-CD-CG-CB

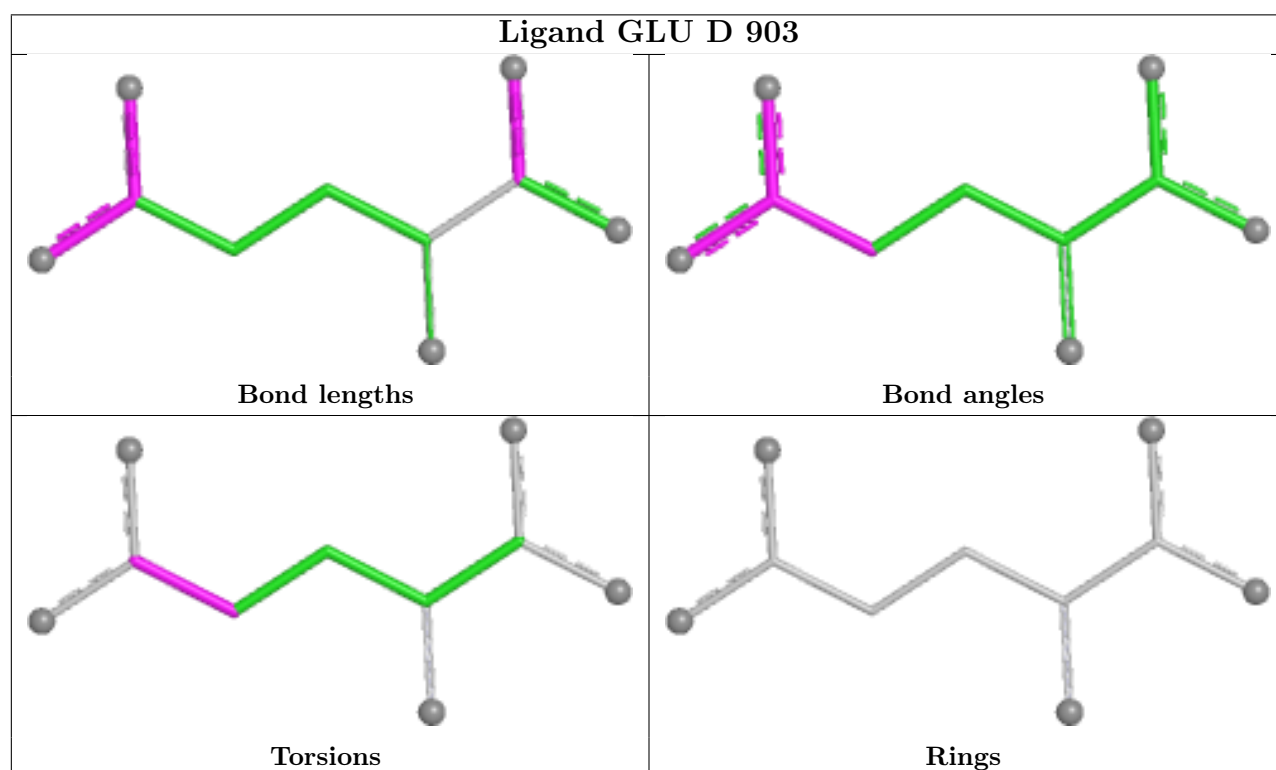
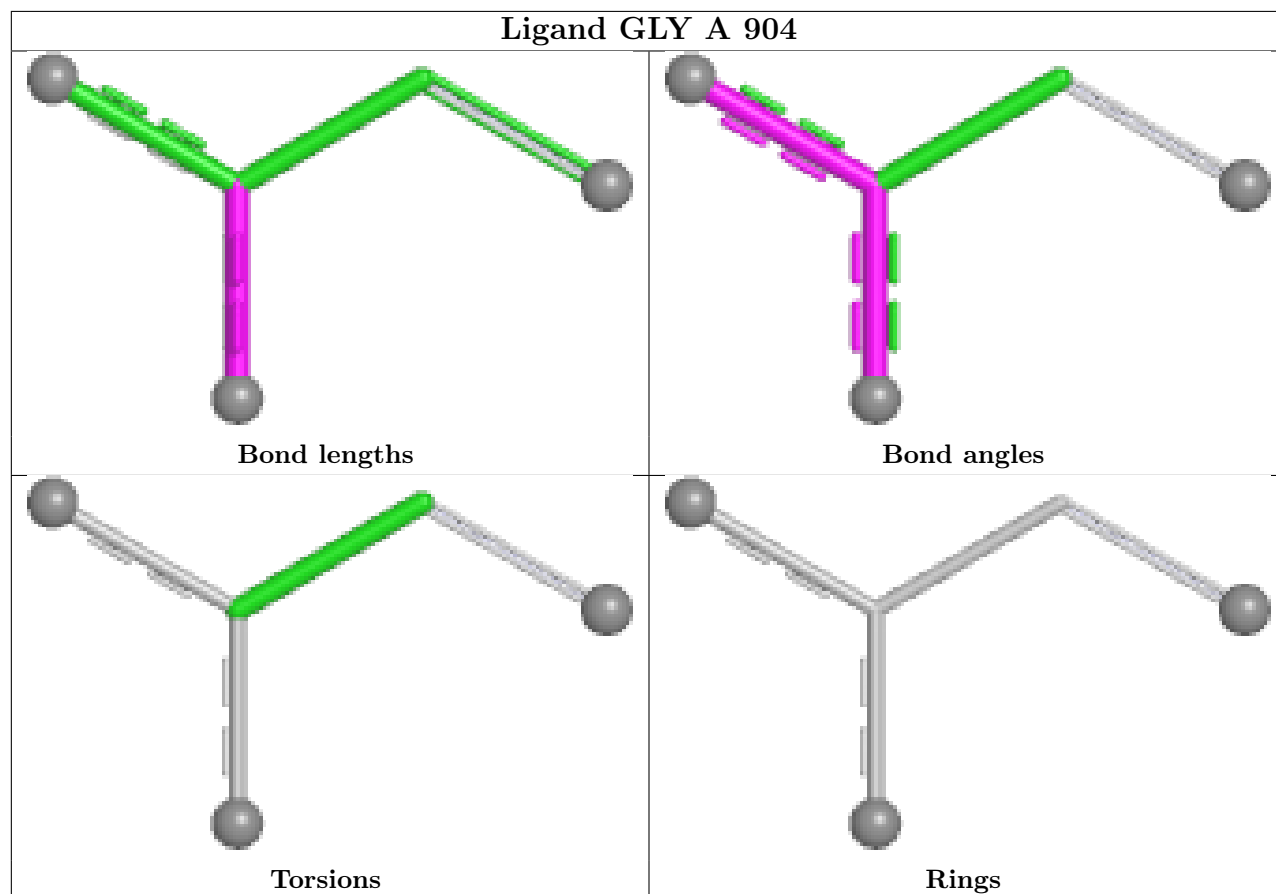
There are no ring outliers.

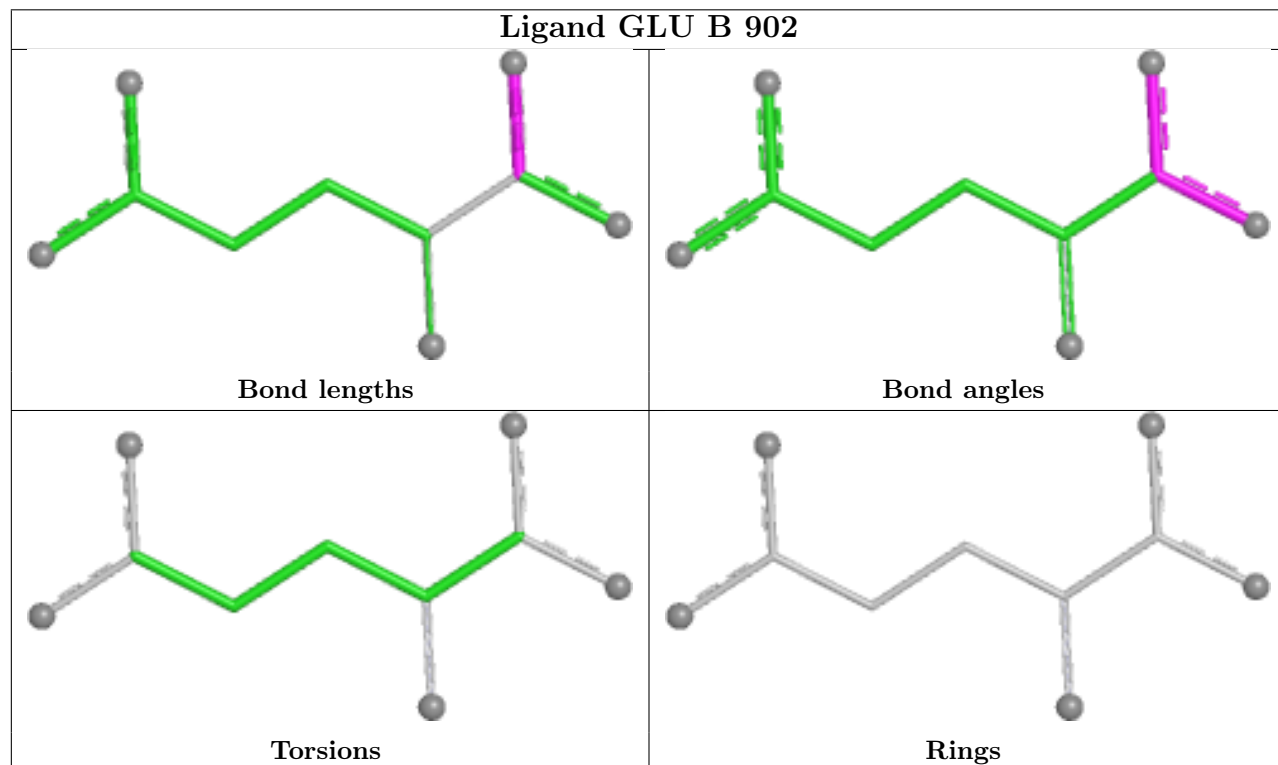
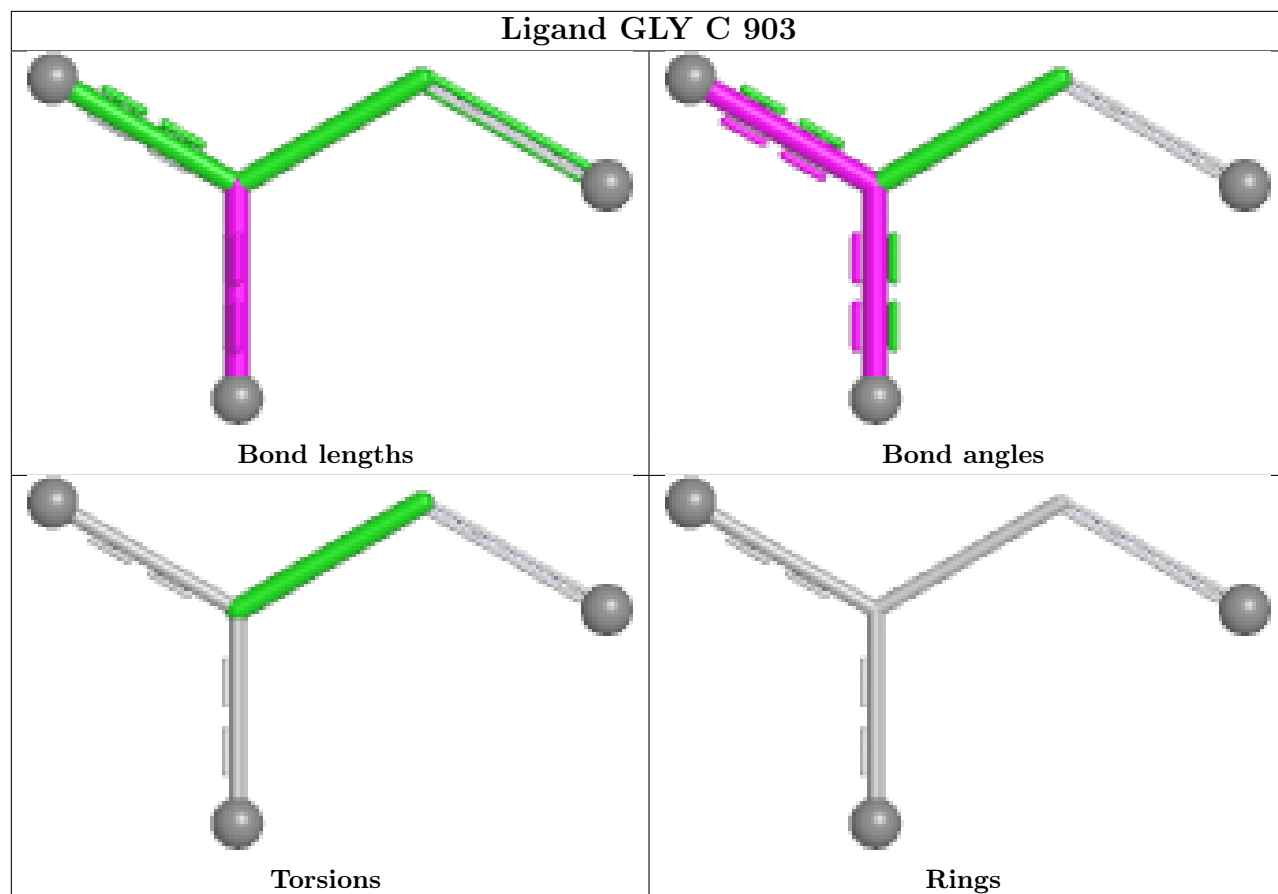
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	901	NAG	1	0
6	D	903	GLU	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

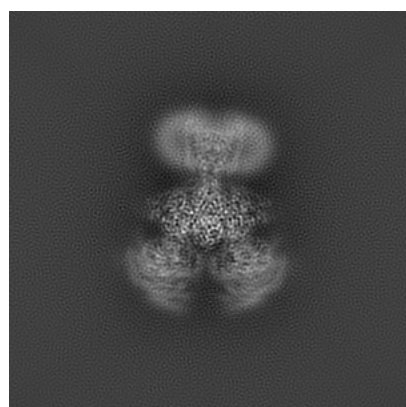
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24946. These allow visual inspection of the internal detail of the map and identification of artifacts.

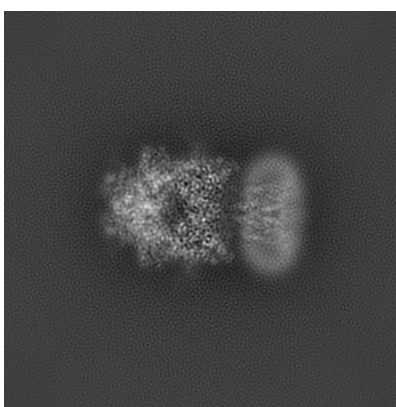
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

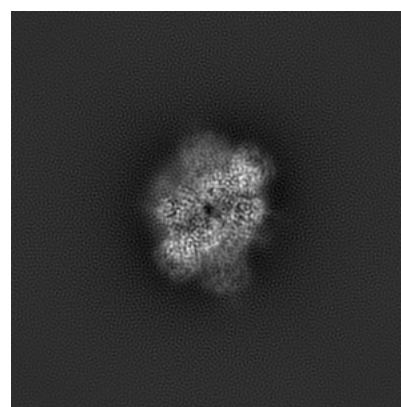
6.1.1 Primary map



X



Y

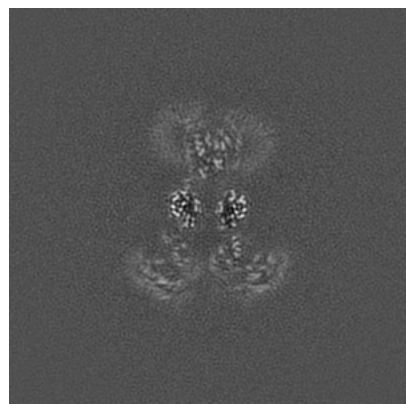


Z

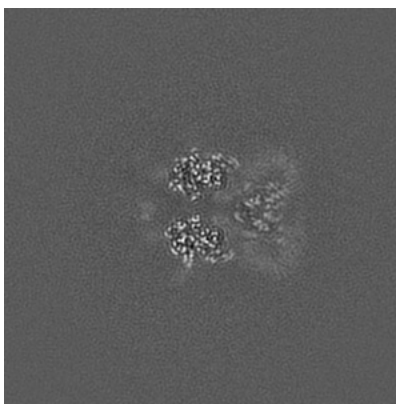
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

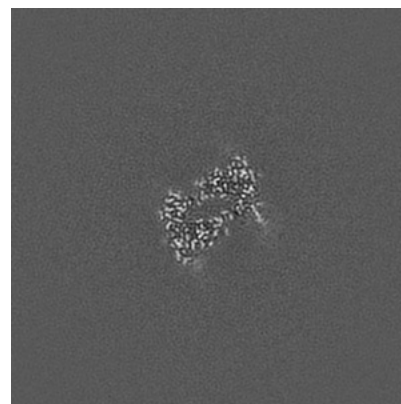
6.2.1 Primary map



X Index: 200



Y Index: 200

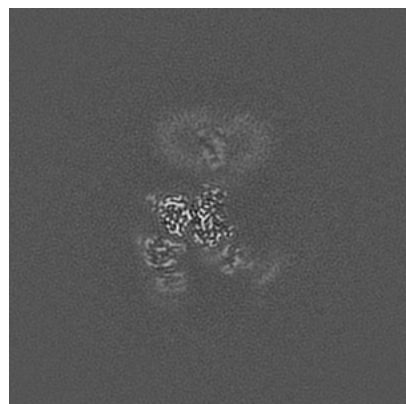


Z Index: 200

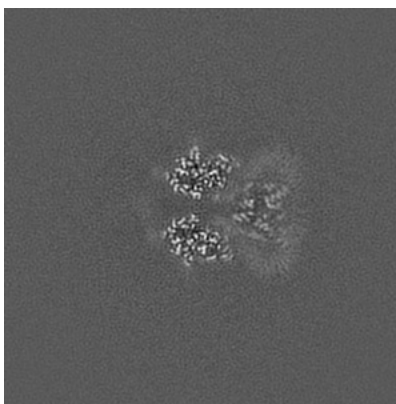
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

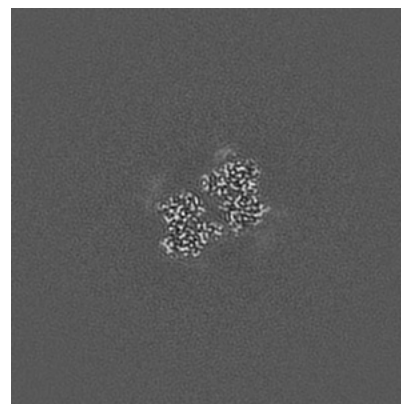
6.3.1 Primary map



X Index: 171



Y Index: 198

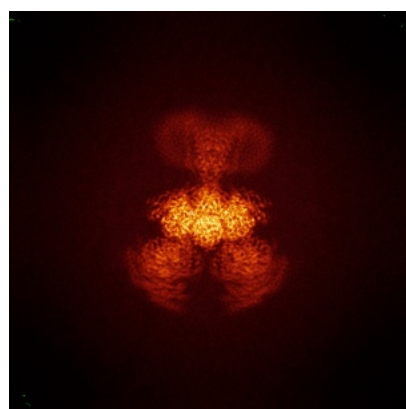


Z Index: 188

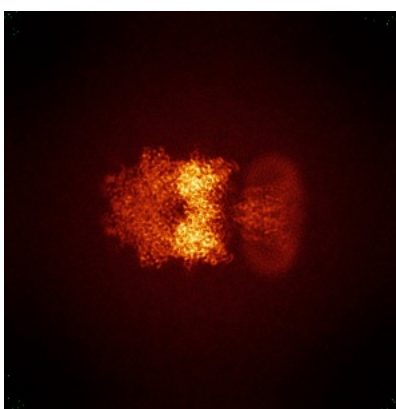
The images above show the largest variance slices of the map in three orthogonal directions.

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

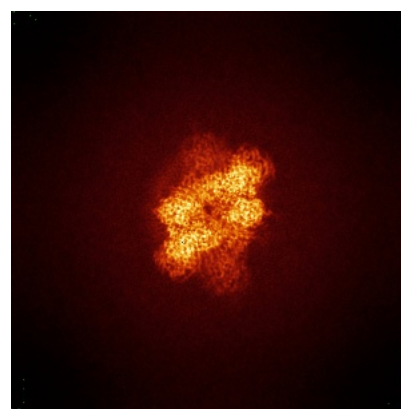
6.4.1 Primary map



X



Y

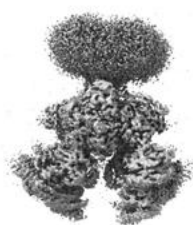


Z

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

6.5 Orthogonal surface views [i](#)

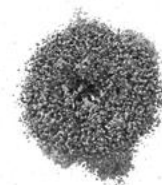
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

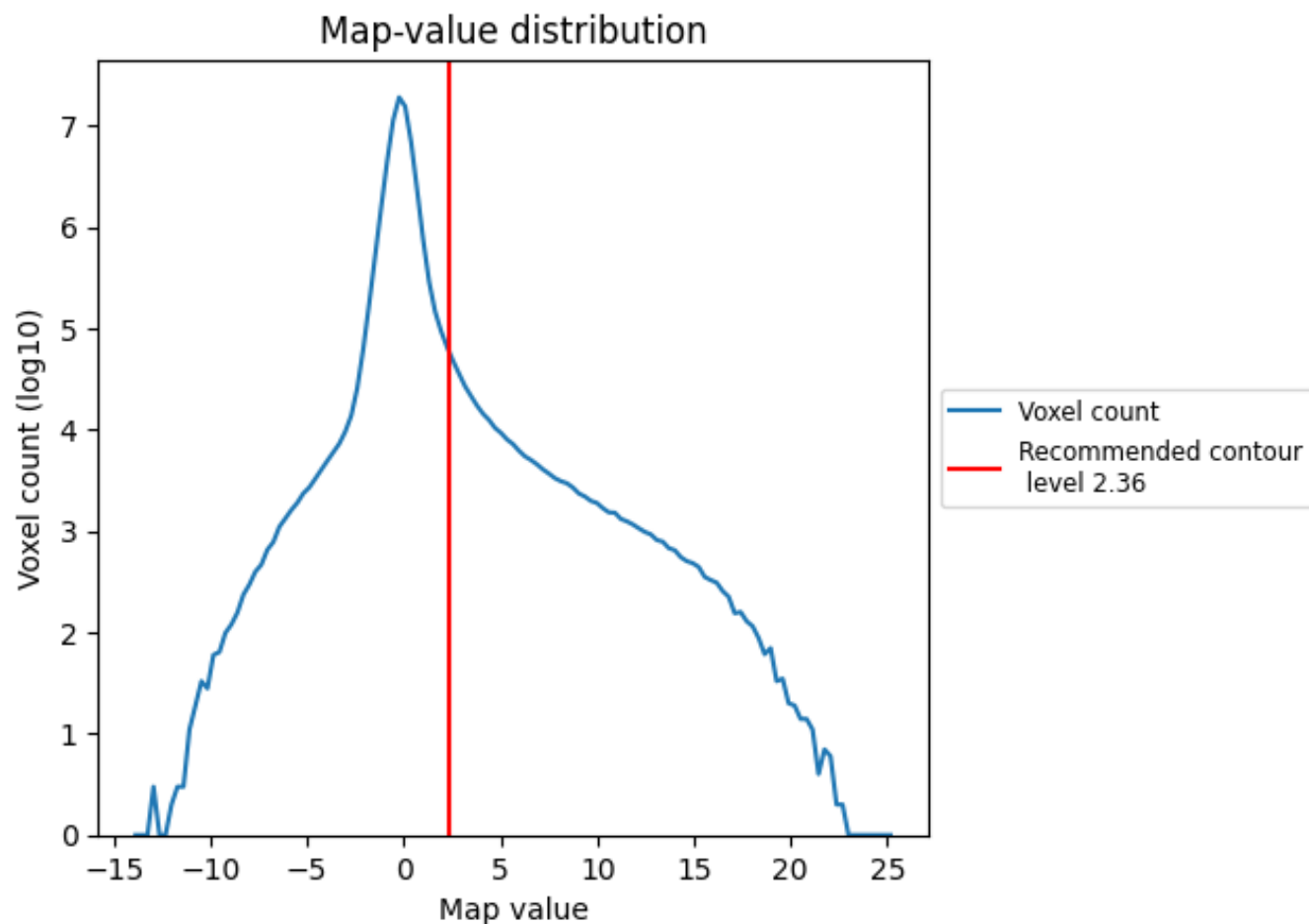
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

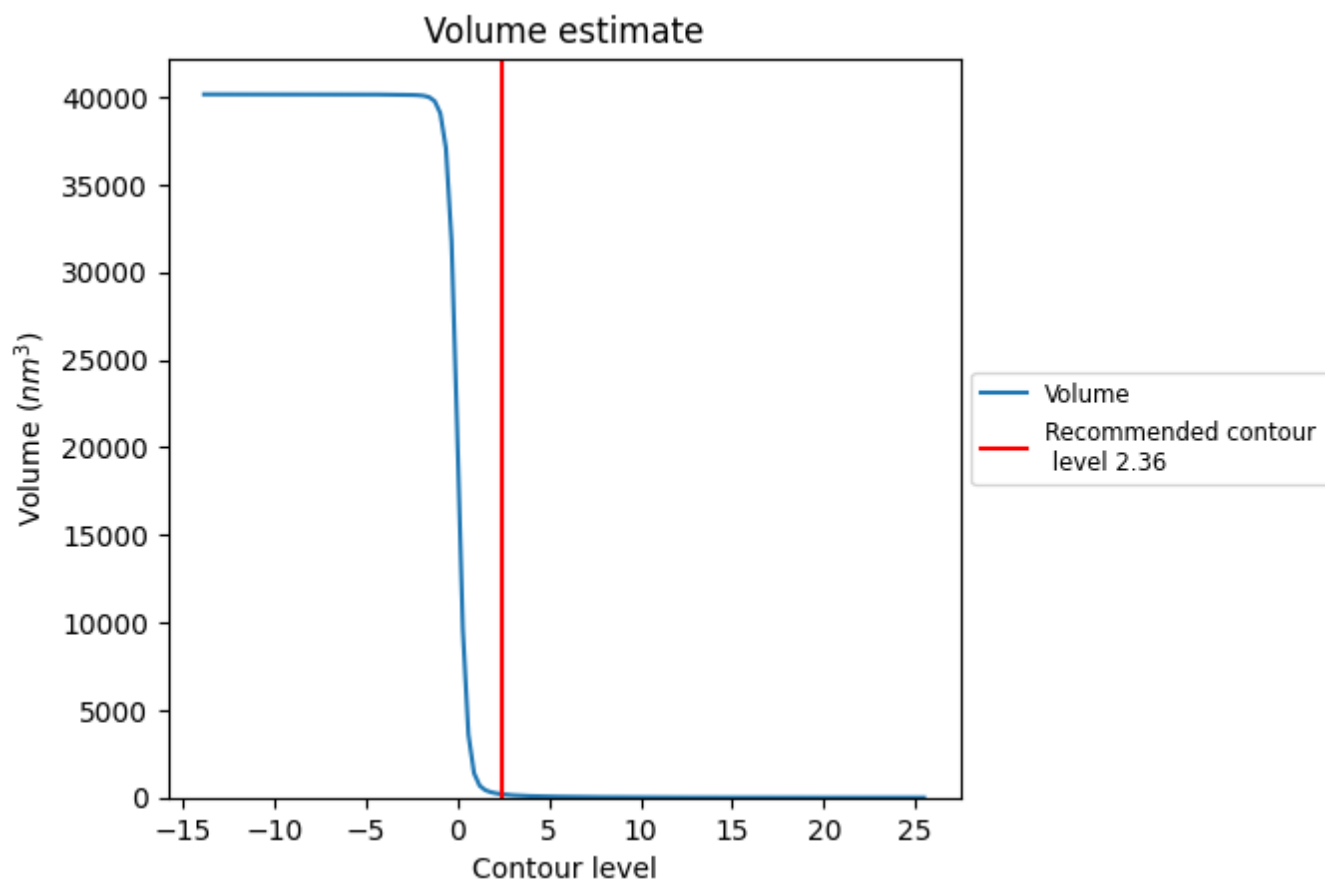
This section contains the results of statistical analysis of the map.

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.

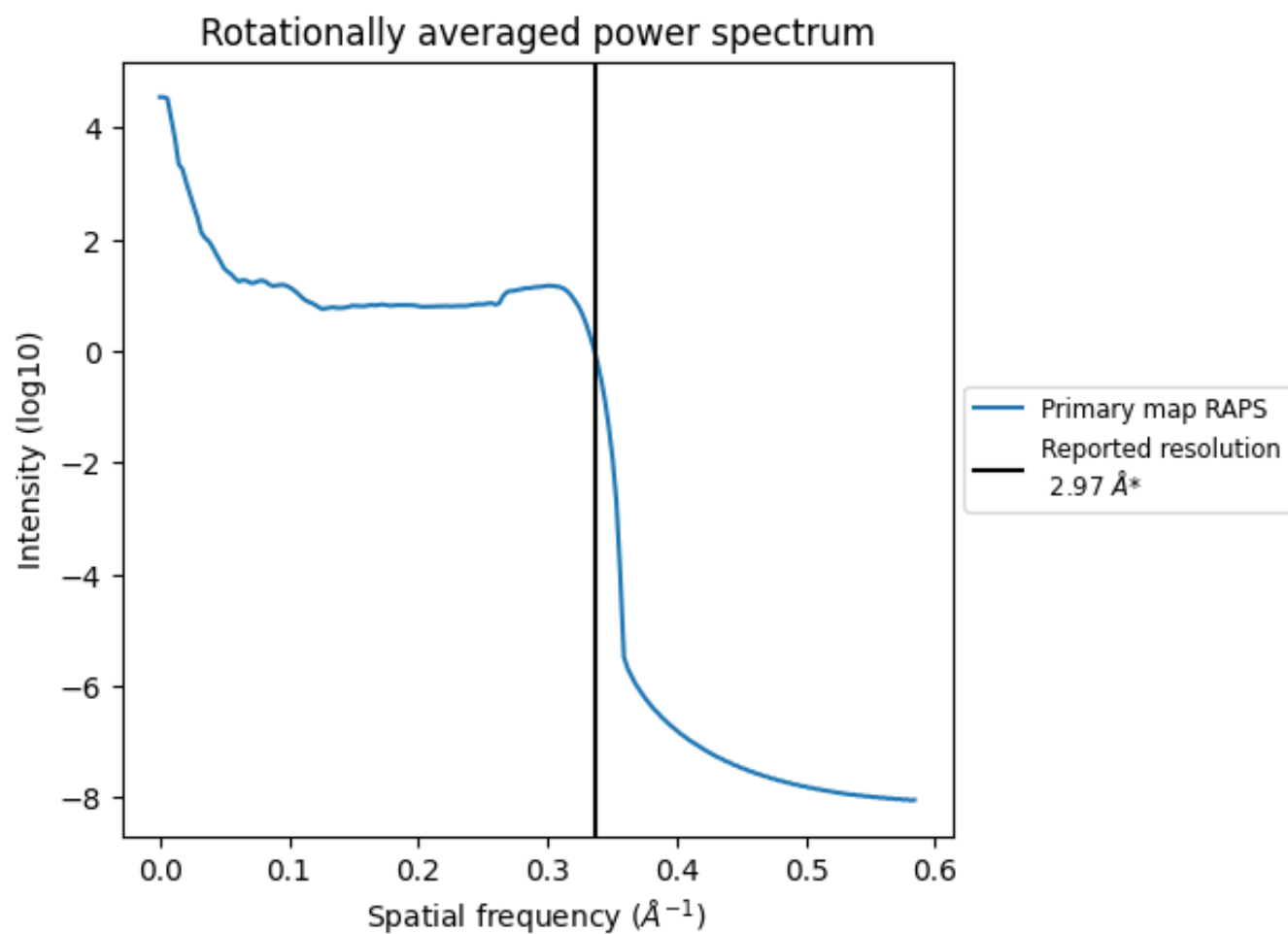
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 201 nm^3 ; this corresponds to an approximate mass of 181 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 0.337 Å⁻¹

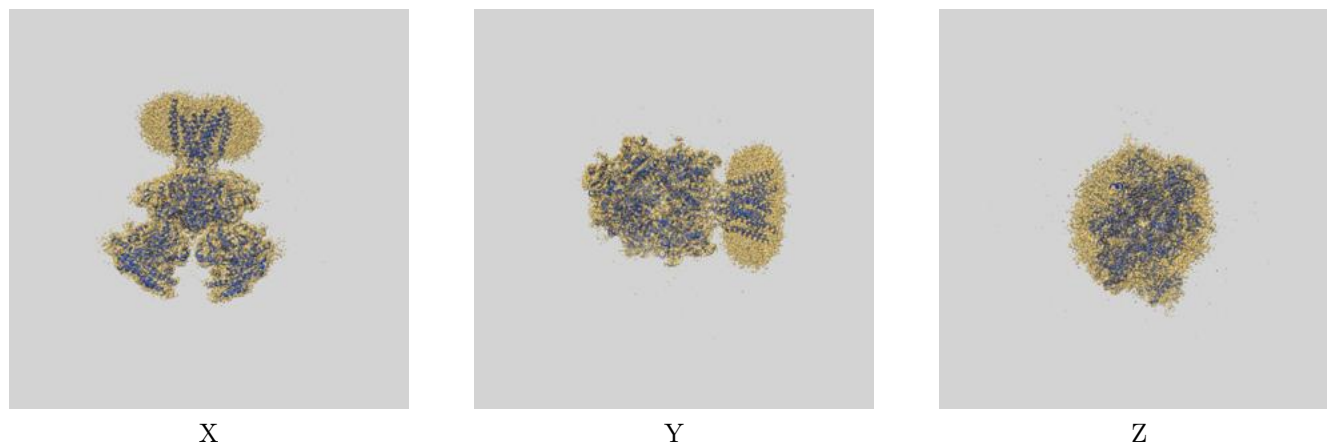
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

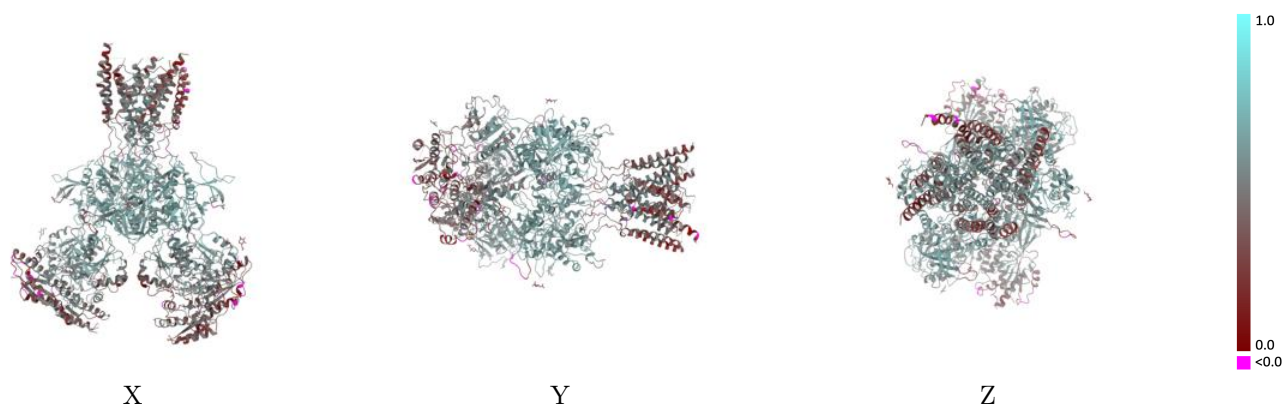
This section contains information regarding the fit between EMDB map EMD-24946 and PDB model 7SAA. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 2.36 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](#)

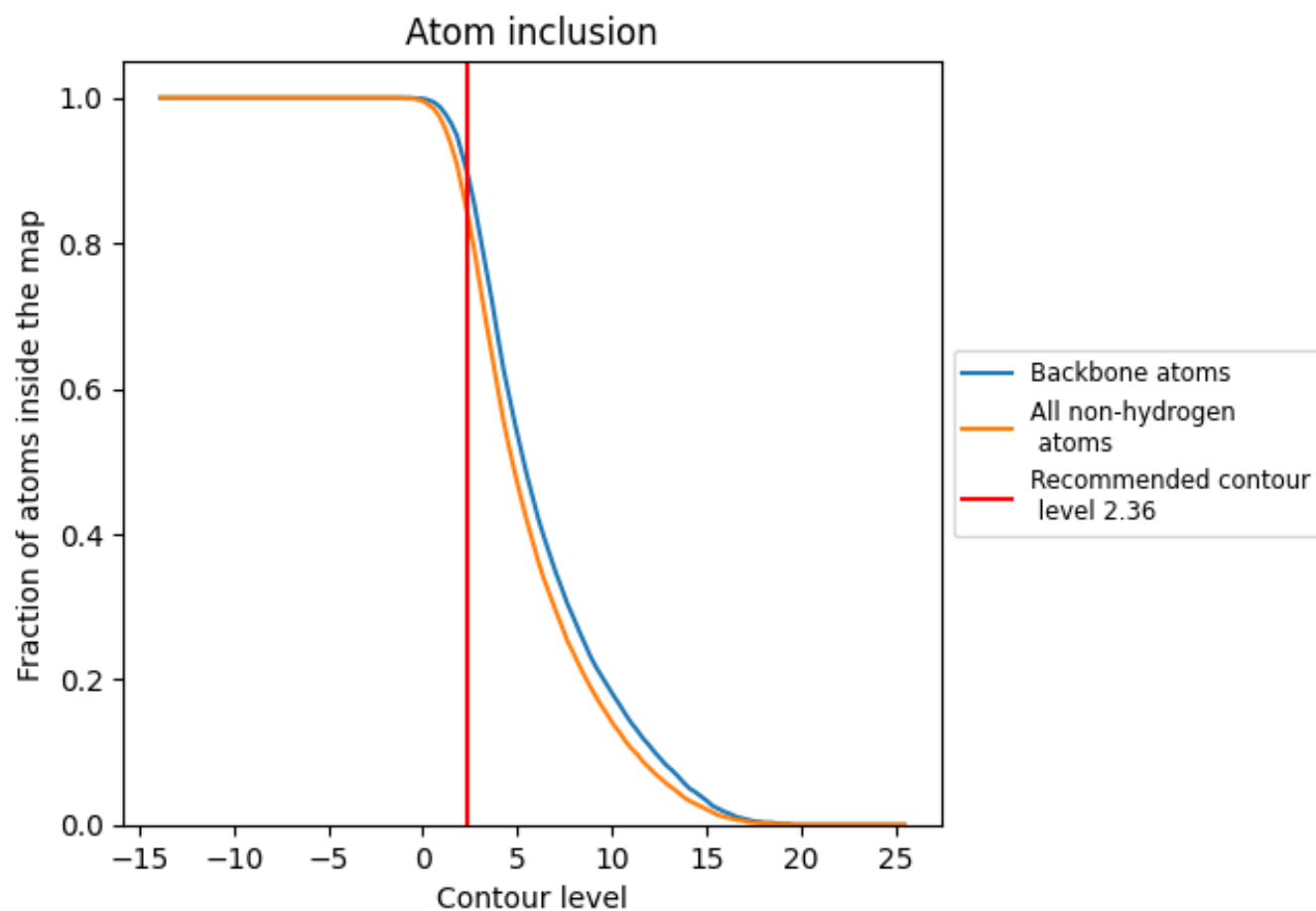


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 90% of all backbone atoms, 84% 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 (2.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8420	0.5050
A	0.8720	0.5270
B	0.8280	0.4960
C	0.8400	0.5000
D	0.8290	0.4970
E	0.8930	0.5730
F	0.5000	0.3660
G	0.8570	0.5560

1.0

0.0

<0.0