



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:47 PM UTC

PDB ID : 5NPC / pdb_00005npc
Title : Crystal Structure of D412N nucleophile mutant cjAgd31B (alpha-transglucosylase from Glycoside Hydrolase Family 31) in complex with unreacted alpha Cyclophellitol Cyclosulfate probe ME647
Authors : Wu, L.; Davies, G.J.
Deposited on : 2017-04-16
Resolution : 1.96 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

<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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

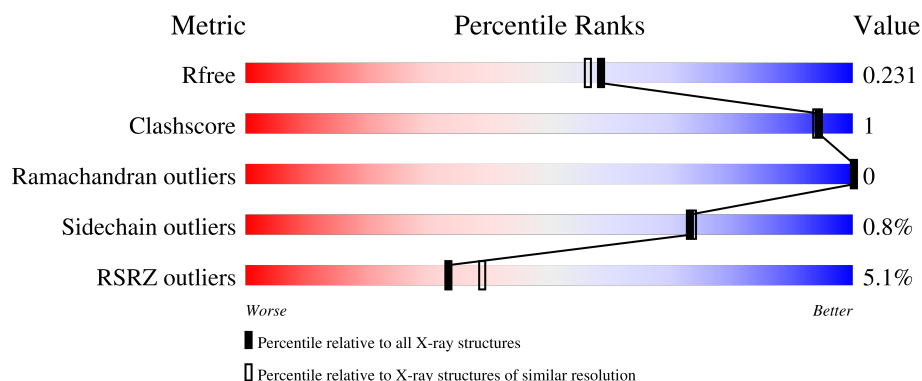
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	5% 89% 7%

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	923	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6768 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
			6283	4013	1079	1170	21			

There are 44 discrepancies between the modelled and reference sequences:

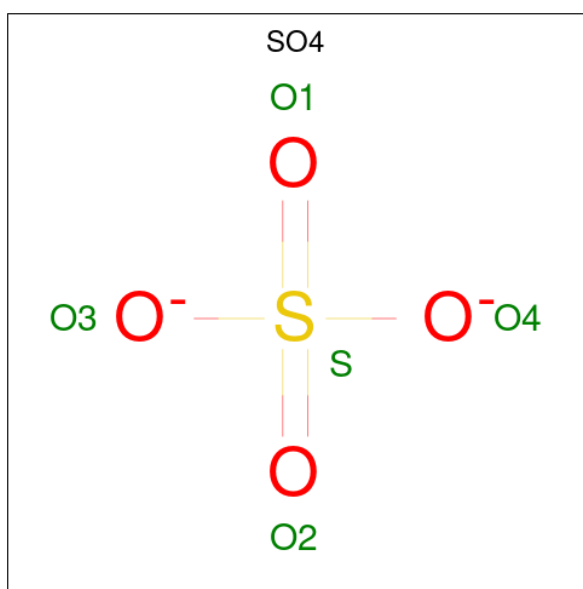
Chain	Residue	Modelled	Actual	Comment	Reference
A	412	ASN	ASP	engineered mutation	UNP B3PEE6
A	817	LYS	-	expression tag	UNP B3PEE6
A	818	GLY	-	expression tag	UNP B3PEE6
A	819	GLY	-	expression tag	UNP B3PEE6
A	820	ARG	-	expression tag	UNP B3PEE6
A	821	ALA	-	expression tag	UNP B3PEE6
A	822	ASP	-	expression 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).



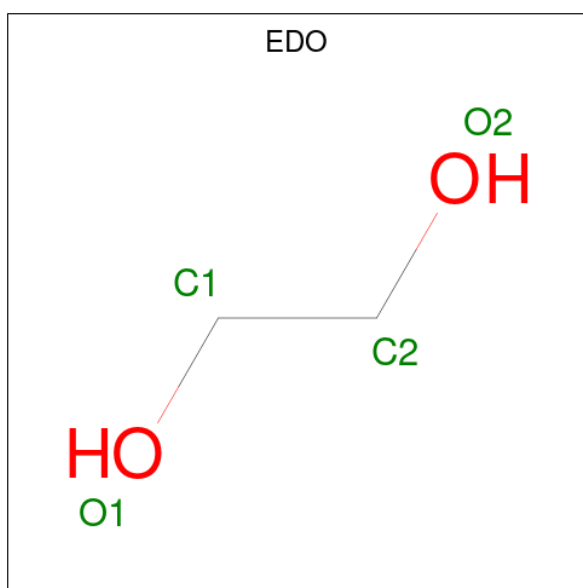
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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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		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



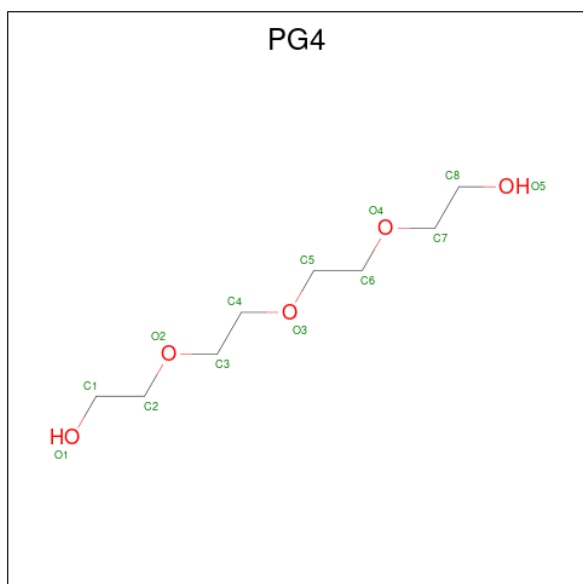
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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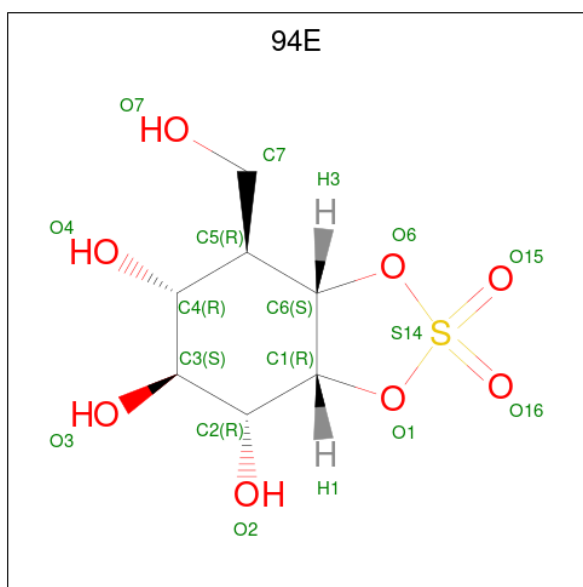
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



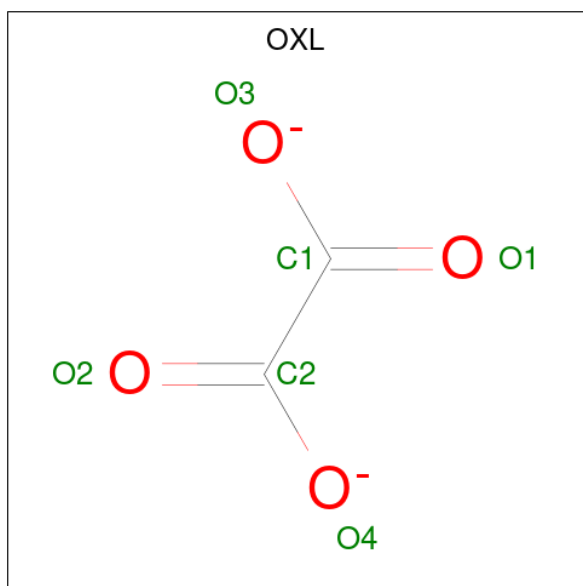
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is (3 {a} {R},4 {R},5 {S},6 {R},7 {R},7 {a} {S})-7-(hydroxymethyl)-2,2-bis(oxidanylidene)-3 {a},4,5,6,7,7 {a}-hexahydrobenzo[d][1,3,2]dioxathiole-4,5,6-triol (CCD ID: 94E) (formula: $C_7H_{12}O_8S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			16	7	8	1		

- 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		

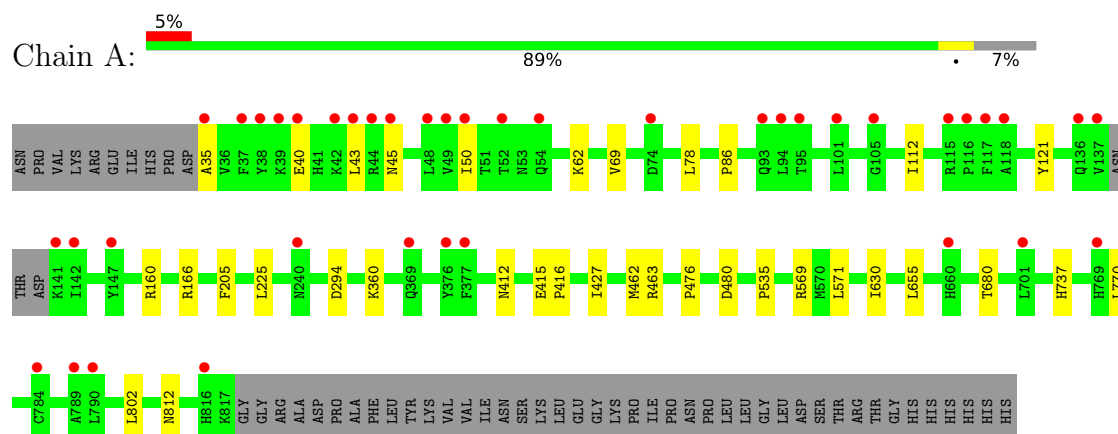
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	362	Total 362	O 362	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 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	197.14Å 197.14Å 102.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.67 – 1.96 65.67 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.67-1.96) 99.9 (65.67-1.96)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.189 , 0.227 0.198 , 0.231	Depositor DCC
R_{free} test set	4175 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6768	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, SO4, 94E, EDO, OXL

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	0.85	1/6453 (0.0%)	0.89	3/8748 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	ASN	CB-CG	-7.12	1.34	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	PRO	N-CA-C	6.65	122.78	113.53
1	A	571	LEU	CA-C-N	-5.00	113.78	119.28
1	A	571	LEU	C-N-CA	-5.00	113.78	119.28

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	6283	0	6108	16	0
2	A	40	0	0	0	0
3	A	48	0	72	0	1
4	A	13	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	16	0	0	1	0
6	A	6	0	0	0	0
7	A	362	0	0	2	0
All	All	6768	0	6198	16	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 1.

All (16) 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:737:HIS:CD2	1:A:812[B]:ASN:HD21	2.26	0.53
1:A:35:ALA:N	7:A:1007:HOH:O	2.41	0.52
1:A:412:ASN:ND2	1:A:463:ARG:HD3	2.27	0.50
1:A:462:MET:O	1:A:476:PRO:HA	2.12	0.50
1:A:415:GLU:N	1:A:416:PRO:HA	2.27	0.48
1:A:50:ILE:HD11	1:A:112:ILE:HD13	1.98	0.46
1:A:62:LYS:NZ	1:A:86:PRO:O	2.48	0.45
1:A:69:VAL:HG21	1:A:121:TYR:OH	2.15	0.45
1:A:480:ASP:OD2	5:A:922:94E:O1	2.34	0.45
1:A:205:PHE:HB2	1:A:225:LEU:HD13	1.99	0.44
1:A:160:ARG:O	1:A:166:ARG:NH2	2.52	0.42
1:A:569:ARG:HD2	7:A:1174:HOH:O	2.20	0.41
1:A:630:ILE:HD12	1:A:655:LEU:HD13	2.01	0.41
1:A:78:LEU:HD22	1:A:427:ILE:HD12	2.03	0.41
1:A:770:LEU:HD22	1:A:802:LEU:HD22	2.03	0.41
1:A:415:GLU:HB2	1:A:416:PRO:C	2.45	0.41

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)
3:A:910:EDO:O1	3:A:910:EDO:O1[11_556]	2.19	0.01

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	782/835 (94%)	751 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	663/705 (94%)	658 (99%)	5 (1%)	73	74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	43	LEU
1	A	294	ASP
1	A	360	LYS
1	A	680	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	449	GLN
1	A	766	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

23 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	901	-	4,4,4	0.50	0	6,6,6	0.30	0
4	PG4	A	921	-	12,12,12	0.70	0	11,11,11	0.57	0
2	SO4	A	902	-	4,4,4	0.41	0	6,6,6	0.38	0
3	EDO	A	919	-	3,3,3	0.35	0	2,2,2	0.40	0
3	EDO	A	911	-	3,3,3	0.51	0	2,2,2	0.31	0
2	SO4	A	907	-	4,4,4	0.52	0	6,6,6	0.22	0
2	SO4	A	905	-	4,4,4	0.48	0	6,6,6	0.35	0
6	OXL	A	923	-	5,5,5	1.35	1 (20%)	6,6,6	5.12	5 (83%)
3	EDO	A	910	-	3,3,3	0.46	0	2,2,2	0.23	0
3	EDO	A	918	-	3,3,3	0.46	0	2,2,2	0.31	0
2	SO4	A	903	-	4,4,4	0.46	0	6,6,6	0.30	0
3	EDO	A	920	-	3,3,3	0.53	0	2,2,2	0.25	0
3	EDO	A	914	-	3,3,3	0.59	0	2,2,2	0.16	0
3	EDO	A	917	-	3,3,3	0.42	0	2,2,2	0.47	0
3	EDO	A	909	-	3,3,3	0.68	0	2,2,2	0.22	0
2	SO4	A	904	-	4,4,4	0.51	0	6,6,6	0.25	0
3	EDO	A	913	-	3,3,3	0.50	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	915	-	3,3,3	0.64	0	2,2,2	0.36	0
2	SO4	A	906	-	4,4,4	0.50	0	6,6,6	0.31	0
5	94E	A	922	-	15,17,17	1.00	1 (6%)	19,27,27	2.10	7 (36%)
2	SO4	A	908	-	4,4,4	0.45	0	6,6,6	0.20	0
3	EDO	A	916	-	3,3,3	0.72	0	2,2,2	0.21	0
3	EDO	A	912	-	3,3,3	0.58	0	2,2,2	0.18	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	EDO	A	909	-	-	1/1/1/1	-
3	EDO	A	913	-	-	1/1/1/1	-
3	EDO	A	915	-	-	0/1/1/1	-
3	EDO	A	910	-	-	1/1/1/1	-
5	94E	A	922	-	-	0/2/36/36	0/2/2/2
3	EDO	A	918	-	-	1/1/1/1	-
3	EDO	A	911	-	-	1/1/1/1	-
3	EDO	A	920	-	-	1/1/1/1	-
3	EDO	A	916	-	-	0/1/1/1	-
4	PG4	A	921	-	-	6/10/10/10	-
3	EDO	A	912	-	-	0/1/1/1	-
3	EDO	A	919	-	-	1/1/1/1	-
3	EDO	A	914	-	-	0/1/1/1	-
6	OXL	A	923	-	-	4/4/4/4	-
3	EDO	A	917	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	922	94E	C5-C4	2.81	1.56	1.53
6	A	923	OXL	O3-C1	-2.07	1.24	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	923	OXL	O4-C2-C1	8.92	130.13	112.83
6	A	923	OXL	O3-C1-O1	-5.12	111.70	123.90
6	A	923	OXL	O4-C2-O2	-4.61	112.92	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	922	94E	O1-S14-O6	4.41	100.02	97.54
6	A	923	OXL	O1-C1-C2	3.69	128.32	120.63
6	A	923	OXL	O3-C1-C2	3.69	119.98	112.83
5	A	922	94E	O6-S14-O15	3.56	114.94	109.49
5	A	922	94E	C4-C3-C2	-3.33	104.99	110.83
5	A	922	94E	O1-S14-O16	2.72	113.65	109.49
5	A	922	94E	O4-C4-C3	-2.55	104.36	110.38
5	A	922	94E	O2-C2-C1	2.23	115.65	109.94
5	A	922	94E	C5-C4-C3	2.09	114.29	110.77

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	921	PG4	O3-C5-C6-O4
4	A	921	PG4	O2-C3-C4-O3
4	A	921	PG4	O4-C7-C8-O5
3	A	911	EDO	O1-C1-C2-O2
3	A	913	EDO	O1-C1-C2-O2
6	A	923	OXL	O1-C1-C2-O2
6	A	923	OXL	O3-C1-C2-O4
3	A	909	EDO	O1-C1-C2-O2
3	A	917	EDO	O1-C1-C2-O2
3	A	918	EDO	O1-C1-C2-O2
3	A	919	EDO	O1-C1-C2-O2
6	A	923	OXL	O3-C1-C2-O2
4	A	921	PG4	C1-C2-O2-C3
6	A	923	OXL	O1-C1-C2-O4
4	A	921	PG4	C8-C7-O4-C6
3	A	910	EDO	O1-C1-C2-O2
3	A	920	EDO	O1-C1-C2-O2
4	A	921	PG4	C5-C6-O4-C7

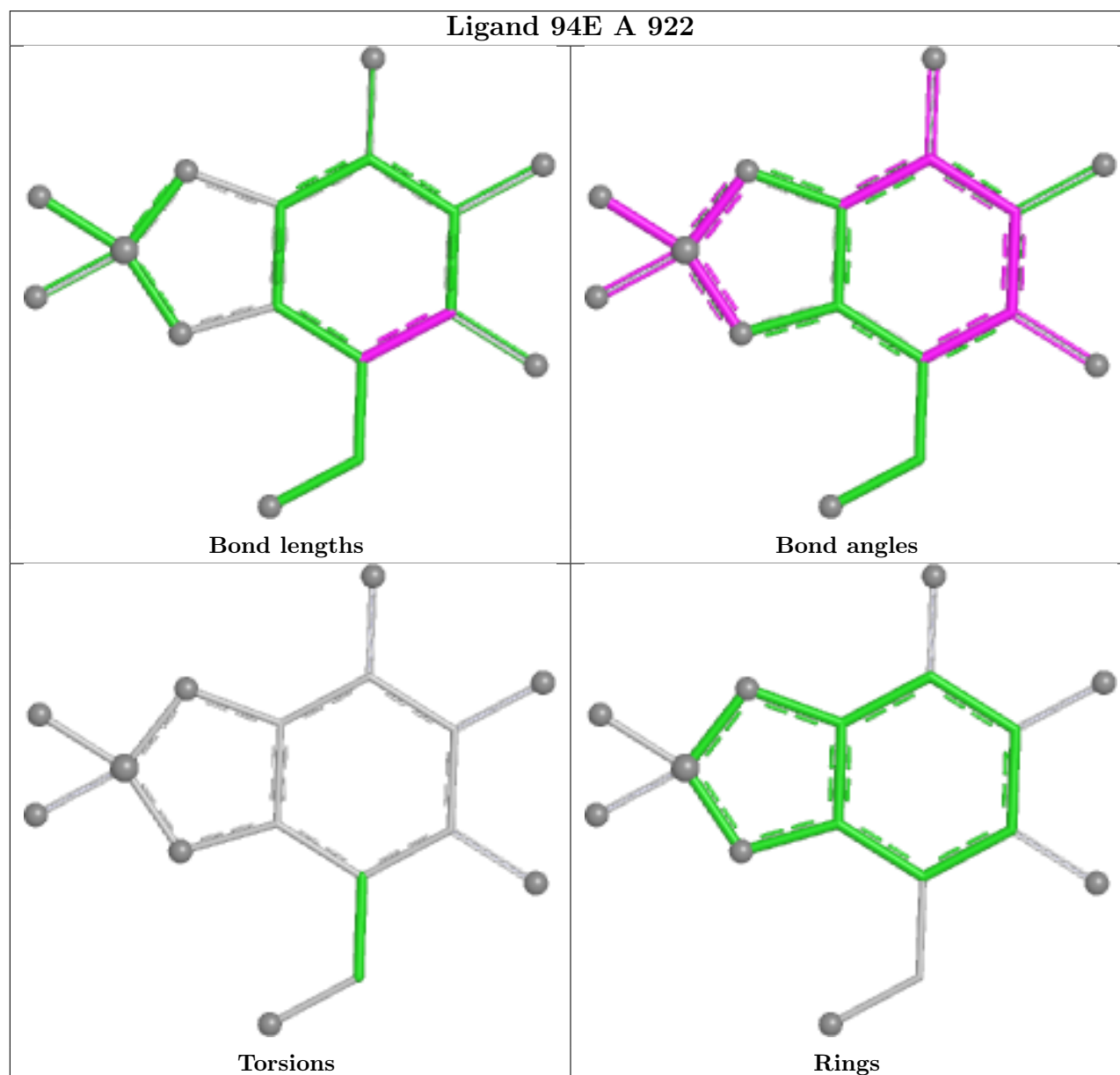
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	910	EDO	0	1
5	A	922	94E	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	780/835 (93%)	0.35	40 (5%) 33 39	16, 35, 64, 97	7 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	VAL	8.6
1	A	43	LEU	3.5
1	A	141	LYS	3.4
1	A	101	LEU	3.4
1	A	35	ALA	3.3
1	A	790	LEU	3.1
1	A	40	GLU	3.0
1	A	376	TYR	2.9
1	A	784	CYS	2.9
1	A	37	PHE	2.9
1	A	660[A]	HIS	2.9
1	A	52	THR	2.8
1	A	118	ALA	2.8
1	A	45	ASN	2.8
1	A	117	PHE	2.8
1	A	50	ILE	2.7
1	A	789	ALA	2.7
1	A	54	GLN	2.7
1	A	115	ARG	2.6
1	A	38	TYR	2.5
1	A	369	GLN	2.5
1	A	142	ILE	2.5
1	A	93	GLN	2.4
1	A	49	VAL	2.4
1	A	377	PHE	2.4
1	A	136	GLN	2.4
1	A	769	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	95	THR	2.3
1	A	94	LEU	2.3
1	A	116	PRO	2.3
1	A	48	LEU	2.2
1	A	42	LYS	2.2
1	A	44	ARG	2.1
1	A	701	LEU	2.1
1	A	240	ASN	2.1
1	A	39	LYS	2.1
1	A	105	GLY	2.0
1	A	74	ASP	2.0
1	A	816	HIS	2.0
1	A	147	TYR	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 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
3	EDO	A	915	4/4	0.72	0.20	48,49,50,56	0
2	SO4	A	908	5/5	0.74	0.11	79,89,92,102	0
2	SO4	A	907	5/5	0.75	0.14	83,85,93,98	0
3	EDO	A	920	4/4	0.77	0.20	71,76,78,79	0
2	SO4	A	905	5/5	0.79	0.10	91,93,103,106	0
3	EDO	A	909	4/4	0.79	0.21	57,61,61,62	0
3	EDO	A	912	4/4	0.80	0.18	54,59,61,63	0
6	OXL	A	923	6/6	0.80	0.14	45,50,51,55	0
3	EDO	A	914	4/4	0.82	0.20	52,59,62,63	0
2	SO4	A	906	5/5	0.83	0.14	67,70,81,91	0

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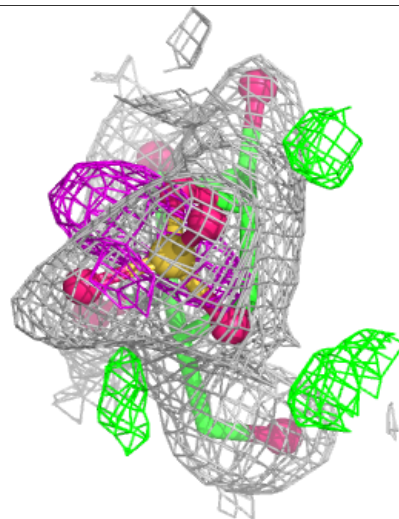
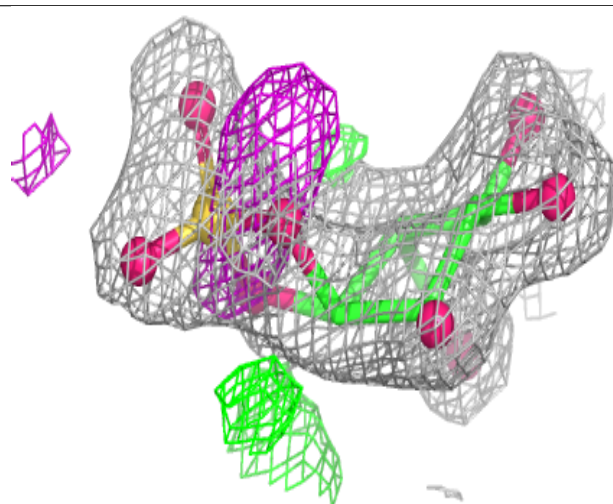
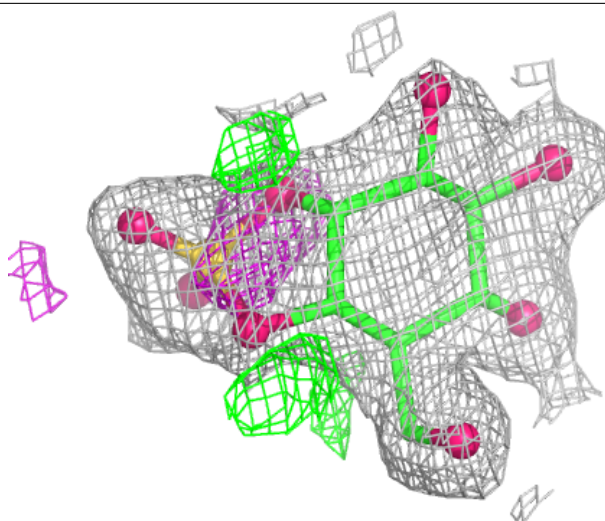
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	913	4/4	0.84	0.17	53,55,56,57	0
3	EDO	A	918	4/4	0.85	0.14	62,64,65,68	0
5	94E	A	922	16/16	0.85	0.15	29,36,49,49	16
3	EDO	A	919	4/4	0.85	0.15	66,66,67,71	0
3	EDO	A	917	4/4	0.86	0.20	65,66,67,67	4
2	SO4	A	903	5/5	0.87	0.09	70,73,80,82	0
4	PG4	A	921	13/13	0.87	0.17	50,55,58,58	0
2	SO4	A	904	5/5	0.88	0.10	67,72,72,81	0
3	EDO	A	916	4/4	0.89	0.15	43,51,54,56	0
3	EDO	A	910	4/4	0.90	0.12	58,60,61,63	0
3	EDO	A	911	4/4	0.91	0.14	50,53,54,57	0
2	SO4	A	902	5/5	0.94	0.08	57,60,67,69	0
2	SO4	A	901	5/5	0.97	0.07	48,50,55,58	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 94E A 922:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.