



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2016 – 11:28 PM EDT

PDB ID : 5FIB
Title : Open form of murine Acid Sphingomyelinase
Authors : Gorelik, A.; Illes, K.; Heinz, L.X.; Superti-Furga, G.; Nagar, B.
Deposited on : 2015-12-22
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

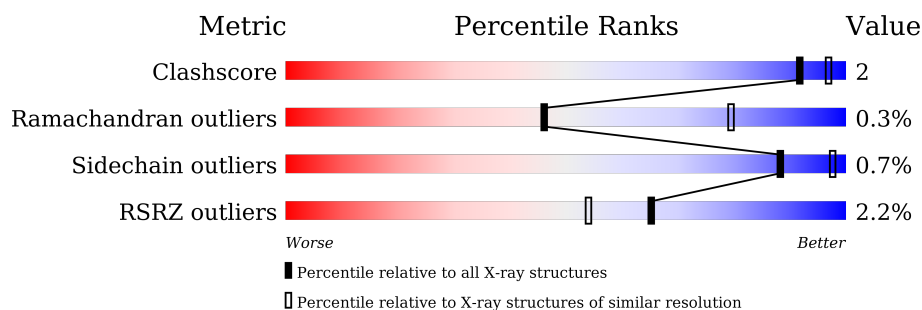
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	538	
1	B	538	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	715	-	-	-	X
3	NAG	A	720	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	719	-	-	-	X
4	FUC	A	710	-	-	-	X
4	FUC	A	718	-	-	-	X
4	FUC	B	716	-	-	-	X
7	SO4	A	726	-	-	-	X
7	SO4	A	730	-	-	-	X
7	SO4	A	731	-	-	-	X
7	SO4	B	722	-	-	-	X
7	SO4	B	723	-	-	-	X
7	SO4	B	724	-	-	-	X
7	SO4	B	726	-	-	-	X
7	SO4	B	727	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 17590 atoms, of which 8565 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 Spingomyelin phosphodiesterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	534	Total	C	H	N	O	S	0	0	0
			8303	2721	4073	735	751	23			
1	B	534	Total	C	H	N	O	S	0	1	0
			8326	2732	4082	737	752	23			

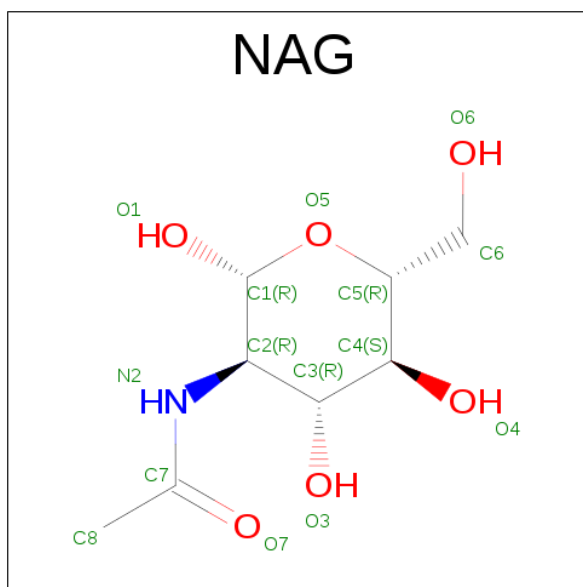
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ASP	-	expression tag	UNP Q04519
A	75	ARG	-	expression tag	UNP Q04519
A	76	HIS	-	expression tag	UNP Q04519
A	77	HIS	-	expression tag	UNP Q04519
A	78	HIS	-	expression tag	UNP Q04519
A	79	HIS	-	expression tag	UNP Q04519
A	80	HIS	-	expression tag	UNP Q04519
A	81	HIS	-	expression tag	UNP Q04519
A	82	LYS	-	expression tag	UNP Q04519
A	83	LEU	-	expression tag	UNP Q04519
B	74	ASP	-	expression tag	UNP Q04519
B	75	ARG	-	expression tag	UNP Q04519
B	76	HIS	-	expression tag	UNP Q04519
B	77	HIS	-	expression tag	UNP Q04519
B	78	HIS	-	expression tag	UNP Q04519
B	79	HIS	-	expression tag	UNP Q04519
B	80	HIS	-	expression tag	UNP Q04519
B	81	HIS	-	expression tag	UNP Q04519
B	82	LYS	-	expression tag	UNP Q04519
B	83	LEU	-	expression tag	UNP Q04519

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	3	Total	Zn	0	0
			3	3		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



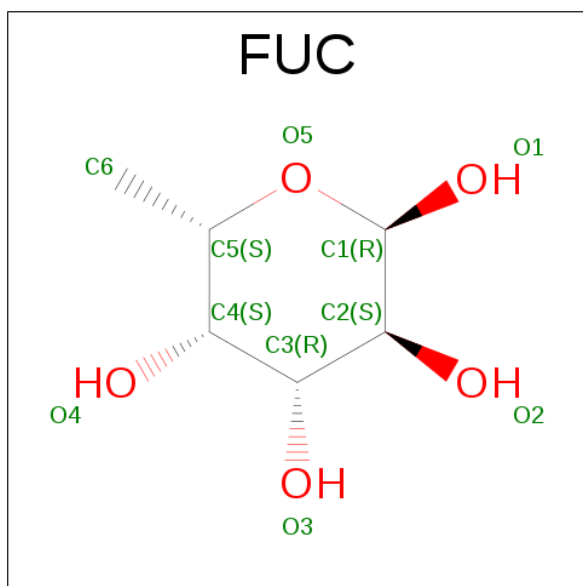
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			26	8	12	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



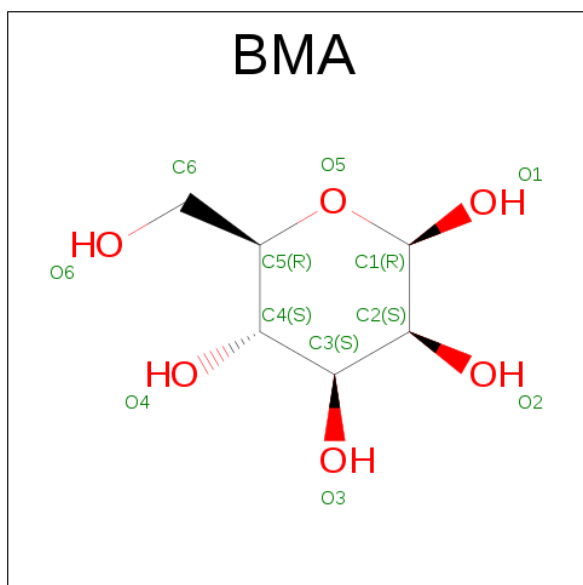
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			21	6	11	4		
4	A	1	Total	C	H	O	0	0
			21	6	11	4		
4	A	1	Total	C	H	O	0	0
			21	6	11	4		
4	A	1	Total	C	H	O	0	0
			21	6	11	4		

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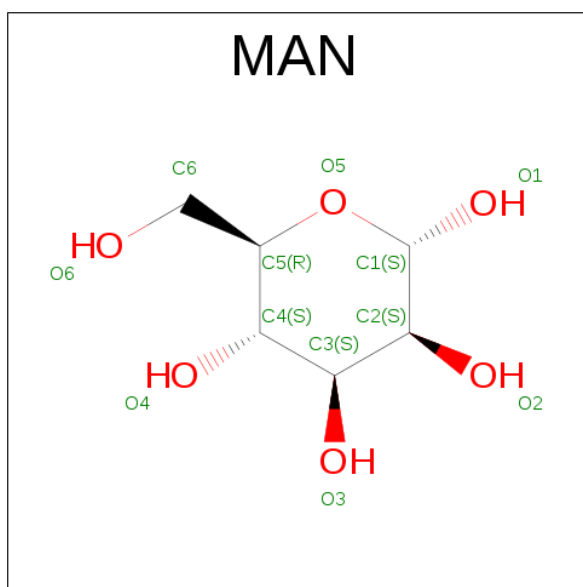
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			21	6	11	4		
4	B	1	Total	C	H	O	0	0
			21	6	11	4		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



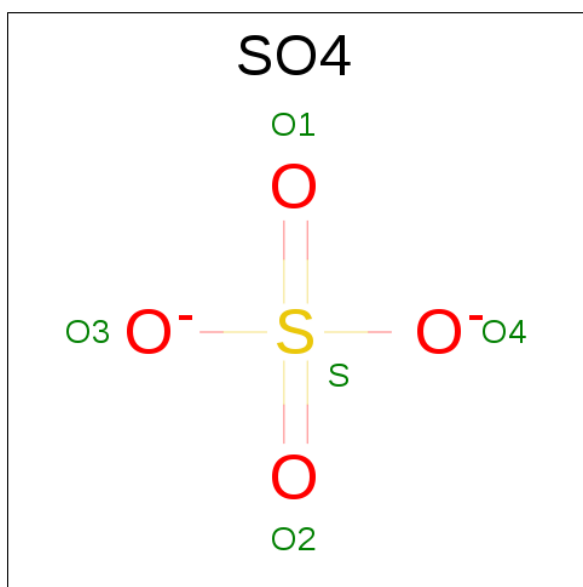
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			20	6	9	5		
5	A	1	Total	C	H	O	0	0
			22	6	11	5		
5	B	1	Total	C	H	O	0	0
			20	6	9	5		
5	B	1	Total	C	H	O	0	0
			20	6	9	5		
5	B	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			22	6	11	5		
6	A	1	Total	C	H	O	0	0
			22	6	11	5		
6	B	1	Total	C	H	O	0	0
			22	6	11	5		
6	B	1	Total	C	H	O	0	0
			22	6	11	5		
6	B	1	Total	C	H	O	0	0
			22	6	11	5		
6	B	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

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

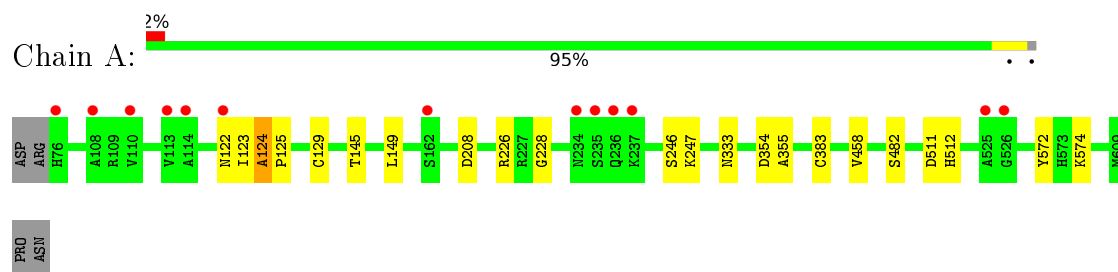
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	14	Total	O	0	0
			14	14		
8	B	16	Total	O	0	0
			16	16		

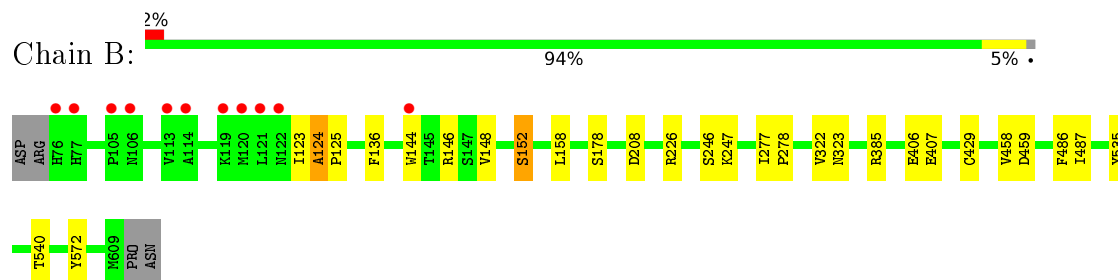
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Sphingomyelin phosphodiesterase



- Molecule 1: Sphingomyelin phosphodiesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	181.17Å 181.17Å 109.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.70 – 2.80 45.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	73.2 (45.70-2.80) 65.4 (45.70-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.190 , 0.237 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17590	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, SO4, FUC, MAN

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	0.25	0/4379	0.42	0/5993
1	B	0.25	0/4395	0.42	0/6016
All	All	0.25	0/8774	0.42	0/12009

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4230	4073	4072	13	1
1	B	4244	4082	4082	19	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	140	129	119	2	0
3	B	98	90	83	3	0
4	A	40	44	40	2	0
4	B	20	22	20	0	1
5	A	22	20	18	0	0
5	B	33	28	25	3	0
6	A	22	22	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	55	55	50	3	0
7	A	50	0	0	1	0
7	B	35	0	0	0	0
8	A	14	0	0	0	0
8	B	16	0	0	1	0
All	All	9025	8565	8529	37	1

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 2.

All (37) 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:152:SER:OG	6:B:718:MAN:O4	1.94	0.84
1:B:152:SER:HG	6:B:718:MAN:HO4	1.32	0.74
3:A:707:NAG:O5	4:A:708:FUC:O2	2.10	0.67
1:A:482:SER:O	1:A:574:LYS:NZ	2.28	0.66
1:B:124:ALA:HB1	1:B:125:PRO:CD	2.29	0.62
1:B:407:GLU:OE1	8:B:801:HOH:O	2.16	0.62
1:B:208:ASP:OD1	1:B:226:ARG:NH1	2.38	0.56
1:A:124:ALA:HB1	1:A:125:PRO:CD	2.36	0.55
1:A:228:GLY:N	7:A:729:SO4:O2	2.41	0.52
1:A:511:ASP:OD1	1:A:512:HIS:N	2.43	0.50
1:B:458:VAL:HG11	1:B:572:TYR:CZ	2.47	0.50
1:A:458:VAL:HG11	1:A:572:TYR:CE2	2.46	0.50
1:A:124:ALA:HB1	1:A:125:PRO:HD2	1.93	0.49
5:B:711:BMA:C2	3:B:715:NAG:HO3	2.17	0.49
1:B:124:ALA:HB1	1:B:125:PRO:HD2	1.95	0.47
1:A:208:ASP:OD1	1:A:226:ARG:NH1	2.48	0.46
1:A:246:SER:OG	1:A:247:LYS:N	2.47	0.46
1:B:406:GLU:OE1	6:B:708:MAN:O3	2.33	0.46
1:B:123:ILE:HG22	1:B:124:ALA:N	2.31	0.46
1:B:144[A]:TRP:CZ2	1:B:148:VAL:HG21	2.51	0.46
1:B:277:ILE:HB	1:B:278:PRO:HD3	1.97	0.45
1:B:158:LEU:HD23	1:B:158:LEU:N	2.32	0.44
1:A:458:VAL:HG11	1:A:572:TYR:CZ	2.52	0.44
1:B:486:PHE:HA	1:B:487:ILE:HA	1.80	0.44
1:B:385:ARG:NH1	1:B:429:CYS:O	2.50	0.44
1:B:322:VAL:O	1:B:323:ASN:HB2	2.19	0.42
1:A:123:ILE:HG22	1:A:124:ALA:N	2.34	0.42
1:A:123:ILE:CG2	1:A:124:ALA:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:707:NAG:H62	4:A:708:FUC:O2	2.20	0.42
1:B:535:TYR:HB2	1:B:540:THR:HG21	2.01	0.42
1:B:123:ILE:HG22	1:B:124:ALA:H	1.85	0.42
1:A:145:THR:HA	1:A:149:LEU:HB2	2.03	0.41
1:A:354:ASP:OD1	1:A:355:ALA:N	2.54	0.41
5:B:711:BMA:HO2	3:B:715:NAG:C3	2.20	0.41
1:B:246:SER:OG	1:B:247:LYS:N	2.54	0.40
1:B:458:VAL:CG1	1:B:459:ASP:N	2.85	0.40
5:B:717:BMA:O2	3:B:720:NAG:H4	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:O	4:B:716:FUC:O3[7_553]	2.07	0.13

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 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	532/538 (99%)	501 (94%)	29 (6%)	2 (0%)	39	74
1	B	533/538 (99%)	502 (94%)	30 (6%)	1 (0%)	52	84
All	All	1065/1076 (99%)	1003 (94%)	59 (6%)	3 (0%)	46	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	ALA
1	A	124	ALA
1	A	333	ASN

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 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	456/460 (99%)	454 (100%)	2 (0%)	93	98
1	B	457/460 (99%)	453 (99%)	4 (1%)	84	96
All	All	913/920 (99%)	907 (99%)	6 (1%)	88	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	CYS
1	A	383	CYS
1	B	136	PHE
1	B	146	ARG
1	B	152	SER
1	B	178	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	HIS
1	A	334	GLN
1	B	290	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 6 are monoatomic - leaving 52 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	A	704	1,3,4	14,14,15	0.46	0	15,19,21	1.07	1 (6%)
4	FUC	A	705	3	10,10,11	1.00	1 (10%)	13,14,16	1.11	1 (7%)
3	NAG	A	706	3	14,14,15	1.82	2 (14%)	15,19,21	1.21	2 (13%)
3	NAG	A	707	1,3,4	14,14,15	0.46	0	15,19,21	0.91	1 (6%)
4	FUC	A	708	3	10,10,11	1.72	3 (30%)	13,14,16	1.62	4 (30%)
3	NAG	A	709	3	14,14,15	0.63	0	15,19,21	0.90	1 (6%)
4	FUC	A	710	3	10,10,11	1.37	1 (10%)	13,14,16	1.96	3 (23%)
5	BMA	A	711	3,6	11,11,12	1.12	0	15,15,17	1.48	3 (20%)
6	MAN	A	712	5	11,11,12	0.97	1 (9%)	15,15,17	1.25	3 (20%)
6	MAN	A	713	5	11,11,12	0.83	1 (9%)	15,15,17	1.14	2 (13%)
3	NAG	A	714	1,3,4	14,14,15	0.54	0	15,19,21	0.39	0
3	NAG	A	715	3,5	14,14,15	0.44	0	15,19,21	0.94	1 (6%)
3	NAG	A	716	1,3	14,14,15	0.24	0	15,19,21	0.36	0
3	NAG	A	717	3	14,14,15	0.32	0	15,19,21	0.77	1 (6%)
4	FUC	A	718	3	10,10,11	1.49	1 (10%)	13,14,16	2.01	3 (23%)
5	BMA	A	719	3	11,11,12	0.58	0	15,15,17	0.93	1 (6%)
3	NAG	A	720	1,3,4	14,14,15	0.38	0	15,19,21	0.45	0
3	NAG	A	721	3,5	14,14,15	0.25	0	15,19,21	0.38	0
7	SO4	A	722	-	4,4,4	0.24	0	6,6,6	0.07	0
7	SO4	A	723	-	4,4,4	0.22	0	6,6,6	0.08	0
7	SO4	A	724	-	4,4,4	0.21	0	6,6,6	0.07	0
7	SO4	A	725	-	4,4,4	0.23	0	6,6,6	0.07	0
7	SO4	A	726	-	4,4,4	0.23	0	6,6,6	0.07	0
7	SO4	A	727	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	A	728	-	4,4,4	0.23	0	6,6,6	0.06	0
7	SO4	A	729	-	4,4,4	0.23	0	6,6,6	0.07	0
7	SO4	A	730	-	4,4,4	0.21	0	6,6,6	0.06	0
7	SO4	A	731	-	4,4,4	0.23	0	6,6,6	0.06	0
3	NAG	B	704	1	14,14,15	0.19	0	15,19,21	0.38	0
4	FUC	B	705	3	10,10,11	1.46	1 (10%)	13,14,16	1.92	3 (23%)
5	BMA	B	706	3,6	11,11,12	0.66	0	15,15,17	1.21	1 (6%)
6	MAN	B	707	5	11,11,12	0.81	1 (9%)	15,15,17	1.68	4 (26%)
6	MAN	B	708	5	11,11,12	1.38	2 (18%)	15,15,17	1.93	4 (26%)
3	NAG	B	709	1,3,4	14,14,15	0.65	1 (7%)	15,19,21	0.59	0
3	NAG	B	710	3,5	14,14,15	0.23	0	15,19,21	0.39	0
5	BMA	B	711	3,6	11,11,12	0.79	0	15,15,17	1.05	2 (13%)
6	MAN	B	712	5	11,11,12	0.70	0	15,15,17	1.06	2 (13%)
6	MAN	B	713	5	11,11,12	0.84	1 (9%)	15,15,17	1.00	1 (6%)
3	NAG	B	714	1,3	14,14,15	0.28	0	15,19,21	0.43	0
3	NAG	B	715	3,5	14,14,15	0.30	0	15,19,21	0.49	0
4	FUC	B	716	3	10,10,11	1.74	3 (30%)	13,14,16	2.79	4 (30%)
5	BMA	B	717	3,6	11,11,12	0.95	0	15,15,17	1.43	3 (20%)
6	MAN	B	718	5	11,11,12	0.77	0	15,15,17	1.04	2 (13%)
3	NAG	B	719	1,3,4	14,14,15	0.58	0	15,19,21	0.54	0
3	NAG	B	720	3,5	14,14,15	0.37	0	15,19,21	0.95	1 (6%)
7	SO4	B	721	-	4,4,4	0.23	0	6,6,6	0.07	0
7	SO4	B	722	-	4,4,4	0.22	0	6,6,6	0.07	0
7	SO4	B	723	-	4,4,4	0.22	0	6,6,6	0.06	0
7	SO4	B	724	-	4,4,4	0.22	0	6,6,6	0.06	0
7	SO4	B	725	-	4,4,4	0.24	0	6,6,6	0.06	0
7	SO4	B	726	-	4,4,4	0.22	0	6,6,6	0.06	0
7	SO4	B	727	-	4,4,4	0.25	0	6,6,6	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	704	1,3,4	-	0/6/23/26	0/1/1/1
4	FUC	A	705	3	-	0/0/17/20	0/1/1/1
3	NAG	A	706	3	-	0/6/23/26	0/1/1/1
3	NAG	A	707	1,3,4	-	0/6/23/26	0/1/1/1
4	FUC	A	708	3	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	709	3	-	0/6/23/26	0/1/1/1
4	FUC	A	710	3	-	0/0/17/20	0/1/1/1
5	BMA	A	711	3,6	-	0/2/19/22	0/1/1/1
6	MAN	A	712	5	-	0/2/19/22	0/1/1/1
6	MAN	A	713	5	-	0/2/19/22	0/1/1/1
3	NAG	A	714	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	A	715	3,5	-	0/6/23/26	0/1/1/1
3	NAG	A	716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	717	3	-	0/6/23/26	0/1/1/1
4	FUC	A	718	3	-	0/0/17/20	0/1/1/1
5	BMA	A	719	3	-	0/2/19/22	0/1/1/1
3	NAG	A	720	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	A	721	3,5	-	0/6/23/26	0/1/1/1
7	SO4	A	722	-	-	0/0/0/0	0/0/0/0
7	SO4	A	723	-	-	0/0/0/0	0/0/0/0
7	SO4	A	724	-	-	0/0/0/0	0/0/0/0
7	SO4	A	725	-	-	0/0/0/0	0/0/0/0
7	SO4	A	726	-	-	0/0/0/0	0/0/0/0
7	SO4	A	727	-	-	0/0/0/0	0/0/0/0
7	SO4	A	728	-	-	0/0/0/0	0/0/0/0
7	SO4	A	729	-	-	0/0/0/0	0/0/0/0
7	SO4	A	730	-	-	0/0/0/0	0/0/0/0
7	SO4	A	731	-	-	0/0/0/0	0/0/0/0
3	NAG	B	704	1	-	0/6/23/26	0/1/1/1
4	FUC	B	705	3	-	0/0/17/20	0/1/1/1
5	BMA	B	706	3,6	-	0/2/19/22	0/1/1/1
6	MAN	B	707	5	-	0/2/19/22	0/1/1/1
6	MAN	B	708	5	-	0/2/19/22	0/1/1/1
3	NAG	B	709	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	B	710	3,5	-	0/6/23/26	0/1/1/1
5	BMA	B	711	3,6	-	0/2/19/22	1/1/1/1
6	MAN	B	712	5	-	0/2/19/22	0/1/1/1
6	MAN	B	713	5	-	0/2/19/22	0/1/1/1
3	NAG	B	714	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	715	3,5	-	0/6/23/26	0/1/1/1
4	FUC	B	716	3	-	0/0/17/20	0/1/1/1
5	BMA	B	717	3,6	-	0/2/19/22	0/1/1/1
6	MAN	B	718	5	-	0/2/19/22	0/1/1/1
3	NAG	B	719	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	B	720	3,5	-	0/6/23/26	0/1/1/1
7	SO4	B	721	-	-	0/0/0/0	0/0/0/0
7	SO4	B	722	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SO4	B	723	-	-	0/0/0/0	0/0/0/0
7	SO4	B	724	-	-	0/0/0/0	0/0/0/0
7	SO4	B	725	-	-	0/0/0/0	0/0/0/0
7	SO4	B	726	-	-	0/0/0/0	0/0/0/0
7	SO4	B	727	-	-	0/0/0/0	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	706	NAG	O5-C1	-4.88	1.35	1.43
3	B	709	NAG	O5-C1	-2.36	1.39	1.43
6	B	713	MAN	C1-C2	2.02	1.57	1.52
4	A	708	FUC	C4-C3	2.04	1.57	1.52
4	A	705	FUC	C1-C2	2.17	1.57	1.52
6	A	713	MAN	C1-C2	2.17	1.57	1.52
4	A	708	FUC	C2-C3	2.42	1.55	1.52
6	B	707	MAN	C1-C2	2.46	1.58	1.52
6	B	708	MAN	C1-C2	2.64	1.58	1.52
4	B	716	FUC	C1-C2	2.71	1.58	1.52
4	B	716	FUC	C4-C3	2.88	1.60	1.52
6	A	712	MAN	C1-C2	2.94	1.59	1.52
4	B	716	FUC	C4-C5	3.05	1.58	1.53
6	B	708	MAN	C2-C3	3.32	1.57	1.52
4	A	708	FUC	C1-C2	3.83	1.61	1.52
4	A	710	FUC	C1-C2	3.90	1.61	1.52
4	B	705	FUC	C1-C2	4.09	1.62	1.52
4	A	718	FUC	C1-C2	4.11	1.62	1.52
3	A	706	NAG	C1-C2	4.16	1.58	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	716	FUC	C1-C2-C3	-6.85	101.26	109.55
5	A	711	BMA	C1-C2-C3	-3.55	105.25	109.55
3	A	706	NAG	O5-C5-C4	-3.27	104.72	110.13
6	B	707	MAN	O2-C2-C3	-3.11	103.92	110.19
6	A	713	MAN	O2-C2-C3	-2.57	105.00	110.19
5	B	717	BMA	O5-C1-C2	-2.49	106.91	110.89
5	B	717	BMA	C1-C2-C3	-2.48	106.55	109.55
6	B	713	MAN	O2-C2-C3	-2.41	105.33	110.19
6	B	708	MAN	O2-C2-C3	-2.38	105.40	110.19
6	A	712	MAN	O2-C2-C3	-2.34	105.47	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	NAG	C3-C4-C5	-2.30	106.12	110.23
5	A	711	BMA	O5-C1-C2	-2.25	107.30	110.89
6	B	712	MAN	O2-C2-C3	-2.23	105.69	110.19
6	B	718	MAN	O2-C2-C3	-2.21	105.74	110.19
4	B	716	FUC	O5-C1-C2	-2.20	107.37	110.89
3	A	715	NAG	O4-C4-C5	-2.03	103.89	109.23
5	A	719	BMA	C1-O5-C5	2.05	115.16	112.14
6	B	708	MAN	C1-O5-C5	2.05	115.16	112.14
4	A	708	FUC	C2-C3-C4	2.06	114.64	111.05
4	A	708	FUC	C3-C4-C5	2.08	112.77	109.66
5	B	711	BMA	O3-C3-C2	2.24	114.12	110.01
5	A	711	BMA	O3-C3-C2	2.33	114.28	110.01
5	B	717	BMA	O3-C3-C2	2.35	114.31	110.01
6	A	712	MAN	C1-O5-C5	2.35	115.60	112.14
3	A	717	NAG	C1-O5-C5	2.43	115.72	112.14
4	B	705	FUC	O5-C1-C2	2.49	114.88	110.89
4	A	718	FUC	O5-C1-C2	2.50	114.89	110.89
4	A	708	FUC	C1-C2-C3	2.52	112.61	109.55
6	B	718	MAN	C1-O5-C5	2.53	115.86	112.14
6	B	707	MAN	O5-C1-C2	2.56	115.00	110.89
4	A	705	FUC	C1-C2-C3	2.62	112.73	109.55
6	A	713	MAN	C1-O5-C5	2.65	116.04	112.14
4	A	710	FUC	O5-C1-C2	2.70	115.21	110.89
3	B	720	NAG	C1-O5-C5	2.70	116.11	112.14
6	B	712	MAN	C1-O5-C5	2.72	116.14	112.14
5	B	711	BMA	C1-O5-C5	2.72	116.14	112.14
3	A	707	NAG	C1-O5-C5	2.79	116.25	112.14
6	A	712	MAN	C1-C2-C3	2.81	112.96	109.55
5	B	706	BMA	C1-O5-C5	2.89	116.39	112.14
6	B	707	MAN	C1-C2-C3	2.89	113.06	109.55
4	B	705	FUC	O5-C5-C4	2.97	114.72	109.58
3	A	706	NAG	C4-C3-C2	3.09	116.13	111.34
6	B	707	MAN	C1-O5-C5	3.16	116.79	112.14
4	A	710	FUC	O5-C5-C4	3.17	115.07	109.58
3	A	709	NAG	C1-O5-C5	3.23	116.88	112.14
6	B	708	MAN	C2-C3-C4	3.29	116.78	111.05
4	A	708	FUC	O2-C2-C1	3.35	115.94	109.23
4	A	718	FUC	O5-C5-C4	3.44	115.53	109.58
4	B	716	FUC	C3-C4-C5	3.99	115.62	109.66
4	B	716	FUC	O2-C2-C1	4.94	119.12	109.23
4	B	705	FUC	C1-C2-C3	4.97	115.57	109.55
4	A	710	FUC	C1-C2-C3	4.97	115.57	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	708	MAN	C1-C2-C3	5.12	115.76	109.55
4	A	718	FUC	C1-C2-C3	5.14	115.78	109.55

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	711	BMA	C1-C2-C3-C4-C5-O5

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	707	NAG	2	0
4	A	708	FUC	2	0
7	A	729	SO4	1	0
6	B	708	MAN	1	0
5	B	711	BMA	2	0
3	B	715	NAG	2	0
4	B	716	FUC	0	1
5	B	717	BMA	1	0
6	B	718	MAN	2	0
3	B	720	NAG	1	0

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 Fit of model and data

6.1 Protein, DNA and RNA chains

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	534/538 (99%)	-0.21	13 (2%) 62 50	16, 38, 91, 130	0
1	B	534/538 (99%)	-0.43	11 (2%) 67 56	14, 32, 83, 120	0
All	All	1068/1076 (99%)	-0.32	24 (2%) 65 54	14, 35, 86, 130	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	SER	5.3
1	A	234	ASN	5.1
1	B	76	HIS	4.1
1	B	120	MET	3.9
1	A	525	ALA	3.9
1	B	114	ALA	3.4
1	A	76	HIS	3.3
1	A	122	ASN	3.1
1	A	526	GLY	3.0
1	A	236	GLN	2.8
1	A	237	LYS	2.6
1	A	110	VAL	2.6
1	B	106	ASN	2.6
1	B	122	ASN	2.5
1	B	144[A]	TRP	2.5
1	B	113	VAL	2.4
1	B	121	LEU	2.4
1	A	108	ALA	2.4
1	B	119	LYS	2.3
1	A	113	VAL	2.2
1	A	114	ALA	2.2
1	B	105	PRO	2.2
1	B	77	HIS	2.2
1	A	162	SER	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
7	SO4	B	726	5/5	0.77	0.65	18.45	79,85,104,136	0
7	SO4	B	722	5/5	0.92	0.43	13.12	63,69,102,118	0
3	NAG	B	719	14/15	0.67	0.42	10.97	83,128,154,156	0
7	SO4	A	731	5/5	0.59	0.53	9.22	94,108,128,155	0
7	SO4	A	730	5/5	0.72	0.61	7.62	73,77,116,138	0
7	SO4	B	724	5/5	0.81	0.37	6.22	72,81,82,122	0
7	SO4	B	723	5/5	0.92	0.26	5.61	73,77,85,112	0
4	FUC	A	710	10/11	0.86	0.27	4.84	70,85,109,109	0
3	NAG	A	720	14/15	0.57	0.54	4.24	92,142,172,177	0
3	NAG	A	715	14/15	0.93	0.30	4.20	71,95,111,114	0
7	SO4	A	726	5/5	0.93	0.27	3.80	52,78,95,110	0
7	SO4	B	727	5/5	0.85	0.34	2.88	78,99,140,145	0
4	FUC	B	716	10/11	0.80	0.46	2.55	87,114,137,153	0
4	FUC	A	718	10/11	0.79	0.44	2.04	85,106,141,142	0
3	NAG	A	714	14/15	0.92	0.19	2.00	59,77,88,97	0
7	SO4	A	729	5/5	0.84	0.36	1.93	77,83,116,117	0
3	NAG	A	709	14/15	0.79	0.27	1.72	56,82,104,107	0
7	SO4	A	725	5/5	0.95	0.30	1.57	77,78,91,105	0
7	SO4	A	728	5/5	0.78	0.25	1.54	94,96,106,133	0
6	MAN	B	708	11/12	0.90	0.18	1.51	40,60,71,82	0
7	SO4	A	724	5/5	0.88	0.22	1.07	60,61,104,125	0
3	NAG	A	716	14/15	0.93	0.17	0.12	46,64,82,84	0
3	NAG	B	714	14/15	0.95	0.13	0.10	35,49,74,88	0
4	FUC	B	705	10/11	0.94	0.13	0.07	37,48,70,84	0
2	ZN	B	702	1/1	0.98	0.19	-0.01	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	FUC	A	708	10/11	0.84	0.17	-0.17	67,106,118,128	0
7	SO4	B	721	5/5	0.90	0.19	-0.24	55,61,78,85	0
7	SO4	A	722	5/5	0.95	0.18	-0.73	56,67,82,84	0
3	NAG	B	709	14/15	0.96	0.10	-0.96	40,52,63,68	0
3	NAG	B	710	14/15	0.96	0.11	-0.96	43,54,61,71	0
2	ZN	B	701	1/1	0.99	0.15	-1.27	24,24,24,24	0
2	ZN	A	702	1/1	0.98	0.16	-1.68	30,30,30,30	0
2	ZN	A	701	1/1	0.99	0.15	-1.68	29,29,29,29	0
2	ZN	A	703	1/1	0.96	0.08	-1.86	47,47,47,47	0
2	ZN	B	703	1/1	0.99	0.04	-4.34	54,54,54,54	0
3	NAG	B	704	14/15	0.78	0.39	-	67,103,130,135	0
3	NAG	A	706	14/15	0.61	0.64	-	101,155,192,206	0
5	BMA	B	717	11/12	0.60	0.55	-	71,138,169,169	0
3	NAG	A	717	14/15	0.84	0.33	-	62,99,123,124	0
7	SO4	A	723	5/5	0.94	0.14	-	34,44,66,73	0
7	SO4	A	727	5/5	0.83	0.56	-	122,122,134,147	0
6	MAN	A	712	11/12	0.70	0.57	-	90,125,150,161	0
3	NAG	A	704	14/15	0.62	0.37	-	68,147,192,192	0
6	MAN	B	713	11/12	0.62	0.56	-	88,143,170,174	0
3	NAG	B	720	14/15	0.73	0.33	-	82,126,153,165	0
3	NAG	B	715	14/15	0.84	0.26	-	63,102,131,145	0
6	MAN	B	707	11/12	0.83	0.23	-	72,90,106,118	0
6	MAN	B	712	11/12	0.59	0.55	-	85,124,156,169	0
6	MAN	A	713	11/12	0.75	0.52	-	94,129,158,164	0
5	BMA	B	711	11/12	0.61	0.41	-	95,132,160,168	0
7	SO4	B	725	5/5	0.90	0.33	-	73,80,100,102	0
6	MAN	B	718	11/12	0.68	0.32	-	104,130,166,169	0
5	BMA	B	706	11/12	0.94	0.15	-	50,73,90,90	0
5	BMA	A	711	11/12	0.73	0.30	-	82,118,148,148	0
4	FUC	A	705	10/11	0.64	0.65	-	115,166,190,212	0
3	NAG	A	721	14/15	0.69	0.43	-	77,129,159,170	0
3	NAG	A	707	14/15	0.94	0.16	-	49,66,78,95	0
5	BMA	A	719	11/12	0.65	0.58	-	100,133,164,180	0

6.5 Other polymers ⓘ

There are no such residues in this entry.