



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 09:30 AM BST

PDB ID : 6RBF
Title : Mucin 2 D3 domain
Authors : Javitt, G.; Fass, D.
Deposited on : 2019-04-10
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

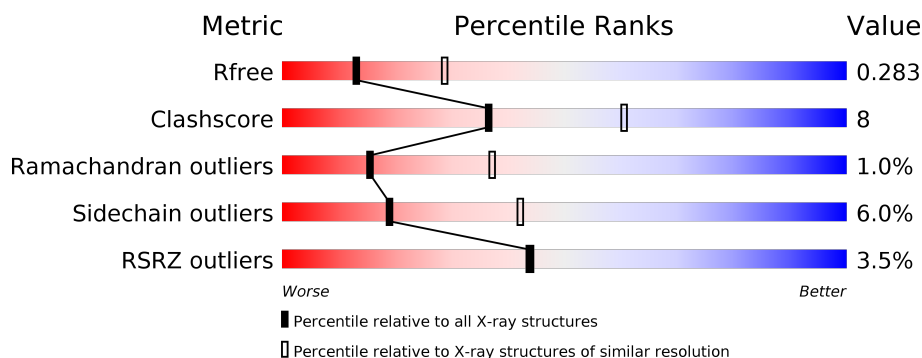
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	410	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 9%</div> </div> </div>
1	B	410	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>19%</div> <div>• 11%</div> </div> </div>
1	C	410	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>• 17%</div> </div> </div>
1	D	410	<div> <div>7%</div> <div> <div></div> <div>61%</div> <div>20%</div> <div>•• 17%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20813 atoms, of which 9800 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Mucin-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	372	Total	C	H	N	O	S	0	1	0
			5357	1752	2544	470	555	36			
1	B	364	Total	C	H	N	O	S	0	0	0
			5286	1724	2520	462	545	35			
1	C	341	Total	C	H	N	O	S	0	1	0
			4948	1626	2352	430	509	31			
1	D	341	Total	C	H	N	O	S	0	2	0
			4905	1621	2318	424	511	31			

There are 32 discrepancies between the modelled and reference sequences:

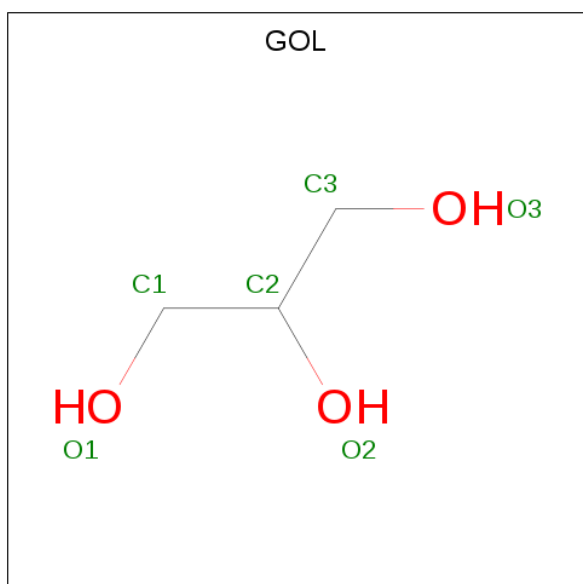
Chain	Residue	Modelled	Actual	Comment	Reference
A	856	ALA	-	expression tag	UNP Q02817
A	857	PRO	-	expression tag	UNP Q02817
A	1260	HIS	-	expression tag	UNP Q02817
A	1261	HIS	-	expression tag	UNP Q02817
A	1262	HIS	-	expression tag	UNP Q02817
A	1263	HIS	-	expression tag	UNP Q02817
A	1264	HIS	-	expression tag	UNP Q02817
A	1265	HIS	-	expression tag	UNP Q02817
B	856	ALA	-	expression tag	UNP Q02817
B	857	PRO	-	expression tag	UNP Q02817
B	1260	HIS	-	expression tag	UNP Q02817
B	1261	HIS	-	expression tag	UNP Q02817
B	1262	HIS	-	expression tag	UNP Q02817
B	1263	HIS	-	expression tag	UNP Q02817
B	1264	HIS	-	expression tag	UNP Q02817
B	1265	HIS	-	expression tag	UNP Q02817
C	856	ALA	-	expression tag	UNP Q02817
C	857	PRO	-	expression tag	UNP Q02817
C	1260	HIS	-	expression tag	UNP Q02817
C	1261	HIS	-	expression tag	UNP Q02817
C	1262	HIS	-	expression tag	UNP Q02817

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1263	HIS	-	expression tag	UNP Q02817
C	1264	HIS	-	expression tag	UNP Q02817
C	1265	HIS	-	expression tag	UNP Q02817
D	856	ALA	-	expression tag	UNP Q02817
D	857	PRO	-	expression tag	UNP Q02817
D	1260	HIS	-	expression tag	UNP Q02817
D	1261	HIS	-	expression tag	UNP Q02817
D	1262	HIS	-	expression tag	UNP Q02817
D	1263	HIS	-	expression tag	UNP Q02817
D	1264	HIS	-	expression tag	UNP Q02817
D	1265	HIS	-	expression tag	UNP Q02817

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

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



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

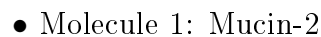


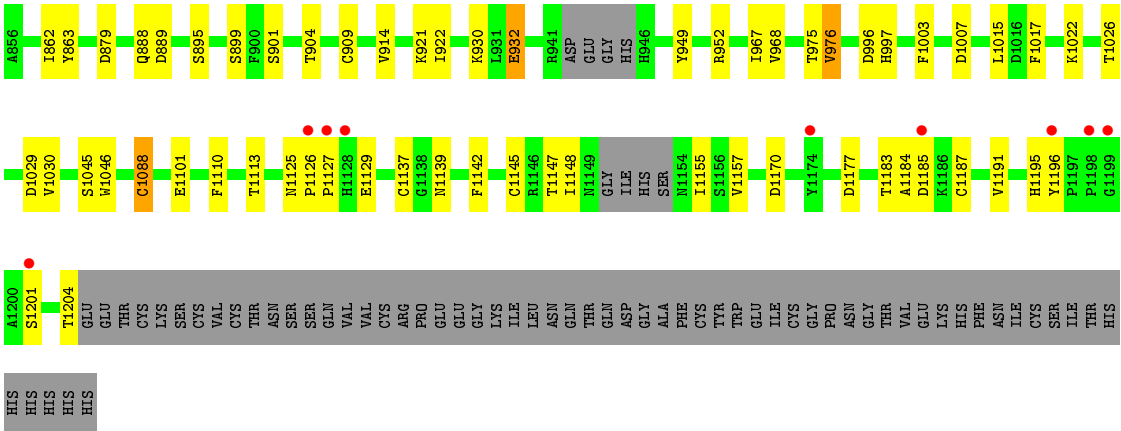
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

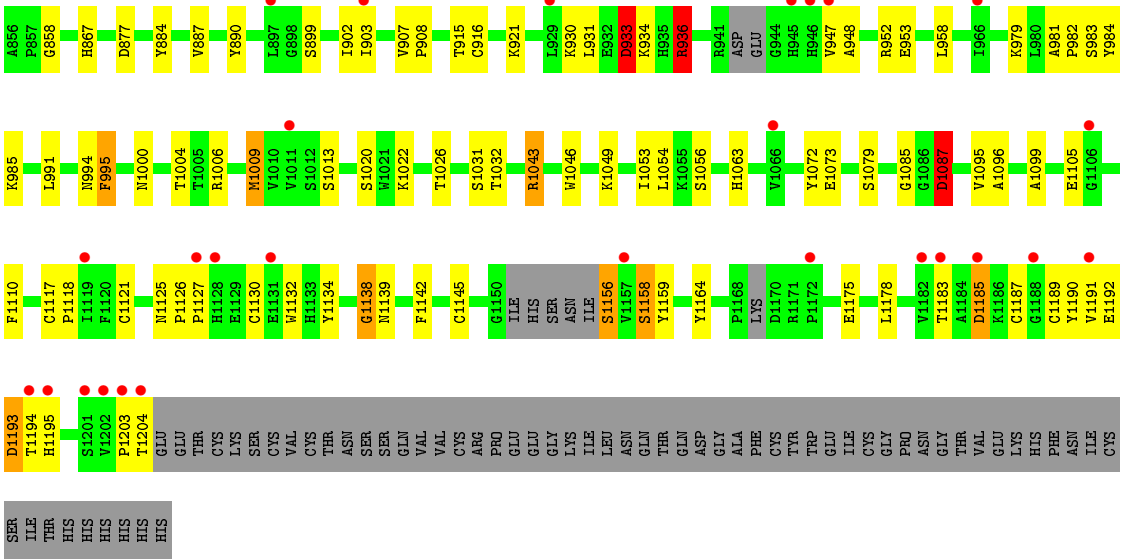
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total	O	0	0
			32	32		
6	B	47	Total	O	0	0
			47	47		
6	C	42	Total	O	0	0
			42	42		
6	D	36	Total	O	0	0
			36	36		

- Molecule 1: Mucin-2





● Molecule 1: Mucin-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	152.46 Å 156.93 Å 93.58 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 2.70 49.48 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.35-2.70) 99.8 (49.48-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.69 Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.217 , 0.283 0.217 , 0.283	Depositor DCC
R_{free} test set	3099 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20813	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GOL, CA, NAG, SO4

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	0.72	3/2889 (0.1%)	0.74	0/3938
1	B	0.73	1/2838 (0.0%)	0.77	0/3866
1	C	0.70	2/2670 (0.1%)	0.75	0/3641
1	D	0.66	1/2664 (0.0%)	0.75	3/3633 (0.1%)
All	All	0.70	7/11061 (0.1%)	0.75	3/15078 (0.0%)

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	D	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1089	GLU	CG-CD	7.03	1.62	1.51
1	C	1088	CYS	CB-SG	6.71	1.93	1.82
1	A	916	CYS	CB-SG	-5.63	1.72	1.81
1	D	916	CYS	CB-SG	-5.51	1.72	1.81
1	A	1130	CYS	CB-SG	-5.35	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1043	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	D	1087	ASP	CB-CG-OD1	-5.31	113.53	118.30
1	D	936	ARG	CG-CD-NE	-5.16	100.96	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1138	GLY	Peptide

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	2813	2544	2542	42	0
1	B	2766	2520	2517	42	0
1	C	2596	2352	2351	30	0
1	D	2587	2318	2316	53	0
2	A	6	8	8	1	0
2	B	12	16	16	0	0
3	A	14	14	13	3	0
3	B	28	28	26	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	15	0	0	0	0
5	C	5	0	0	1	0
5	D	10	0	0	1	0
6	A	32	0	0	0	0
6	B	47	0	0	0	0
6	C	42	0	0	2	0
6	D	36	0	0	0	0
All	All	11013	9800	9789	163	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.

The worst 5 of 163 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:C:1022:LYS:NZ	1:C:1029:ASP:OD1	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1302:NAG:H83	3:A:1302:NAG:H3	1.55	0.85
1:D:1054:LEU:HD21	1:D:1095:VAL:HG22	1.64	0.78
1:B:889:ASP:OD2	1:B:899:SER:HB3	1.87	0.74
1:D:1043:ARG:NH2	1:D:1087:ASP:OD1	2.23	0.72

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 X-ray entries followed by that with respect to entries of similar resolution.

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	367/410 (90%)	334 (91%)	32 (9%)	1 (0%)	41	66
1	B	358/410 (87%)	327 (91%)	25 (7%)	6 (2%)	9	23
1	C	336/410 (82%)	304 (90%)	30 (9%)	2 (1%)	25	50
1	D	335/410 (82%)	291 (87%)	39 (12%)	5 (2%)	10	26
All	All	1396/1640 (85%)	1256 (90%)	126 (9%)	14 (1%)	15	37

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	942	ASP
1	B	1122	ASP
1	B	943	GLU
1	D	933	ASP
1	B	890	TYR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	315/366 (86%)	300 (95%)	15 (5%)	25	53
1	B	312/366 (85%)	293 (94%)	19 (6%)	18	41
1	C	289/366 (79%)	276 (96%)	13 (4%)	27	55
1	D	285/366 (78%)	260 (91%)	25 (9%)	10	23
All	All	1201/1464 (82%)	1129 (94%)	72 (6%)	19	42

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1210	SER
1	C	1101	GLU
1	D	1185	ASP
1	B	1216	SER
1	C	976	VAL

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1304	1	14,14,15	0.72	1 (7%)	17,19,21	0.78	0
5	SO4	D	1302	-	4,4,4	0.22	0	6,6,6	0.21	0
5	SO4	B	1305	-	4,4,4	0.16	0	6,6,6	0.36	0
3	NAG	B	1301	1	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
5	SO4	B	1307	-	4,4,4	0.25	0	6,6,6	0.52	0
5	SO4	C	1301	-	4,4,4	0.29	0	6,6,6	0.17	0
2	GOL	B	1302	-	5,5,5	2.39	2 (40%)	5,5,5	0.88	0
3	NAG	A	1302	1	14,14,15	0.88	2 (14%)	17,19,21	1.49	3 (17%)
2	GOL	A	1301	-	5,5,5	1.21	0	5,5,5	1.01	0
5	SO4	D	1301	-	4,4,4	0.20	0	6,6,6	0.23	0
2	GOL	B	1303	-	5,5,5	1.46	1 (20%)	5,5,5	0.81	0
5	SO4	B	1306	-	4,4,4	0.22	0	6,6,6	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
2	GOL	B	1302	-	-	2/4/4/4	-
3	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
2	GOL	A	1301	-	-	2/4/4/4	-
2	GOL	B	1303	-	-	2/4/4/4	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1302	GOL	C1-C2	3.68	1.66	1.51
2	B	1302	GOL	C3-C2	3.31	1.65	1.51
3	B	1304	NAG	O5-C1	2.34	1.47	1.43
3	A	1302	NAG	C1-C2	2.31	1.55	1.52
2	B	1303	GOL	C1-C2	2.26	1.61	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	NAG	C2-N2-C7	3.66	128.12	122.90
3	A	1302	NAG	C1-C2-N2	3.42	116.33	110.49
3	B	1301	NAG	C1-O5-C5	2.85	116.05	112.19
3	A	1302	NAG	O4-C4-C3	-2.03	105.65	110.35

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1302	GOL	O1-C1-C2-C3
2	B	1303	GOL	C1-C2-C3-O3
2	B	1303	GOL	O2-C2-C3-O3
3	B	1304	NAG	C4-C5-C6-O6
3	A	1302	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1301	SO4	1	0
3	A	1302	NAG	3	0
2	A	1301	GOL	1	0
5	D	1301	SO4	1	0

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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	372/410 (90%)	0.04	7 (1%) 66 69	25, 52, 89, 127	0
1	B	364/410 (88%)	0.13	7 (1%) 66 69	27, 47, 77, 116	0
1	C	341/410 (83%)	0.17	9 (2%) 56 57	25, 48, 98, 121	0
1	D	341/410 (83%)	0.28	27 (7%) 12 10	27, 56, 111, 172	0
All	All	1418/1640 (86%)	0.15	50 (3%) 44 44	25, 51, 98, 172	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1128	HIS	6.7
1	B	1208	CYS	5.3
1	A	1207	THR	5.3
1	D	1172	PRO	5.0
1	D	946	HIS	4.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	1301	6/6	0.80	0.29	50,61,68,71	0
2	GOL	B	1302	6/6	0.83	0.28	42,77,117,117	0
5	SO4	D	1302	5/5	0.83	0.27	92,98,126,169	0
2	GOL	B	1303	6/6	0.84	0.26	51,69,89,89	0
5	SO4	B	1307	5/5	0.85	0.16	73,77,101,109	0
3	NAG	A	1302	14/15	0.87	0.16	56,71,83,85	0
5	SO4	C	1301	5/5	0.88	0.16	71,82,95,102	0
3	NAG	B	1301	14/15	0.91	0.17	54,74,100,102	0
4	CA	D	1303	1/1	0.93	0.07	83,83,83,83	0
3	NAG	B	1304	14/15	0.93	0.26	66,76,91,91	0
5	SO4	D	1301	5/5	0.93	0.13	85,101,114,117	0
4	CA	B	1308	1/1	0.95	0.05	65,65,65,65	0
4	CA	A	1303	1/1	0.95	0.06	66,66,66,66	0
4	CA	C	1302	1/1	0.97	0.06	57,57,57,57	0
5	SO4	B	1306	5/5	0.97	0.19	57,58,68,71	0
5	SO4	B	1305	5/5	0.98	0.17	48,63,67,67	0

6.5 Other polymers ⓘ

There are no such residues in this entry.