



Full wwPDB X-ray Structure Validation Report

May 7, 2014 – 11:49 PM EDT

PDB ID : 4OJC
Title : Crystal structure of the wild-type full-length trimeric ectodomain of the C. elegans fusion protein EFF-1
Authors : Krey, T.; Rey, F.A.
Deposited on : 2014-01-21
Resolution : 2.93 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

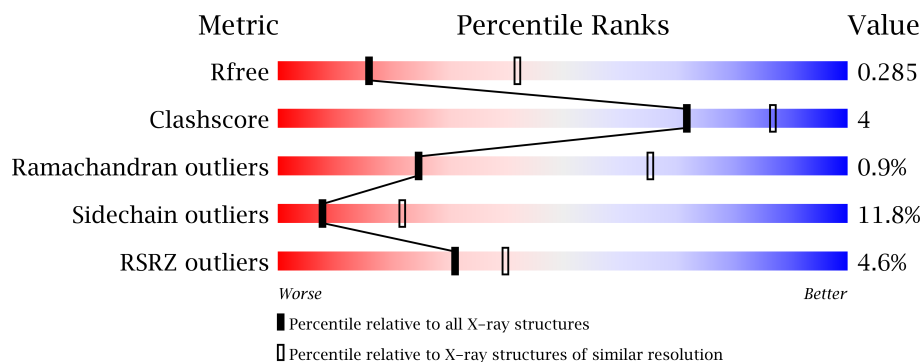
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.93 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}	66092	1424 (2.98-2.90)
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RSRZ outliers	66119	1425 (2.98-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	580	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	A	1107	-	X
4	SO4	A	1112	-	X
4	SO4	A	1114	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3773 atoms, of which 0 are hydrogen and 0 are deuterium.

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 EFF-1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3639	2277	645	690	27			

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ARG	-	EXPRESSION TAG	UNP G5ECA1
A	22	SER	-	EXPRESSION TAG	UNP G5ECA1
A	562	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	563	PRO	-	EXPRESSION TAG	UNP G5ECA1
A	564	PHE	-	EXPRESSION TAG	UNP G5ECA1
A	565	GLU	-	EXPRESSION TAG	UNP G5ECA1
A	566	ASP	-	EXPRESSION TAG	UNP G5ECA1
A	567	ASP	-	EXPRESSION TAG	UNP G5ECA1
A	568	ASP	-	EXPRESSION TAG	UNP G5ECA1
A	569	ASP	-	EXPRESSION TAG	UNP G5ECA1
A	570	LYS	-	EXPRESSION TAG	UNP G5ECA1
A	571	ALA	-	EXPRESSION TAG	UNP G5ECA1
A	572	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	573	TRP	-	EXPRESSION TAG	UNP G5ECA1
A	574	SER	-	EXPRESSION TAG	UNP G5ECA1
A	575	HIS	-	EXPRESSION TAG	UNP G5ECA1
A	576	PRO	-	EXPRESSION TAG	UNP G5ECA1
A	577	GLN	-	EXPRESSION TAG	UNP G5ECA1
A	578	PHE	-	EXPRESSION TAG	UNP G5ECA1
A	579	GLU	-	EXPRESSION TAG	UNP G5ECA1
A	580	LYS	-	EXPRESSION TAG	UNP G5ECA1
A	581	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	582	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	583	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	584	SER	-	EXPRESSION TAG	UNP G5ECA1
A	585	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	586	GLY	-	EXPRESSION TAG	UNP G5ECA1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	587	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	588	SER	-	EXPRESSION TAG	UNP G5ECA1
A	589	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	590	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	591	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	592	SER	-	EXPRESSION TAG	UNP G5ECA1
A	593	TRP	-	EXPRESSION TAG	UNP G5ECA1
A	594	SER	-	EXPRESSION TAG	UNP G5ECA1
A	595	HIS	-	EXPRESSION TAG	UNP G5ECA1
A	596	PRO	-	EXPRESSION TAG	UNP G5ECA1
A	597	GLN	-	EXPRESSION TAG	UNP G5ECA1
A	598	PHE	-	EXPRESSION TAG	UNP G5ECA1
A	599	GLU	-	EXPRESSION TAG	UNP G5ECA1
A	600	LYS	-	EXPRESSION TAG	UNP G5ECA1

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		

There are 41 discrepancies between the modelled and reference sequences:

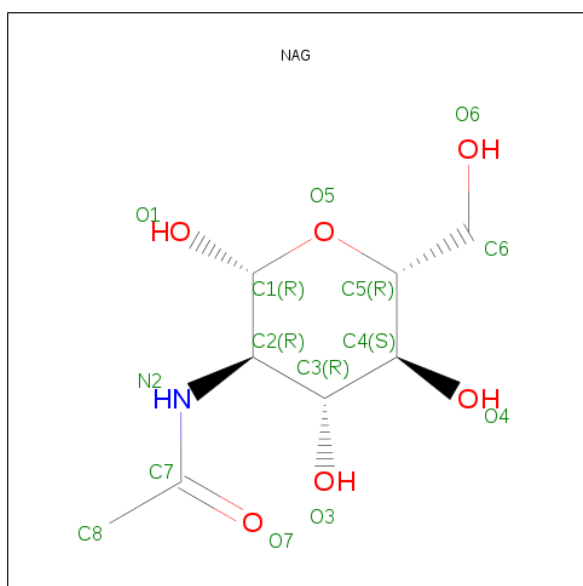
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ARG	-	EXPRESSION TAG	UNP G5ECA1
A	22	SER	-	EXPRESSION TAG	UNP G5ECA1
A	562	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	563	PRO	-	EXPRESSION TAG	UNP G5ECA1
A	564	PHE	-	EXPRESSION TAG	UNP G5ECA1
A	565	GLU	-	EXPRESSION TAG	UNP G5ECA1
A	566	ASP	-	EXPRESSION TAG	UNP G5ECA1
A	567	ASP	-	EXPRESSION TAG	UNP G5ECA1
A	568	ASP	-	EXPRESSION TAG	UNP G5ECA1
A	569	ASP	-	EXPRESSION TAG	UNP G5ECA1
A	570	LYS	-	EXPRESSION TAG	UNP G5ECA1
A	571	ALA	-	EXPRESSION TAG	UNP G5ECA1
A	572	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	573	TRP	-	EXPRESSION TAG	UNP G5ECA1
A	574	SER	-	EXPRESSION TAG	UNP G5ECA1
A	575	HIS	-	EXPRESSION TAG	UNP G5ECA1
A	576	PRO	-	EXPRESSION TAG	UNP G5ECA1
A	577	GLN	-	EXPRESSION TAG	UNP G5ECA1

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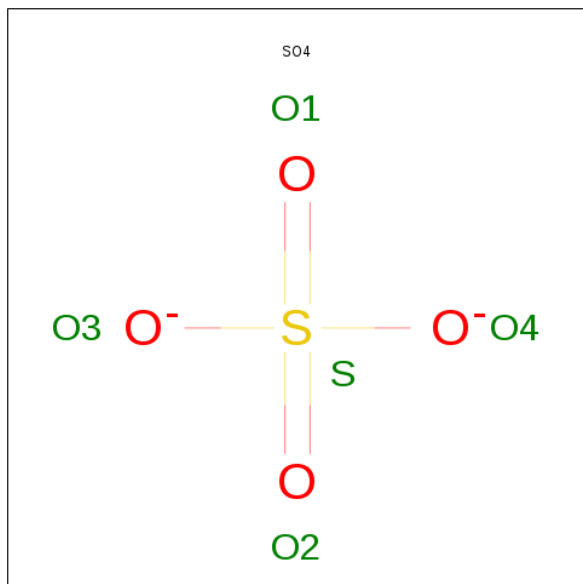
Chain	Residue	Modelled	Actual	Comment	Reference
A	578	PHE	-	EXPRESSION TAG	UNP G5ECA1
A	579	GLU	-	EXPRESSION TAG	UNP G5ECA1
A	580	LYS	-	EXPRESSION TAG	UNP G5ECA1
A	581	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	582	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	583	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	584	SER	-	EXPRESSION TAG	UNP G5ECA1
A	585	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	586	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	587	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	588	SER	-	EXPRESSION TAG	UNP G5ECA1
A	589	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	590	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	591	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	592	SER	-	EXPRESSION TAG	UNP G5ECA1
A	593	TRP	-	EXPRESSION TAG	UNP G5ECA1
A	594	SER	-	EXPRESSION TAG	UNP G5ECA1
A	595	HIS	-	EXPRESSION TAG	UNP G5ECA1
A	596	PRO	-	EXPRESSION TAG	UNP G5ECA1
A	597	GLN	-	EXPRESSION TAG	UNP G5ECA1
A	598	PHE	-	EXPRESSION TAG	UNP G5ECA1
A	599	GLU	-	EXPRESSION TAG	UNP G5ECA1
A	600	LYS	-	EXPRESSION TAG	UNP G5ECA1

- Molecule 3 is SUGAR (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	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	173.70Å 173.70Å 173.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.42 – 2.93 46.42 – 2.93	Depositor EDS
% Data completeness (in resolution range)	92.9 (46.42-2.93) 92.9 (46.42-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.220 , 0.278 0.229 , 0.285	Depositor DCC
R_{free} test set	991 reflections (5.98%)	DCC
Wilson B-factor (Å ²)	89.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.2	EDS
Estimated twinning fraction	0.023 for -l,-k,-h	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 17555 reflections (0.011%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3773	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	0/3715	0.79	1/5017 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	102	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3639	0	3529	32	0
2	A	28	0	25	1	0
3	A	42	0	39	1	0
4	A	45	0	0	1	0
5	A	19	0	0	0	0
All	All	3773	0	3593	32	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 4.

All (32) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:409:ARG:HD3	1:A:435:SER:HB3	1.76	0.68
1:A:282:GLU:HG2	1:A:283:GLU:H	1.66	0.59
1:A:196:ASN:ND2	3:A:1105:NAG:O7	2.39	0.56
1:A:336:TYR:HE2	1:A:552:ILE:HG22	1.73	0.53
1:A:75:CYS:SG	1:A:104:THR:HG22	2.49	0.53
1:A:410:ILE:HG22	1:A:489:ALA:HB2	1.90	0.52
1:A:246:LEU:HD22	1:A:254:LEU:HB2	1.91	0.52
1:A:198:THR:HG22	1:A:275:THR:OG1	2.10	0.52
1:A:334:GLN:O	1:A:552:ILE:HG23	2.10	0.51
1:A:71:HIS:HA	1:A:106:ARG:NH1	2.26	0.50
1:A:169:PHE:HB2	1:A:185:LEU:HB3	1.94	0.50
1:A:419:VAL:HB	1:A:506:GLU:HG3	1.94	0.49
1:A:336:TYR:CE2	1:A:552:ILE:HG22	2.48	0.49
1:A:69:GLY:HA2	1:A:385:ASN:OD1	2.13	0.49
1:A:339:ILE:HG23	1:A:547:LYS:HA	1.95	0.48
1:A:475:PRO:HG2	1:A:477:ILE:HG22	1.94	0.48
1:A:164:CYS:HB3	1:A:190:ARG:HG3	1.97	0.46
1:A:195:LYS:N	1:A:195:LYS:HD2	2.26	0.46
1:A:215:TYR:CD1	1:A:246:LEU:HD12	2.51	0.45
1:A:557:MET:HG2	1:A:558:ILE:HG12	1.99	0.44
1:A:305:MET:HB2	1:A:311:PHE:CE2	2.52	0.44
1:A:77:ARG:HB2	1:A:404:PHE:HE2	1.82	0.44
1:A:114:HIS:CE1	1:A:207:PRO:HG3	2.53	0.44
1:A:147:HIS:CD2	1:A:186:CYS:HB3	2.53	0.43
1:A:77:ARG:HG3	2:A:1102:NAG:H81	2.01	0.43
1:A:480:GLN:HG2	1:A:504:TYR:CE1	2.53	0.42
1:A:234:ARG:NH1	4:A:1108:SO4:S	2.91	0.42
1:A:470:MET:HG3	1:A:472:ILE:HD11	2.01	0.42
1:A:233:ILE:HG23	1:A:244:ARG:HD2	2.01	0.41
1:A:557:MET:SD	1:A:557:MET:N	2.79	0.41
1:A:329:LYS:HD2	1:A:335:THR:HB	2.01	0.41
1:A:357:GLU:N	1:A:357:GLU:OE1	2.45	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 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	449/580 (77%)	407 (91%)	38 (8%)	4 (1%)	25 65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	552	ILE
1	A	179	GLU
1	A	307	ASP
1	A	317	VAL

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	406/502 (81%)	358 (88%)	48 (12%)	8 22

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	THR
1	A	50	THR
1	A	60	ARG
1	A	62	MET
1	A	77	ARG
1	A	78	LEU
1	A	102	LEU
1	A	108	GLU
1	A	132	ILE
1	A	134	GLU

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Mol	Chain	Res	Type
1	A	135	CYS
1	A	152	CYS
1	A	154	GLU
1	A	162	SER
1	A	175	ILE
1	A	180	ASP
1	A	189	VAL
1	A	195	LYS
1	A	196	ASN
1	A	199	PHE
1	A	228	LYS
1	A	237	LEU
1	A	244	ARG
1	A	246	LEU
1	A	263	SER
1	A	274	ARG
1	A	281	THR
1	A	295	ASN
1	A	307	ASP
1	A	321	ASP
1	A	341	SER
1	A	365	SER
1	A	375	GLN
1	A	392	LEU
1	A	397	GLU
1	A	409	ARG
1	A	410	ILE
1	A	416	SER
1	A	426	LEU
1	A	441	SER
1	A	466	SER
1	A	474	LEU
1	A	488	ARG
1	A	497	LYS
1	A	547	LYS
1	A	552	ILE
1	A	554	ASP
1	A	557	MET

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 chains 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 ⓘ

2 carbohydrates 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	A	1101	1,2	12,14,15	2.31	6 (50%)	15,19,21	2.41	5 (33%)
2	NAG	A	1102	2	12,14,15	2.78	5 (41%)	15,19,21	2.74	9 (60%)

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	A	1101	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1102	2	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1102	NAG	C3-C2	5.21	1.60	1.52
2	A	1101	NAG	C2-N2	5.07	1.51	1.46
2	A	1102	NAG	C2-N2	4.98	1.51	1.46
2	A	1102	NAG	C4-C3	3.84	1.62	1.52
2	A	1102	NAG	O4-C4	3.24	1.50	1.43
2	A	1102	NAG	C4-C5	3.18	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	NAG	C4-C5	3.11	1.59	1.53
2	A	1101	NAG	C4-C3	2.95	1.60	1.52
2	A	1101	NAG	C7-N2	2.51	1.44	1.34
2	A	1101	NAG	C3-C2	2.21	1.56	1.52
2	A	1101	NAG	O4-C4	2.20	1.48	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	NAG	C2-N2-C7	7.02	131.88	123.39
2	A	1102	NAG	C2-N2-C7	6.28	131.00	123.39
2	A	1102	NAG	O4-C4-C3	3.52	118.23	110.36
2	A	1101	NAG	C4-C3-C2	3.17	117.39	110.74
2	A	1102	NAG	C6-C5-C4	3.08	120.58	113.04
2	A	1102	NAG	C8-C7-N2	-3.02	110.40	116.12
2	A	1102	NAG	O7-C7-N2	2.93	127.86	121.90
2	A	1101	NAG	O3-C3-C4	2.88	116.80	110.36
2	A	1102	NAG	O5-C5-C4	2.64	114.00	110.65
2	A	1102	NAG	O3-C3-C4	2.59	116.15	110.36
2	A	1102	NAG	C3-C2-N2	2.54	115.43	111.62
2	A	1101	NAG	C6-C5-C4	2.23	118.50	113.04
2	A	1101	NAG	C3-C4-C5	-2.18	106.26	110.17
2	A	1102	NAG	C4-C3-C2	2.12	115.19	110.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

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
3	NAG	A	1103	1	12,14,15	1.25	1 (8%)	15,19,21	2.31	5 (33%)
3	NAG	A	1104	1	12,14,15	2.00	4 (33%)	15,19,21	2.84	6 (40%)
3	NAG	A	1105	1	12,14,15	2.85	4 (33%)	15,19,21	2.97	5 (33%)
4	SO4	A	1106	-	4,4,4	0.20	0	6,6,6	0.05	0
4	SO4	A	1107	-	4,4,4	0.93	0	6,6,6	0.32	0
4	SO4	A	1108	-	4,4,4	0.38	0	6,6,6	0.20	0
4	SO4	A	1109	-	4,4,4	0.46	0	6,6,6	0.18	0
4	SO4	A	1110	-	4,4,4	0.22	0	6,6,6	0.34	0
4	SO4	A	1111	-	4,4,4	0.28	0	6,6,6	0.15	0
4	SO4	A	1112	-	4,4,4	0.27	0	6,6,6	0.17	0
4	SO4	A	1113	-	4,4,4	0.32	0	6,6,6	0.11	0
4	SO4	A	1114	-	4,4,4	0.08	0	6,6,6	0.13	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	1103	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1104	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1105	1	-	0/6/23/26	0/1/1/1
4	SO4	A	1106	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1107	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1108	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1109	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1110	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1111	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1112	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1113	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1114	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1105	NAG	C3-C2	6.01	1.61	1.52
3	A	1105	NAG	C2-N2	5.21	1.52	1.46
3	A	1105	NAG	C4-C3	3.85	1.62	1.52
3	A	1104	NAG	C4-C3	3.55	1.61	1.52
3	A	1104	NAG	C4-C5	3.28	1.60	1.53
3	A	1104	NAG	C3-C2	3.13	1.57	1.52
3	A	1104	NAG	C2-N2	2.90	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1105	NAG	C4-C5	2.90	1.59	1.53
3	A	1103	NAG	C4-C5	2.04	1.57	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1105	NAG	C2-N2-C7	8.13	133.23	123.39
3	A	1104	NAG	C3-C2-N2	7.25	122.50	111.62
3	A	1103	NAG	O5-C5-C4	5.39	117.50	110.65
3	A	1105	NAG	C6-C5-C4	4.99	125.24	113.04
3	A	1104	NAG	O5-C5-C4	4.44	116.28	110.65
3	A	1104	NAG	C2-N2-C7	4.44	128.76	123.39
3	A	1103	NAG	O3-C3-C2	-3.87	101.27	109.16
3	A	1105	NAG	C4-C3-C2	3.53	118.15	110.74
3	A	1103	NAG	C4-C3-C2	3.23	117.52	110.74
3	A	1104	NAG	C3-C4-C5	3.21	115.92	110.17
3	A	1104	NAG	O5-C5-C6	3.11	110.24	106.98
3	A	1105	NAG	O5-C5-C6	2.95	110.08	106.98
3	A	1103	NAG	C3-C4-C5	2.85	115.28	110.17
3	A	1103	NAG	C2-N2-C7	-2.63	120.21	123.39
3	A	1104	NAG	C4-C3-C2	2.24	115.45	110.74
3	A	1105	NAG	O7-C7-N2	2.14	126.26	121.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	461/580 (79%)	0.23	22 (4%)	29 37	57, 86, 134, 177	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	553	GLY	6.1
1	A	34	ARG	5.0
1	A	157	LYS	4.1
1	A	552	ILE	3.2
1	A	221	VAL	3.1
1	A	35	ALA	3.0
1	A	338	SER	2.8
1	A	158	SER	2.6
1	A	156	ASP	2.5
1	A	281	THR	2.5
1	A	554	ASP	2.4
1	A	141	THR	2.4
1	A	549	ILE	2.4
1	A	220	PHE	2.4
1	A	551	SER	2.3
1	A	496	ASP	2.3
1	A	557	MET	2.3
1	A	216	ALA	2.3
1	A	224	TYR	2.2
1	A	159	ASP	2.1
1	A	259	GLY	2.0
1	A	280	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	1102	14/15	0.31	0.57	107,111,113,113	0
2	NAG	A	1101	14/15	0.19	0.05	101,105,107,107	0

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	A	1114	5/5	0.37	5.86	207,212,213,213	0
4	SO4	A	1107	5/5	0.27	5.42	49,53,54,55	5
4	SO4	A	1112	5/5	0.23	2.04	162,167,168,168	0
3	NAG	A	1104	14/15	0.33	1.94	128,132,135,135	0
3	NAG	A	1105	14/15	0.33	1.52	143,146,149,149	0
4	SO4	A	1113	5/5	0.34	1.29	150,155,155,156	0
3	NAG	A	1103	14/15	0.17	0.43	84,88,90,90	0
4	SO4	A	1109	5/5	0.18	0.10	112,116,117,117	0
4	SO4	A	1110	5/5	0.14	-0.12	120,124,125,125	0
4	SO4	A	1111	5/5	0.12	-1.80	99,103,104,107	0
4	SO4	A	1108	5/5	0.15	-2.46	140,144,145,145	0
4	SO4	A	1106	5/5	0.37	-	84,89,90,91	5

6.5 Other polymers ⓘ

There are no such residues in this entry.