



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:30 PM UTC

PDB ID : 5NPD / pdb_00005npd
Title : Crystal Structure of D412N nucleophile mutant cjAgd31B (alpha-transglucosylase from Glycoside Hydrolase Family 31) in complex with alpha Cyclophellitol Aziridine probe CF021
Authors : Wu, L.; Davies, G.J.
Deposited on : 2017-04-16
Resolution : 1.95 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

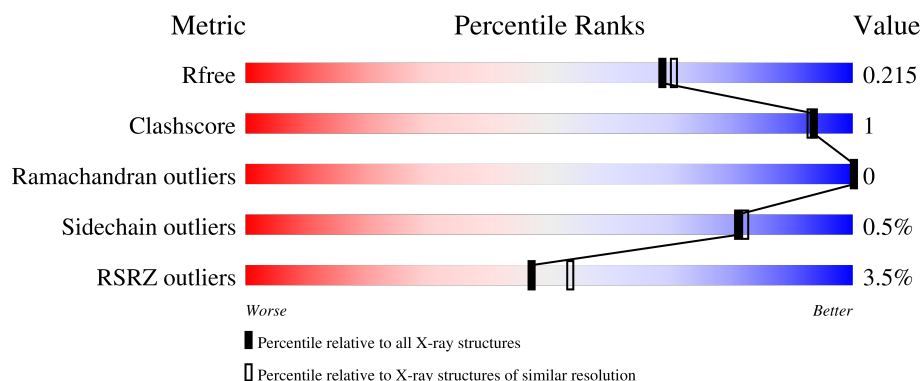
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

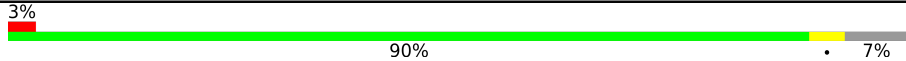
The reported resolution of this entry is 1.95 Å.

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 of 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	835	

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
6	OXL	A	916	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6860 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 Oligosaccharide 4-alpha-D-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	780	Total	C	N	O	S	3	6	0
			6278	4010	1075	1172	21			

There are 44 discrepancies between the modelled and reference sequences:

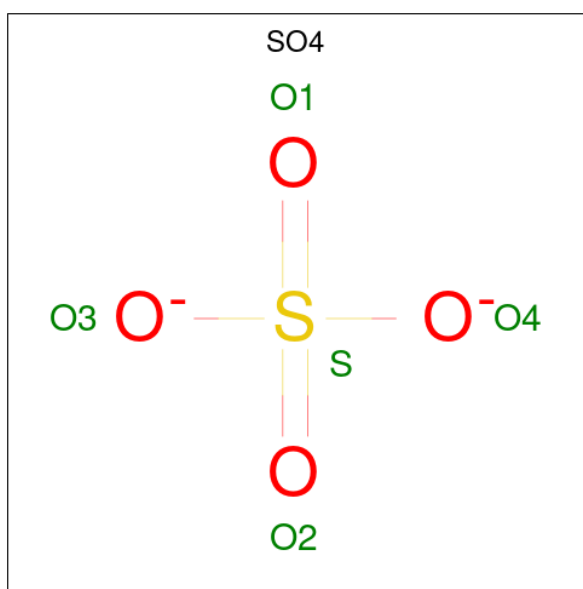
Chain	Residue	Modelled	Actual	Comment	Reference
A	412	ASN	ASP	engineered mutation	UNP B3PEE6
A	817	LYS	-	expression tag	UNP B3PEE6
A	818	GLY	-	expression tag	UNP B3PEE6
A	819	GLY	-	expression tag	UNP B3PEE6
A	820	ARG	-	expression tag	UNP B3PEE6
A	821	ALA	-	expression tag	UNP B3PEE6
A	822	ASP	-	expression tag	UNP B3PEE6
A	823	PRO	-	expression tag	UNP B3PEE6
A	824	ALA	-	expression tag	UNP B3PEE6
A	825	PHE	-	expression tag	UNP B3PEE6
A	826	LEU	-	expression tag	UNP B3PEE6
A	827	TYR	-	expression tag	UNP B3PEE6
A	828	LYS	-	expression tag	UNP B3PEE6
A	829	VAL	-	expression tag	UNP B3PEE6
A	830	VAL	-	expression tag	UNP B3PEE6
A	831	ILE	-	expression tag	UNP B3PEE6
A	832	ASN	-	expression tag	UNP B3PEE6
A	833	SER	-	expression tag	UNP B3PEE6
A	834	LYS	-	expression tag	UNP B3PEE6
A	835	LEU	-	expression tag	UNP B3PEE6
A	836	GLU	-	expression tag	UNP B3PEE6
A	837	GLY	-	expression tag	UNP B3PEE6
A	838	LYS	-	expression tag	UNP B3PEE6
A	839	PRO	-	expression tag	UNP B3PEE6
A	840	ILE	-	expression tag	UNP B3PEE6
A	841	PRO	-	expression tag	UNP B3PEE6
A	842	ASN	-	expression tag	UNP B3PEE6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	843	PRO	-	expression tag	UNP B3PEE6
A	844	LEU	-	expression tag	UNP B3PEE6
A	845	LEU	-	expression tag	UNP B3PEE6
A	846	GLY	-	expression tag	UNP B3PEE6
A	847	LEU	-	expression tag	UNP B3PEE6
A	848	ASP	-	expression tag	UNP B3PEE6
A	849	SER	-	expression tag	UNP B3PEE6
A	850	THR	-	expression tag	UNP B3PEE6
A	851	ARG	-	expression tag	UNP B3PEE6
A	852	THR	-	expression tag	UNP B3PEE6
A	853	GLY	-	expression tag	UNP B3PEE6
A	854	HIS	-	expression tag	UNP B3PEE6
A	855	HIS	-	expression tag	UNP B3PEE6
A	856	HIS	-	expression tag	UNP B3PEE6
A	857	HIS	-	expression tag	UNP B3PEE6
A	858	HIS	-	expression tag	UNP B3PEE6
A	859	HIS	-	expression tag	UNP B3PEE6

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



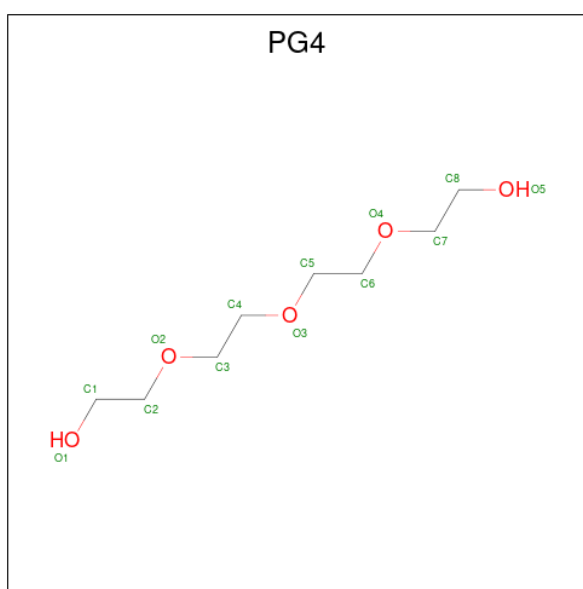
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



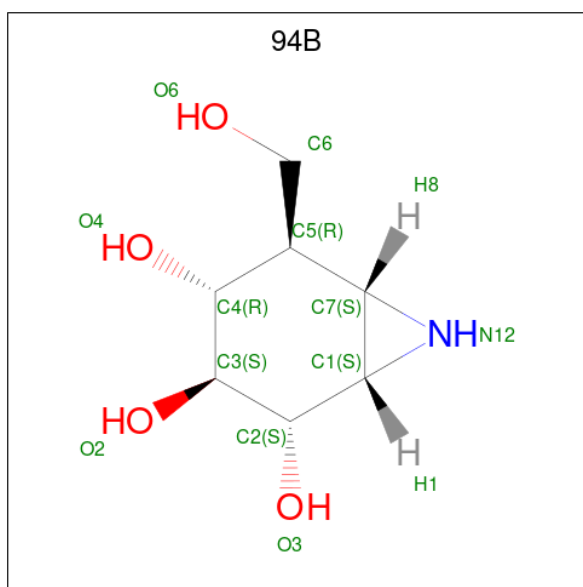
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



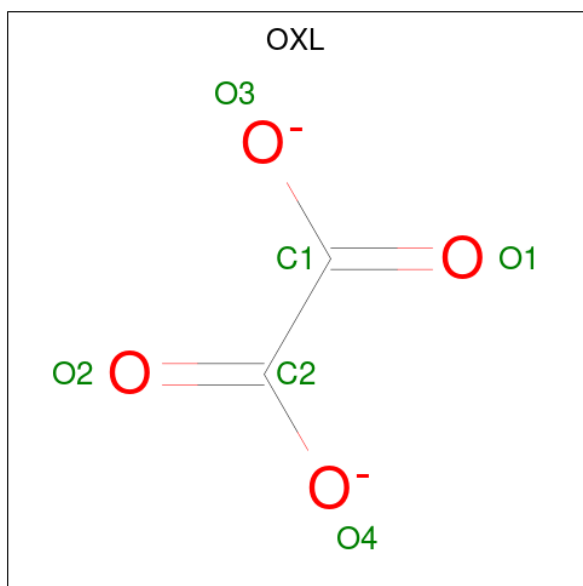
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is (1 {S},2 {S},3 {S},4 {R},5 {R},6 {S})-5-(hydroxymethyl)-7-azabicyclo[4.1.0]heptane-2,3,4-triol (CCD ID: 94B) (formula: C₇H₁₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 6 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



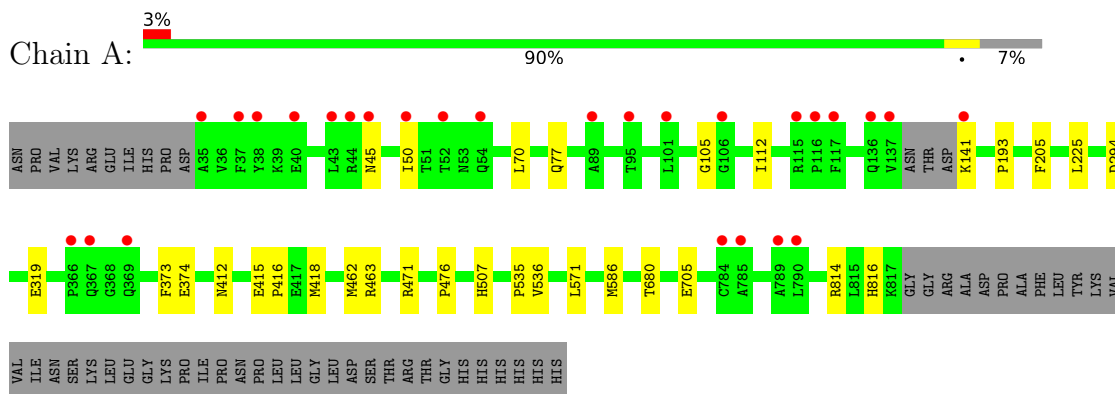
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	2	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	492	Total 492	O 492	0	0

i

- Molecule 1: Oligosaccharide 4-alpha-D-glucosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	197.31 Å 197.31 Å 102.77 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.39 – 1.95 47.39 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.39-1.95) 100.0 (47.39-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 1.95 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.171 , 0.210 0.181 , 0.215	Depositor DCC
R_{free} test set	4331 reflections (3.69%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.808	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6860	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: OXL, 94B, PG4, EDO, 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	0.89	0/6448	0.91	9/8742 (0.1%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ASN	CB-CG-ND2	-7.21	105.58	116.40
1	A	535	PRO	N-CA-C	5.96	121.81	113.53
1	A	105	GLY	N-CA-C	-5.61	104.89	112.57
1	A	586	MET	CA-C-N	-5.57	114.52	120.03
1	A	586	MET	C-N-CA	-5.57	114.52	120.03

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	6278	0	6098	17	0
2	A	35	0	0	0	0
3	A	13	0	18	0	0
4	A	24	0	36	0	1
5	A	12	0	0	1	0
6	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	492	0	0	4	1
All	All	6860	0	6152	18	2

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 1.

The worst 5 of 18 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)
5:A:915:94B:N12	7:A:1002:HOH:O	2.05	0.89
1:A:374:GLU:O	1:A:418:MET:HE1	1.96	0.66
1:A:319:GLU:OE1	7:A:1003:HOH:O	2.15	0.63
1:A:816:HIS:CD2	7:A:1001:HOH:O	2.58	0.56
1:A:50:ILE:HD11	1:A:112:ILE:HD13	1.88	0.55

All (2) 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)
7:A:1309:HOH:O	7:A:1309:HOH:O[7_556]	1.82	0.38
4:A:909:EDO:O2	4:A:909:EDO:O2[11_556]	2.18	0.02

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	782/835 (94%)	755 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	663/705 (94%)	660 (100%)	3 (0%)	81	82

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	294	ASP
1	A	680	THR
1	A	705	GLU

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

Mol	Chain	Res	Type
1	A	379	ASN
1	A	720	ASN
1	A	766	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	904	-	4,4,4	0.50	0	6,6,6	0.36	0
2	SO4	A	905	-	4,4,4	0.55	0	6,6,6	0.13	0
3	PG4	A	908	-	12,12,12	0.55	0	11,11,11	0.78	0
4	EDO	A	910	-	3,3,3	0.50	0	2,2,2	0.14	0
6	OXL	A	916	-	5,5,5	1.50	1 (20%)	6,6,6	4.61	5 (83%)
4	EDO	A	913	-	3,3,3	0.44	0	2,2,2	0.32	0
2	SO4	A	906	-	4,4,4	0.45	0	6,6,6	0.19	0
2	SO4	A	902	-	4,4,4	0.50	0	6,6,6	0.37	0
4	EDO	A	912	-	3,3,3	0.59	0	2,2,2	0.16	0
2	SO4	A	901	-	4,4,4	0.51	0	6,6,6	0.37	0
2	SO4	A	907	-	4,4,4	0.65	0	6,6,6	0.35	0
4	EDO	A	911	-	3,3,3	0.51	0	2,2,2	0.29	0
4	EDO	A	909	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	A	914	-	3,3,3	0.38	0	2,2,2	0.30	0
2	SO4	A	903	-	4,4,4	0.51	0	6,6,6	0.16	0
5	94B	A	915	-	13,13,13	1.47	1 (7%)	15,20,20	2.06	5 (33%)

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	PG4	A	908	-	-	4/10/10/10	-
4	EDO	A	910	-	-	0/1/1/1	-
4	EDO	A	913	-	-	1/1/1/1	-
4	EDO	A	914	-	-	1/1/1/1	-
4	EDO	A	912	-	-	0/1/1/1	-
4	EDO	A	911	-	-	0/1/1/1	-
6	OXL	A	916	-	-	4/4/4/4	-
5	94B	A	915	-	-	0/2/27/27	0/2/2/2
4	EDO	A	909	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	915	94B	C7-C1	4.18	1.52	1.48
6	A	916	OXL	O3-C1	-2.02	1.25	1.30

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	916	OXL	O4-C2-C1	7.47	127.32	112.83
6	A	916	OXL	O3-C1-O1	-5.02	111.95	123.90
6	A	916	OXL	O3-C1-C2	4.38	121.32	112.83
6	A	916	OXL	O4-C2-O2	-4.26	113.77	123.90
5	A	915	94B	C7-N12-C1	4.20	61.95	60.38

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	908	PG4	O2-C3-C4-O3
3	A	908	PG4	O3-C5-C6-O4
6	A	916	OXL	O1-C1-C2-O2
4	A	914	EDO	O1-C1-C2-O2
3	A	908	PG4	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	909	EDO	0	1
5	A	915	94B	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	780/835 (93%)	0.25	27 (3%)	47 53	16, 34, 60, 100	7 (0%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	VAL	8.1
1	A	35	ALA	4.0
1	A	784	CYS	3.9
1	A	790	LEU	3.2
1	A	37	PHE	3.2

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 oligosaccharides 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(Å ²)	Q < 0.9
4	EDO	A	910	4/4	0.47	0.19	109,112,114,117	0
2	SO4	A	905	5/5	0.75	0.17	86,87,93,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	906	5/5	0.78	0.09	77,91,93,99	0
6	OXL	A	916	6/6	0.82	0.14	49,52,54,58	0
4	EDO	A	913	4/4	0.83	0.21	70,70,72,75	0
2	SO4	A	903	5/5	0.83	0.11	73,79,88,88	0
5	94B	A	915	12/12	0.86	0.15	28,35,37,40	12
4	EDO	A	912	4/4	0.87	0.17	47,50,54,55	0
2	SO4	A	904	5/5	0.87	0.10	69,76,82,82	0
2	SO4	A	907	5/5	0.88	0.12	53,54,70,80	0
4	EDO	A	911	4/4	0.88	0.16	50,54,56,57	0
3	PG4	A	908	13/13	0.88	0.14	43,50,52,53	0
4	EDO	A	909	4/4	0.89	0.13	54,55,55,58	0
2	SO4	A	902	5/5	0.94	0.07	54,57,63,66	0
4	EDO	A	914	4/4	0.94	0.10	41,47,47,49	0
2	SO4	A	901	5/5	0.98	0.12	41,46,50,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.