



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 07:44 PM UTC

PDB ID : 8VAO / pdb_00008vao
EMDB ID : EMD-43097
Title : Simulation-driven design of prefusion stabilized SARS-CoV-2 spike S2 antigen
Authors : Zhou, L.; McLellan, J.S.
Deposited on : 2023-12-11
Resolution : 2.80 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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

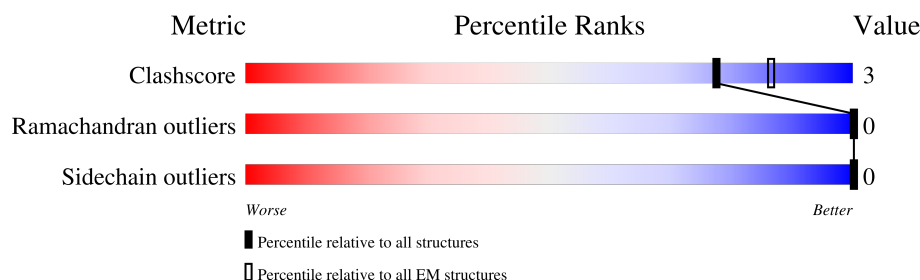
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	512	
1	B	512	
1	C	512	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20280 atoms, of which 10068 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 Spike protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0
			6676	2136	3314	563	644	19		
1	B	437	Total	C	H	N	O	S	0	0
			6676	2136	3314	563	644	19		
1	C	437	Total	C	H	N	O	S	0	0
			6676	2136	3314	563	644	19		

There are 33 discrepancies between the modelled and reference sequences:

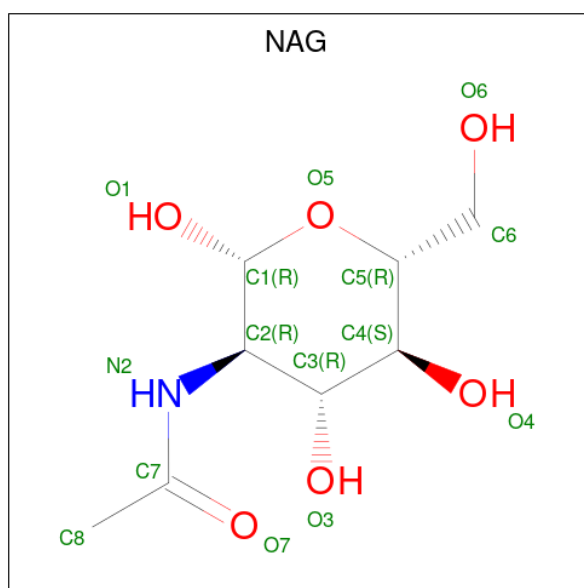
Chain	Residue	Modelled	Actual	Comment	Reference
A	704	CYS	SER	engineered mutation	UNP P0DTC2
A	790	CYS	LYS	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	957	GLU	GLN	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	991	TRP	VAL	engineered mutation	UNP P0DTC2
A	998	TRP	THR	engineered mutation	UNP P0DTC2
B	704	CYS	SER	engineered mutation	UNP P0DTC2
B	790	CYS	LYS	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	957	GLU	GLN	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	991	TRP	VAL	engineered mutation	UNP P0DTC2
B	998	TRP	THR	engineered mutation	UNP P0DTC2
C	704	CYS	SER	engineered mutation	UNP P0DTC2
C	790	CYS	LYS	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	957	GLU	GLN	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	991	TRP	VAL	engineered mutation	UNP P0DTC2
C	998	TRP	THR	engineered mutation	UNP P0DTC2

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



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	B	1	Total	C	H	N	O	0
			28	8	14	1	5	

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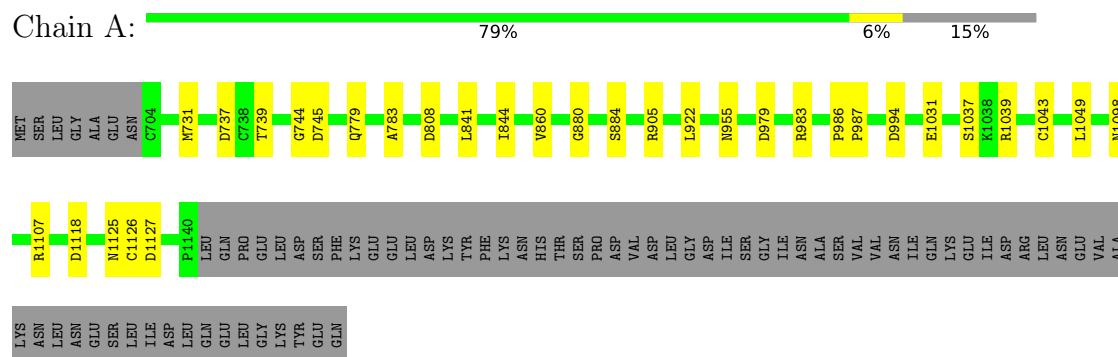
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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	C	1	Total	C	H	N	O	0
			28	8	14	1	5	

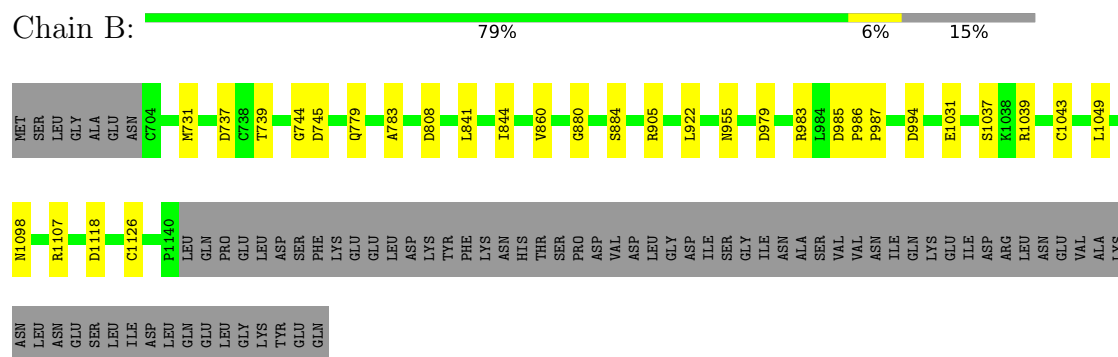
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

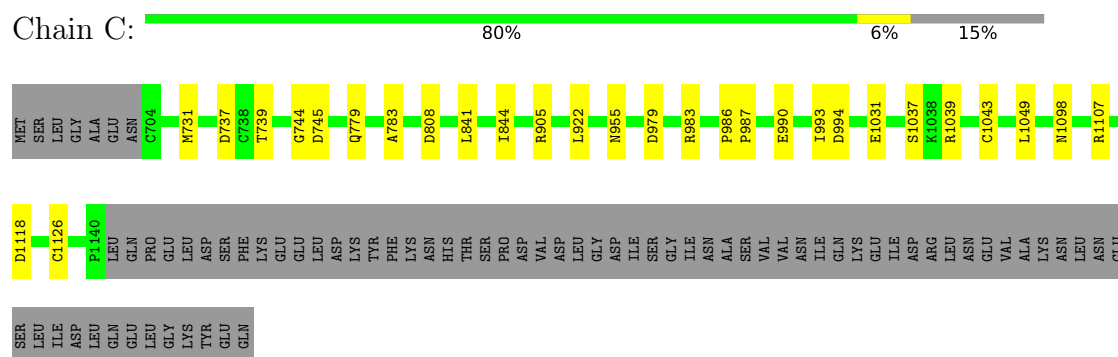
- Molecule 1: Spike protein S2



- Molecule 1: Spike protein S2



- Molecule 1: Spike protein S2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	249447	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	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	0.11	0/3434	0.26	0/4678
1	B	0.11	0/3434	0.26	0/4678
1	C	0.11	0/3434	0.26	0/4678
All	All	0.11	0/10302	0.26	0/14034

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	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1107	ARG	Sidechain
1	B	1107	ARG	Sidechain
1	C	1107	ARG	Sidechain

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	3362	3314	3313	21	0
1	B	3362	3314	3313	21	0
1	C	3362	3314	3313	19	0
2	A	42	42	39	0	0
2	B	42	42	39	0	0
2	C	42	42	39	0	0
All	All	10212	10068	10056	58	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 3.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1037:SER:OG	1:B:1043:CYS:SG	2.40	0.80
1:C:1037:SER:OG	1:C:1043:CYS:SG	2.40	0.79
1:A:1037:SER:OG	1:A:1043:CYS:SG	2.40	0.78
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.36	0.59
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.36	0.59
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.36	0.57
1:C:731:MET:SD	1:C:955:ASN:ND2	2.81	0.52
1:A:731:MET:SD	1:A:955:ASN:ND2	2.81	0.52
1:B:745:ASP:OD1	1:B:745:ASP:C	2.54	0.50
1:C:745:ASP:C	1:C:745:ASP:OD1	2.54	0.50
1:A:1098:ASN:O	1:A:1098:ASN:ND2	2.45	0.50
1:A:745:ASP:OD1	1:A:745:ASP:C	2.54	0.50
1:C:841:LEU:O	1:C:844:ILE:HG22	2.12	0.49
1:B:841:LEU:O	1:B:844:ILE:HG22	2.12	0.49
1:B:1098:ASN:O	1:B:1098:ASN:ND2	2.44	0.49
1:B:731:MET:SD	1:B:955:ASN:ND2	2.81	0.49
1:C:1098:ASN:ND2	1:C:1098:ASN:O	2.45	0.49
1:A:841:LEU:O	1:A:844:ILE:HG22	2.12	0.49
1:A:1031:GLU:OE2	1:C:1039:ARG:NH1	2.46	0.48
1:A:737:ASP:OD1	1:A:739:THR:HG22	2.13	0.48
1:B:737:ASP:OD1	1:B:739:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:737:ASP:OD1	1:C:739:THR:HG22	2.13	0.48
1:A:1039:ARG:NH1	1:B:1031:GLU:OE2	2.44	0.47
1:C:779:GLN:O	1:C:783:ALA:HB3	2.16	0.46
1:C:808:ASP:OD1	1:C:808:ASP:C	2.59	0.46
1:A:779:GLN:O	1:A:783:ALA:HB3	2.16	0.45
1:B:779:GLN:O	1:B:783:ALA:HB3	2.16	0.45
1:C:1126:CYS:SG	1:C:1126:CYS:O	2.74	0.45
1:A:808:ASP:OD1	1:A:808:ASP:C	2.59	0.45
1:A:986:PRO:N	1:A:987:PRO:HD2	2.32	0.45
1:A:1126:CYS:SG	1:A:1126:CYS:O	2.74	0.44
1:B:808:ASP:C	1:B:808:ASP:OD1	2.59	0.44
1:B:1126:CYS:SG	1:B:1126:CYS:O	2.74	0.44
1:B:986:PRO:N	1:B:987:PRO:HD2	2.32	0.44
1:C:986:PRO:N	1:C:987:PRO:HD2	2.32	0.44
1:B:994:ASP:O	1:B:994:ASP:OD1	2.37	0.43
1:A:994:ASP:OD1	1:A:994:ASP:O	2.37	0.43
1:C:994:ASP:O	1:C:994:ASP:OD1	2.37	0.42
1:B:880:GLY:O	1:B:884:SER:N	2.49	0.42
1:A:744:GLY:O	1:A:745:ASP:CG	2.63	0.42
1:B:985:ASP:OD1	1:B:985:ASP:N	2.51	0.42
1:A:880:GLY:O	1:A:884:SER:N	2.49	0.41
1:B:1039:ARG:NH1	1:C:1031:GLU:OE2	2.49	0.41
1:A:1118:ASP:OD1	1:A:1118:ASP:C	2.63	0.41
1:C:744:GLY:O	1:C:745:ASP:CG	2.63	0.41
1:C:1118:ASP:OD1	1:C:1118:ASP:C	2.63	0.41
1:B:1118:ASP:OD1	1:B:1118:ASP:C	2.63	0.41
1:B:922:LEU:C	1:B:922:LEU:HD23	2.46	0.41
1:A:979:ASP:OD1	1:A:983:ARG:NH1	2.54	0.40
1:B:744:GLY:O	1:B:745:ASP:CG	2.63	0.40
1:B:979:ASP:OD1	1:B:983:ARG:NH1	2.54	0.40
1:B:860:VAL:O	1:B:860:VAL:HG23	2.22	0.40
1:C:922:LEU:C	1:C:922:LEU:HD23	2.46	0.40
1:C:979:ASP:OD1	1:C:983:ARG:NH1	2.54	0.40
1:A:1125:ASN:OD1	1:A:1127:ASP:HB2	2.22	0.40
1:C:990:GLU:HA	1:C:993:ILE:HG22	2.03	0.40
1:A:860:VAL:O	1:A:860:VAL:HG23	2.22	0.40
1:A:922:LEU:HD23	1:A:922:LEU:C	2.46	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	435/512 (85%)	425 (98%)	10 (2%)	0	100	100
1	B	435/512 (85%)	425 (98%)	10 (2%)	0	100	100
1	C	435/512 (85%)	425 (98%)	10 (2%)	0	100	100
All	All	1305/1536 (85%)	1275 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	375/443 (85%)	375 (100%)	0	100	100
1	B	375/443 (85%)	375 (100%)	0	100	100
1	C	375/443 (85%)	375 (100%)	0	100	100
All	All	1125/1329 (85%)	1125 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	784	GLN
1	A	913	GLN
1	A	914	ASN

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Mol	Chain	Res	Type
1	A	935	GLN
1	A	949	GLN
1	A	1048	HIS
1	A	1101	HIS
1	B	784	GLN
1	B	913	GLN
1	B	914	ASN
1	B	935	GLN
1	B	949	GLN
1	B	1048	HIS
1	B	1101	HIS
1	C	784	GLN
1	C	913	GLN
1	C	914	ASN
1	C	935	GLN
1	C	949	GLN
1	C	1048	HIS
1	C	1101	HIS

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
2	NAG	B	1302	1	14,14,15	0.18	0	17,19,21	0.61	1 (5%)
2	NAG	A	1302	1	14,14,15	0.17	0	17,19,21	0.60	1 (5%)
2	NAG	C	1301	1	14,14,15	0.16	0	17,19,21	0.57	0
2	NAG	B	1303	1	14,14,15	0.18	0	17,19,21	0.54	0
2	NAG	C	1302	1	14,14,15	0.16	0	17,19,21	0.60	1 (5%)
2	NAG	B	1301	1	14,14,15	0.15	0	17,19,21	0.56	0
2	NAG	A	1303	1	14,14,15	0.17	0	17,19,21	0.54	0
2	NAG	C	1303	1	14,14,15	0.17	0	17,19,21	0.55	0
2	NAG	A	1301	1	14,14,15	0.15	0	17,19,21	0.57	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
2	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1302	NAG	C1-O5-C5	2.14	115.05	112.19
2	A	1302	NAG	C1-O5-C5	2.12	115.03	112.19
2	C	1302	NAG	C1-O5-C5	2.11	115.02	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	NAG	O5-C5-C6-O6
2	B	1301	NAG	O5-C5-C6-O6
2	C	1301	NAG	O5-C5-C6-O6
2	A	1302	NAG	O5-C5-C6-O6
2	B	1302	NAG	O5-C5-C6-O6
2	C	1302	NAG	O5-C5-C6-O6
2	A	1301	NAG	C4-C5-C6-O6
2	B	1301	NAG	C4-C5-C6-O6
2	C	1301	NAG	C4-C5-C6-O6
2	A	1301	NAG	C1-C2-N2-C7
2	B	1301	NAG	C1-C2-N2-C7
2	C	1301	NAG	C1-C2-N2-C7
2	A	1301	NAG	C3-C2-N2-C7
2	B	1301	NAG	C3-C2-N2-C7
2	C	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43097. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.