



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:51 pm GMT

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 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

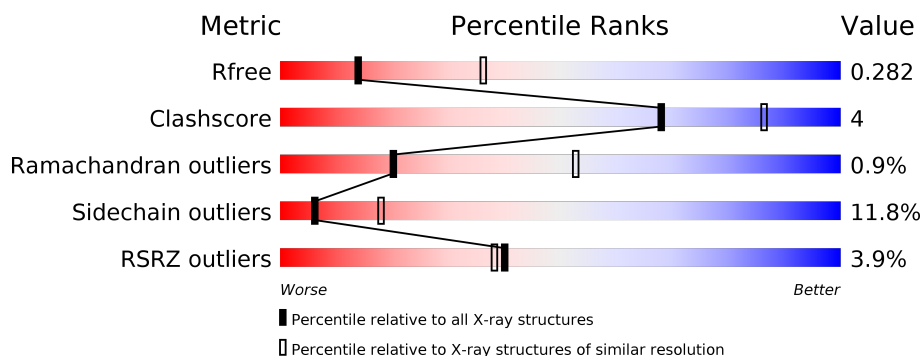
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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}	100719	2289 (2.98-2.90)
Clashscore	112137	2543 (2.98-2.90)
Ramachandran outliers	110173	2475 (2.98-2.90)
Sidechain outliers	110143	2477 (2.98-2.90)
RSRZ outliers	101464	2301 (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. 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	580	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3773 atoms, of which 0 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 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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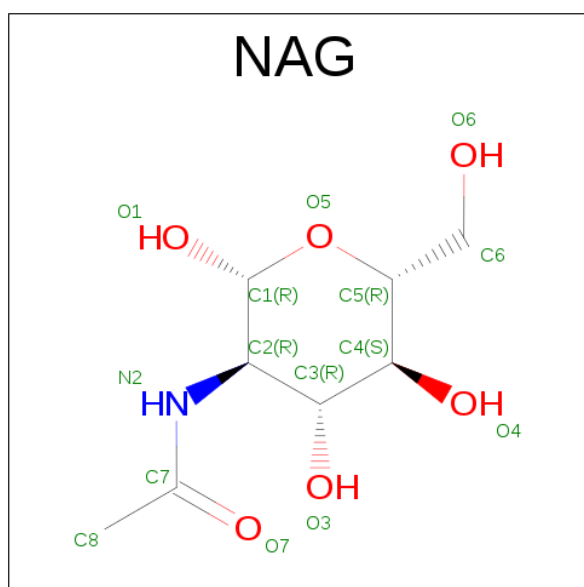
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Chain	Residue	Modelled	Actual	Comment	Reference
A	587	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	588	SER	-	EXPRESSION TAG	UNP G5ECA1
A	589	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	590	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	591	GLY	-	EXPRESSION TAG	UNP G5ECA1
A	592	SER	-	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		

- 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		

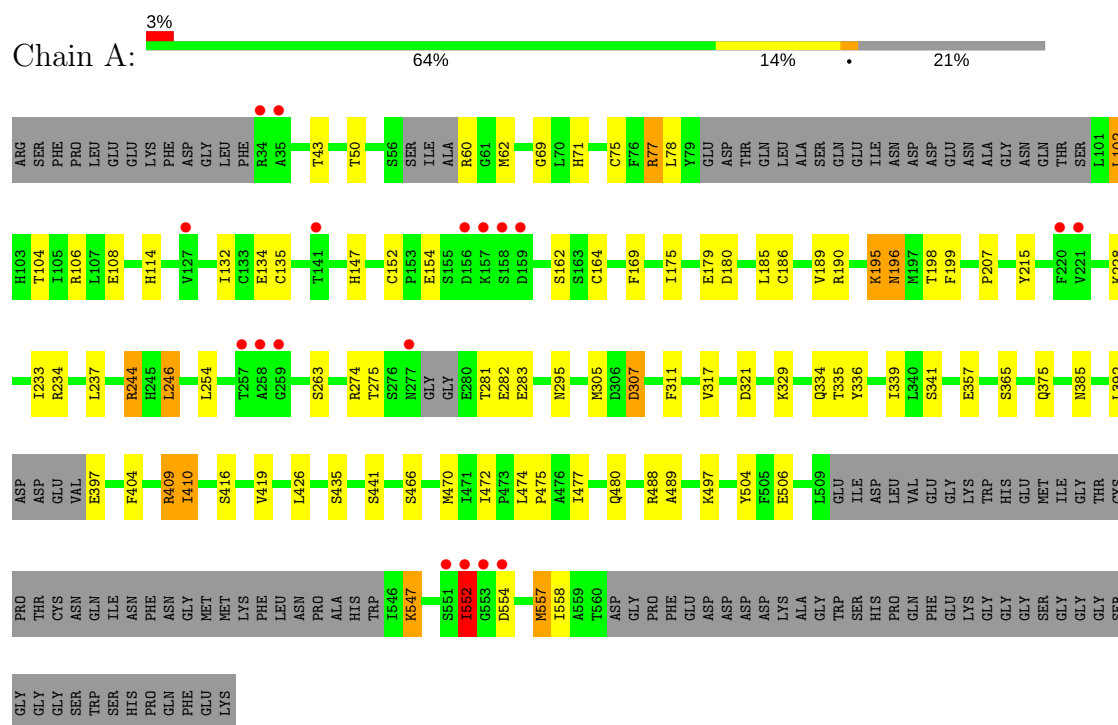
- Molecule 5 is water.

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

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 the various outlier classes 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: EFF-1A



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 0.228 , 0.282	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 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -l,-k,-h	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.

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: 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(°)	Ideal(°)
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 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 4.

All (32) 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: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:75:CYS:SG	1:A:104:THR:HG22	2.49	0.53
1:A:336:TYR:HE2	1:A:552:ILE:HG22	1.73	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%)	20	53

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%)	6	18

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

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Mol	Chain	Res	Type
1	A	108	GLU
1	A	132	ILE
1	A	134	GLU
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 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 ⓘ

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	14,14,15	1.97	6 (42%)	15,19,21	2.53	7 (46%)
2	NAG	A	1102	2	14,14,15	2.90	7 (50%)	15,19,21	2.78	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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	NAG	O4-C4	2.32	1.48	1.43
2	A	1102	NAG	O5-C1	2.60	1.48	1.43
2	A	1101	NAG	C7-N2	2.68	1.44	1.34
2	A	1101	NAG	C1-C2	2.68	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	NAG	C4-C3	3.08	1.60	1.52
2	A	1102	NAG	C2-N2	3.13	1.51	1.46
2	A	1101	NAG	C2-N2	3.18	1.51	1.46
2	A	1101	NAG	C4-C5	3.19	1.59	1.53
2	A	1102	NAG	C4-C5	3.26	1.60	1.53
2	A	1102	NAG	O4-C4	3.42	1.50	1.43
2	A	1102	NAG	C3-C2	3.68	1.60	1.52
2	A	1102	NAG	C4-C3	4.01	1.62	1.52
2	A	1102	NAG	C1-C2	6.36	1.61	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1102	NAG	C8-C7-N2	-3.16	110.40	116.11
2	A	1101	NAG	C3-C4-C5	-2.24	106.26	110.22
2	A	1102	NAG	O5-C1-C2	-2.17	108.45	111.47
2	A	1101	NAG	O7-C7-N2	2.06	125.89	121.92
2	A	1101	NAG	C6-C5-C4	2.35	118.50	113.00
2	A	1102	NAG	O3-C3-C4	2.66	116.15	110.36
2	A	1102	NAG	C4-C3-C2	2.85	115.19	111.02
2	A	1101	NAG	O3-C3-C4	2.96	116.80	110.36
2	A	1102	NAG	O7-C7-N2	3.09	127.86	121.92
2	A	1102	NAG	C6-C5-C4	3.24	120.58	113.00
2	A	1101	NAG	O5-C1-C2	3.30	116.07	111.47
2	A	1102	NAG	O4-C4-C3	3.62	118.23	110.36
2	A	1102	NAG	C1-C2-N2	3.95	117.24	110.49
2	A	1101	NAG	C4-C3-C2	4.35	117.39	111.02
2	A	1102	NAG	C2-N2-C7	5.52	131.00	122.94
2	A	1101	NAG	C2-N2-C7	6.13	131.88	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1102	NAG	1	0

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	14,14,15	1.25	2 (14%)	15,19,21	2.54	6 (40%)
3	NAG	A	1104	1	14,14,15	1.79	3 (21%)	15,19,21	1.88	5 (33%)
3	NAG	A	1105	1	14,14,15	2.27	5 (35%)	15,19,21	4.08	6 (40%)
4	SO4	A	1106	-	4,4,4	0.21	0	6,6,6	0.05	0
4	SO4	A	1107	-	4,4,4	0.52	0	6,6,6	0.28	0
4	SO4	A	1108	-	4,4,4	0.31	0	6,6,6	0.18	0
4	SO4	A	1109	-	4,4,4	0.19	0	6,6,6	0.17	0
4	SO4	A	1110	-	4,4,4	0.27	0	6,6,6	0.35	0
4	SO4	A	1111	-	4,4,4	0.32	0	6,6,6	0.22	0
4	SO4	A	1112	-	4,4,4	0.34	0	6,6,6	0.22	0
4	SO4	A	1113	-	4,4,4	0.41	0	6,6,6	0.06	0
4	SO4	A	1114	-	4,4,4	0.23	0	6,6,6	0.11	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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1103	NAG	O4-C4	2.00	1.47	1.43
3	A	1103	NAG	C4-C5	2.10	1.57	1.53
3	A	1104	NAG	C3-C2	2.28	1.57	1.52
3	A	1105	NAG	C4-C5	2.98	1.59	1.53
3	A	1105	NAG	C1-C2	3.03	1.56	1.52
3	A	1105	NAG	C2-N2	3.27	1.52	1.46
3	A	1104	NAG	C4-C5	3.36	1.60	1.53
3	A	1104	NAG	C4-C3	3.70	1.61	1.52
3	A	1105	NAG	C4-C3	4.02	1.62	1.52
3	A	1105	NAG	C3-C2	4.22	1.61	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1105	NAG	C1-O5-C5	-9.76	98.71	112.17
3	A	1103	NAG	O3-C3-C2	-3.79	101.27	109.39
3	A	1104	NAG	O5-C1-C2	-2.79	107.59	111.47
3	A	1104	NAG	C1-C2-N2	2.01	113.91	110.49
3	A	1105	NAG	O7-C7-N2	2.25	126.26	121.92
3	A	1103	NAG	C3-C4-C5	2.87	115.28	110.22
3	A	1104	NAG	C4-C3-C2	3.03	115.45	111.02
3	A	1103	NAG	O5-C1-C2	3.06	115.73	111.47
3	A	1104	NAG	C3-C4-C5	3.24	115.92	110.22
3	A	1103	NAG	C1-O5-C5	3.51	117.01	112.17
3	A	1104	NAG	C2-N2-C7	3.99	128.76	122.94
3	A	1103	NAG	C4-C3-C2	4.43	117.52	111.02
3	A	1103	NAG	C1-C2-N2	4.65	118.43	110.49
3	A	1105	NAG	C4-C3-C2	4.87	118.15	111.02
3	A	1105	NAG	C6-C5-C4	5.23	125.24	113.00
3	A	1105	NAG	C1-C2-N2	6.18	121.05	110.49
3	A	1105	NAG	C2-N2-C7	7.05	133.23	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1105	NAG	1	0
4	A	1108	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 ⓘ

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%)	0.30	18 (3%) 40 38	57, 86, 134, 177	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	553	GLY	7.5
1	A	552	ILE	4.1
1	A	157	LYS	3.7
1	A	34	ARG	3.6
1	A	554	ASP	3.1
1	A	551	SER	3.0
1	A	158	SER	2.6
1	A	141	THR	2.6
1	A	159	ASP	2.5
1	A	35	ALA	2.5
1	A	221	VAL	2.4
1	A	258	ALA	2.4
1	A	257	THR	2.1
1	A	127	VAL	2.1
1	A	259	GLY	2.1
1	A	156	ASP	2.1
1	A	277	ASN	2.1
1	A	220	PHE	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 [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
2	NAG	A	1102	14/15	0.85	0.33	0.73	107,111,113,113	0
2	NAG	A	1101	14/15	0.91	0.21	-0.04	101,105,107,107	0

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
4	SO4	A	1113	5/5	0.89	0.35	1.54	150,155,155,156	0
3	NAG	A	1104	14/15	0.86	0.31	1.52	128,132,135,135	0
3	NAG	A	1103	14/15	0.96	0.18	0.22	84,88,90,90	0
4	SO4	A	1110	5/5	0.92	0.15	-0.04	120,124,125,125	0
4	SO4	A	1108	5/5	0.91	0.15	-3.45	140,144,145,145	0
4	SO4	A	1106	5/5	0.99	0.34	-	84,89,90,91	5
4	SO4	A	1111	5/5	0.97	0.12	-	99,103,104,107	0
4	SO4	A	1112	5/5	0.68	0.23	-	162,167,168,168	0
4	SO4	A	1109	5/5	0.95	0.16	-	112,116,117,117	0
3	NAG	A	1105	14/15	0.58	0.36	-	143,146,149,149	0
4	SO4	A	1107	5/5	0.95	0.34	-	49,53,54,55	5
4	SO4	A	1114	5/5	0.64	0.46	-	207,212,213,213	0

6.5 Other polymers [i](#)

There are no such residues in this entry.