



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 06:16 AM EDT

PDB ID : 7P4D / pdb_00007p4d
Title : Crystal Structure of Agd31B, alpha-transglucosylase in Glycoside Hydrolase Family 31, in complex with covalent Cyclophellitol Sulfamidate probe KK130
Authors : Wu, L.; Davies, G.J.
Deposited on : 2021-07-11
Resolution : 1.85 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

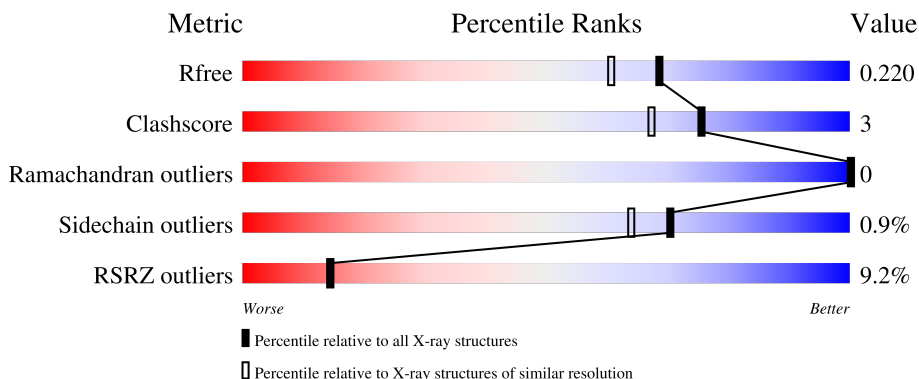
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	AAA	836	

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
4	OXL	AAA	903	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13000 atoms, of which 6159 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	AAA	780	Total	C	H	N	O	S	170	5	0
			12389	4006	6116	1073	1173	21			

There are 44 discrepancies between the modelled and reference sequences:

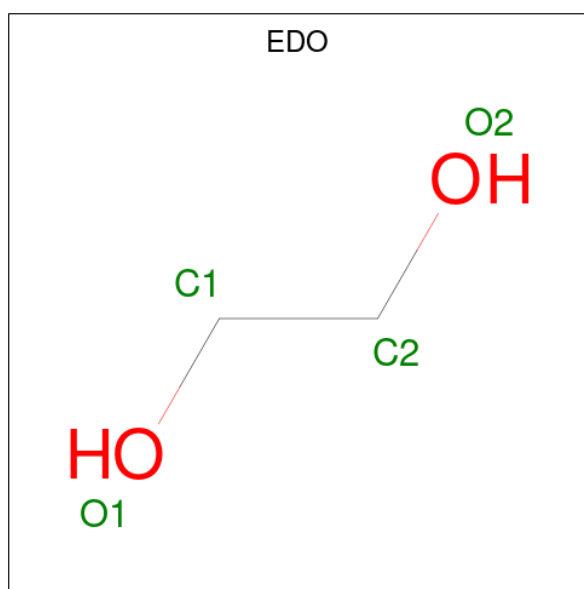
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	24	MET	-	initiating methionine	UNP B3PEE6
AAA	817	LYS	-	expression tag	UNP B3PEE6
AAA	818	GLY	-	expression tag	UNP B3PEE6
AAA	819	GLY	-	expression tag	UNP B3PEE6
AAA	820	ARG	-	expression tag	UNP B3PEE6
AAA	821	ALA	-	expression tag	UNP B3PEE6
AAA	822	ASP	-	expression tag	UNP B3PEE6
AAA	823	PRO	-	expression tag	UNP B3PEE6
AAA	824	ALA	-	expression tag	UNP B3PEE6
AAA	825	PHE	-	expression tag	UNP B3PEE6
AAA	826	LEU	-	expression tag	UNP B3PEE6
AAA	827	TYR	-	expression tag	UNP B3PEE6
AAA	828	LYS	-	expression tag	UNP B3PEE6
AAA	829	VAL	-	expression tag	UNP B3PEE6
AAA	830	VAL	-	expression tag	UNP B3PEE6
AAA	831	ILE	-	expression tag	UNP B3PEE6
AAA	832	ASN	-	expression tag	UNP B3PEE6
AAA	833	SER	-	expression tag	UNP B3PEE6
AAA	834	LYS	-	expression tag	UNP B3PEE6
AAA	835	LEU	-	expression tag	UNP B3PEE6
AAA	836	GLU	-	expression tag	UNP B3PEE6
AAA	837	GLY	-	expression tag	UNP B3PEE6
AAA	838	LYS	-	expression tag	UNP B3PEE6
AAA	839	PRO	-	expression tag	UNP B3PEE6
AAA	840	ILE	-	expression tag	UNP B3PEE6
AAA	841	PRO	-	expression tag	UNP B3PEE6
AAA	842	ASN	-	expression tag	UNP B3PEE6

Continued on next page...

Continued from previous page...

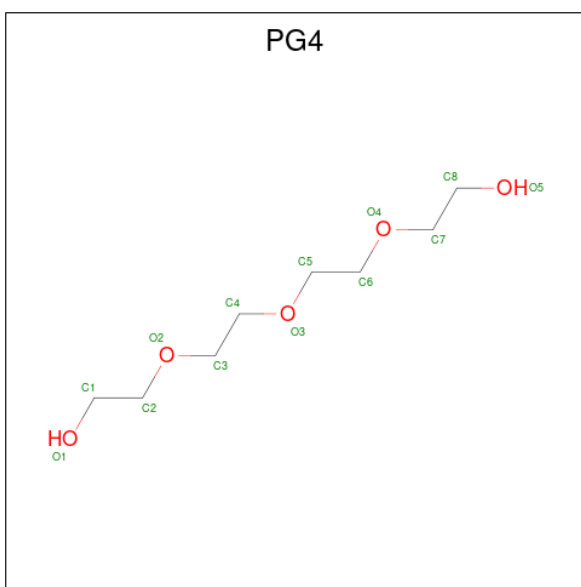
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	843	PRO	-	expression tag	UNP B3PEE6
AAA	844	LEU	-	expression tag	UNP B3PEE6
AAA	845	LEU	-	expression tag	UNP B3PEE6
AAA	846	GLY	-	expression tag	UNP B3PEE6
AAA	847	LEU	-	expression tag	UNP B3PEE6
AAA	848	ASP	-	expression tag	UNP B3PEE6
AAA	849	SER	-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

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



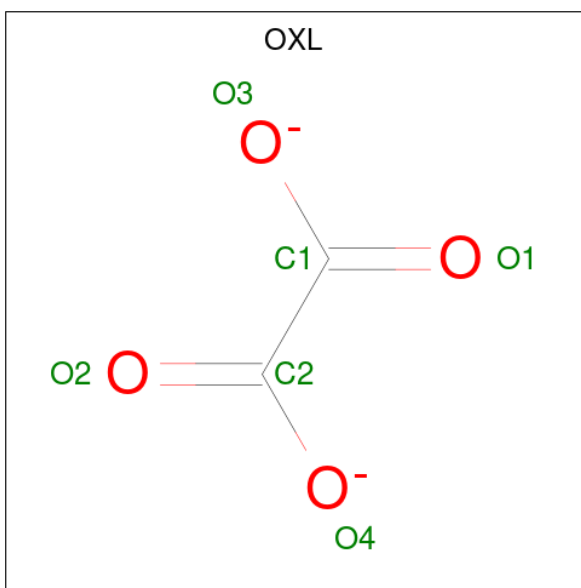
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



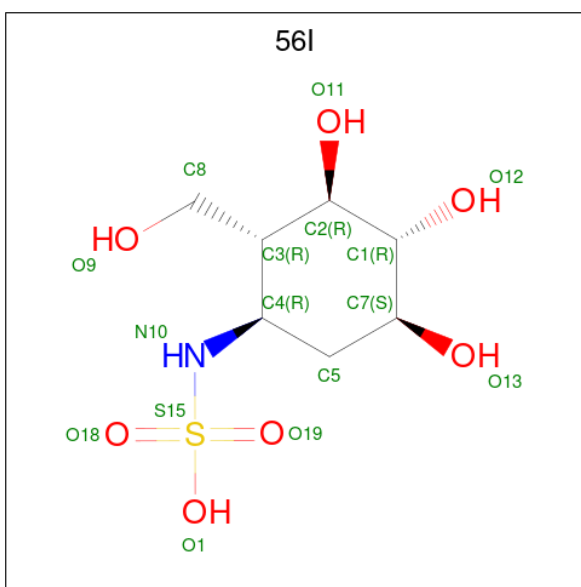
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			31	8	18	5		

- Molecule 4 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



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

- Molecule 5 is [(1R,2R,3R,4R,5S)-2-(hydroxymethyl)-3,4,5-tris(oxidanyl)cyclohexyl]sulfamic acid (CCD ID: 56I) (formula: C₇H₁₅NO₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	AAA	1	Total	C	H	N	O	S	4	0
			29	7	13	1	7	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

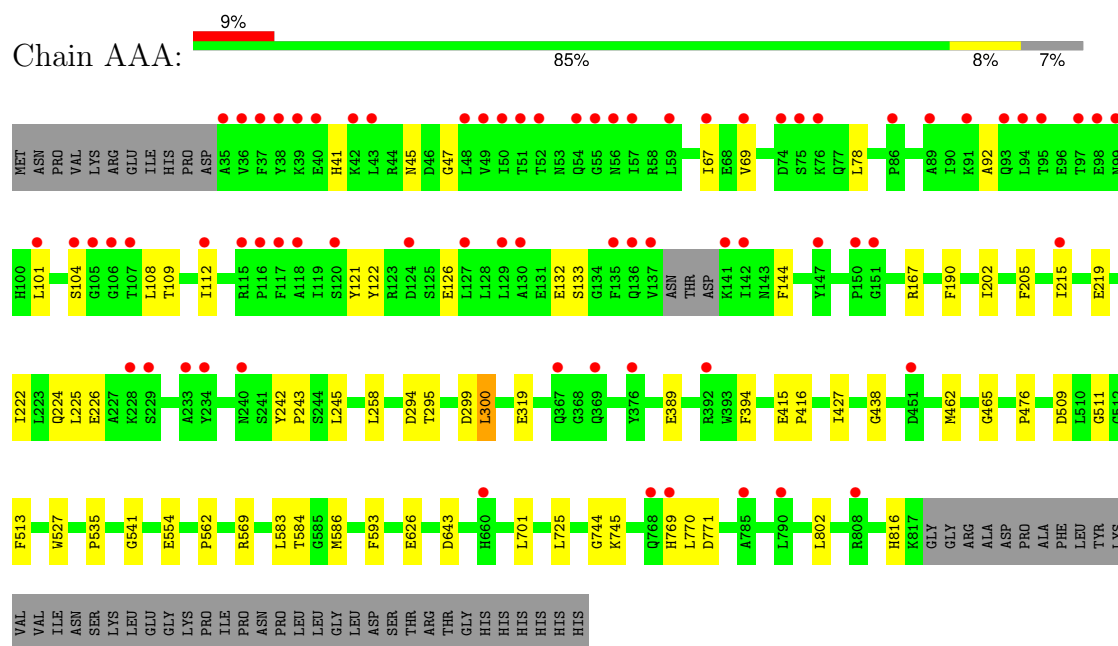
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	485	Total	O	0	0
			485	485		

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	197.08Å 197.08Å 102.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	98.54 – 1.85 98.54 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (98.54-1.85) 99.9 (98.54-1.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.188 , 0.222 0.186 , 0.220	Depositor DCC
R_{free} test set	4584 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13000	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: SO4, PG4, EDO, OXL, 56I

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	AAA	1.08	3/6439 (0.0%)	1.28	8/8730 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	299	ASP	C-O	5.55	1.29	1.23
1	AAA	295	THR	C-O	5.47	1.30	1.23
1	AAA	465	GLY	C-O	5.02	1.27	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	535	PRO	N-CA-C	5.85	121.66	113.53
1	AAA	319	GLU	CB-CG-CD	5.83	122.52	112.60
1	AAA	438	GLY	CA-C-N	5.24	127.61	120.54
1	AAA	438	GLY	C-N-CA	5.24	127.61	120.54
1	AAA	744	GLY	CA-C-O	-5.19	118.42	122.52
1	AAA	593	PHE	CA-CB-CG	5.05	118.85	113.80
1	AAA	389	GLU	CA-C-N	5.04	125.53	119.94
1	AAA	389	GLU	C-N-CA	5.04	125.53	119.94

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	AAA	6273	6116	6090	38	0
2	AAA	8	12	12	1	0
3	AAA	13	18	18	1	0
4	AAA	6	0	0	0	0
5	AAA	16	13	0	0	0
6	AAA	40	0	0	0	0
7	AAA	485	0	0	5	0
All	All	6841	6159	6120	38	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 3.

All (38) 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:AAA:554:GLU:OE1	7:AAA:1001:HOH:O	2.06	0.73
1:AAA:104:SER:HG	1:AAA:109:THR:HG1	1.37	0.72
1:AAA:771[B]:ASP:OD1	1:AAA:771[B]:ASP:C	2.39	0.65
1:AAA:243:PRO:HB3	1:AAA:586:MET:HE1	1.78	0.65
1:AAA:132:GLU:OE1	1:AAA:133:SER:OG	2.22	0.57
1:AAA:569:ARG:HD2	7:AAA:1225:HOH:O	2.06	0.55
1:AAA:205:PHE:HB2	1:AAA:225:LEU:HD13	1.89	0.54
1:AAA:69:VAL:HG21	1:AAA:121:TYR:OH	2.10	0.52
1:AAA:92:ALA:HB1	1:AAA:104:SER:O	2.12	0.49
1:AAA:626:GLU:HG2	7:AAA:1402:HOH:O	2.12	0.49
1:AAA:78:LEU:HD22	1:AAA:427:ILE:HD12	1.94	0.49
1:AAA:769:HIS:NE2	1:AAA:816:HIS:HB3	2.27	0.49
1:AAA:415:GLU:N	1:AAA:416:PRO:HA	2.27	0.49
1:AAA:725:LEU:N	1:AAA:725:LEU:HD12	2.28	0.48
1:AAA:462:MET:O	1:AAA:476:PRO:HA	2.14	0.47
1:AAA:643:ASP:HB2	7:AAA:1382:HOH:O	2.13	0.47
1:AAA:78:LEU:HG	2:AAA:901:EDO:H12	1.97	0.47
1:AAA:101:LEU:HB2	1:AAA:112:ILE:HB	1.97	0.47
1:AAA:513:PHE:HA	1:AAA:541:GLY:HA2	1.97	0.46
1:AAA:562:PRO:HB2	3:AAA:902:PG4:H82	1.97	0.46
1:AAA:45:ASN:C	1:AAA:47:GLY:H	2.23	0.46
1:AAA:202:ILE:HG13	1:AAA:245:LEU:HD21	1.97	0.46
1:AAA:511:GLY:H	1:AAA:527:TRP:CG	2.34	0.46
1:AAA:41:HIS:CE1	1:AAA:101:LEU:HD21	2.51	0.46
1:AAA:243:PRO:HB3	1:AAA:586:MET:CE	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:122:TYR:HA	1:AAA:126:GLU:O	2.17	0.45
1:AAA:745:LYS:NZ	7:AAA:1016:HOH:O	2.46	0.44
1:AAA:583:LEU:HB3	1:AAA:584:THR:HG23	1.99	0.43
1:AAA:243:PRO:CB	1:AAA:586:MET:HE1	2.48	0.43
1:AAA:67:ILE:HG22	1:AAA:108:LEU:HD21	1.99	0.43
1:AAA:509:ASP:OD2	1:AAA:513:PHE:HB2	2.18	0.42
1:AAA:258:LEU:HD12	1:AAA:258:LEU:HA	1.93	0.42
1:AAA:770:LEU:HD22	1:AAA:802:LEU:HD22	2.01	0.41
1:AAA:144:PHE:O	1:AAA:224:GLN:HA	2.21	0.41
1:AAA:219:GLU:HB2	1:AAA:222:ILE:HB	2.03	0.41
1:AAA:242:TYR:N	1:AAA:243:PRO:CD	2.84	0.41
1:AAA:167:ARG:HA	1:AAA:215:ILE:HG22	2.02	0.40
1:AAA:300:LEU:C	1:AAA:300:LEU:HD12	2.47	0.40

There are no symmetry-related clashes.

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	AAA	781/836 (93%)	744 (95%)	37 (5%)	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	AAA	662/706 (94%)	656 (99%)	6 (1%)	70 64

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

Mol	Chain	Res	Type
1	AAA	190	PHE
1	AAA	226	GLU
1	AAA	294	ASP
1	AAA	300	LEU
1	AAA	394	PHE
1	AAA	701	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

13 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	PG4	AAA	902	-	12,12,12	0.33	0	11,11,11	0.51	0
6	SO4	AAA	911	-	4,4,4	0.33	0	6,6,6	0.09	0
5	56I	AAA	905	1	16,16,16	1.22	2 (12%)	18,24,24	1.76	3 (16%)
6	SO4	AAA	912	-	4,4,4	0.32	0	6,6,6	0.10	0
6	SO4	AAA	906	-	4,4,4	0.40	0	6,6,6	0.19	0
6	SO4	AAA	907	-	4,4,4	0.34	0	6,6,6	0.18	0
6	SO4	AAA	910	-	4,4,4	0.32	0	6,6,6	0.11	0
4	OXL	AAA	903	-	5,5,5	2.33	2 (40%)	6,6,6	2.28	2 (33%)
6	SO4	AAA	909	-	4,4,4	0.31	0	6,6,6	0.05	0
6	SO4	AAA	908	-	4,4,4	0.28	0	6,6,6	0.14	0
2	EDO	AAA	904	-	3,3,3	0.21	0	2,2,2	0.24	0
2	EDO	AAA	901	-	3,3,3	0.42	0	2,2,2	0.45	0
6	SO4	AAA	913	-	4,4,4	0.25	0	6,6,6	0.10	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	PG4	AAA	902	-	-	5/10/10/10	-
5	56I	AAA	905	1	-	2/7/27/27	0/1/1/1
4	OXL	AAA	903	-	-	2/4/4/4	-
2	EDO	AAA	904	-	-	1/1/1/1	-
2	EDO	AAA	901	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	903	OXL	C2-C1	3.65	1.60	1.54
4	AAA	903	OXL	O3-C1	-3.29	1.21	1.30
5	AAA	905	56I	S15-N10	3.11	1.63	1.59
5	AAA	905	56I	O18-S15	2.76	1.45	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AAA	905	56I	O18-S15-N10	-5.09	100.37	108.88
4	AAA	903	OXL	O4-C2-C1	4.60	121.75	112.83
5	AAA	905	56I	C5-C4-C3	3.19	114.57	111.55
4	AAA	903	OXL	O2-C2-C1	-2.56	115.29	120.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AAA	905	56I	C5-C7-C1	2.18	113.81	110.67

There are no chirality outliers.

All (11) torsion outliers are listed below:

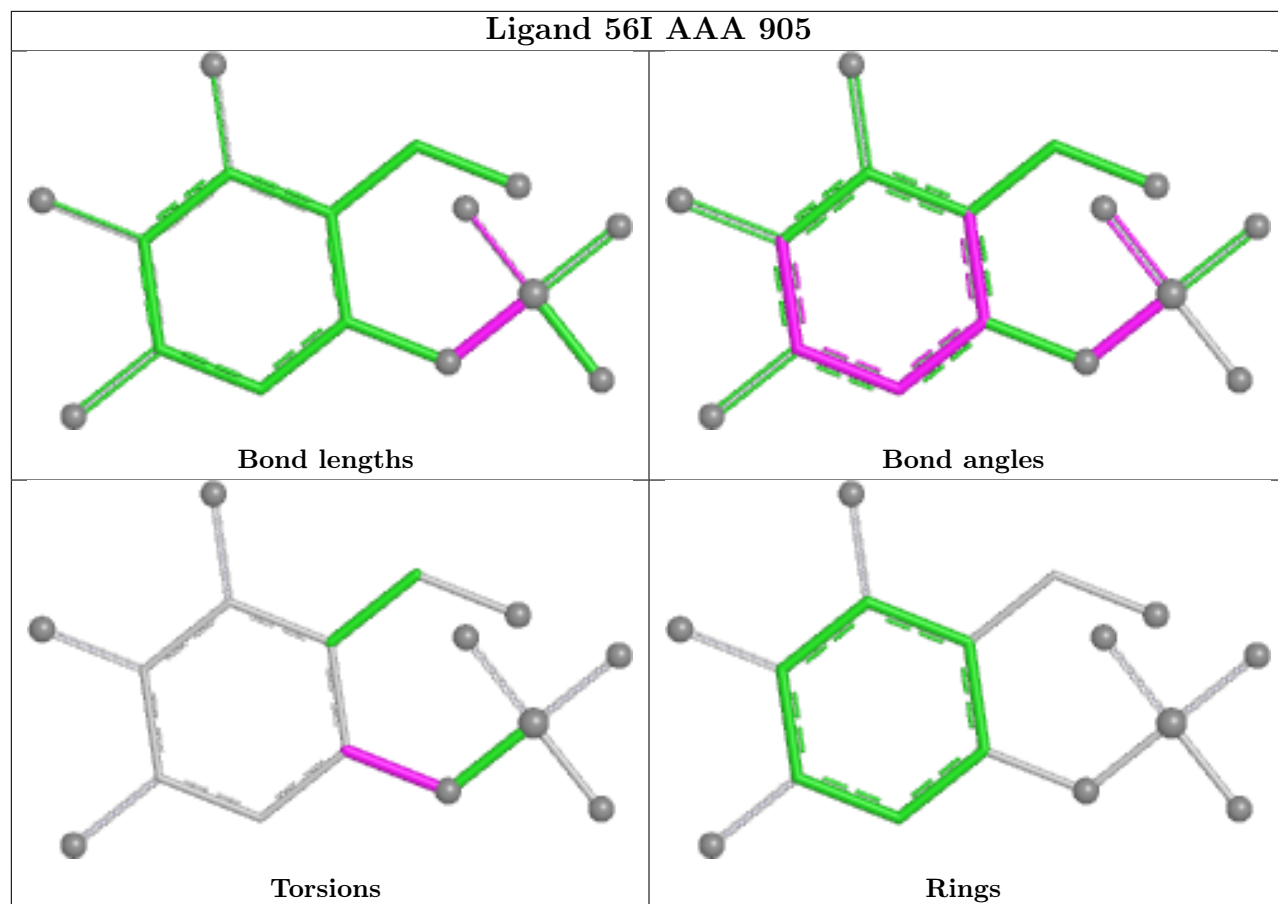
Mol	Chain	Res	Type	Atoms
3	AAA	902	PG4	O1-C1-C2-O2
3	AAA	902	PG4	C4-C3-O2-C2
5	AAA	905	56I	C3-C4-N10-S15
3	AAA	902	PG4	O3-C5-C6-O4
3	AAA	902	PG4	C1-C2-O2-C3
2	AAA	904	EDO	O1-C1-C2-O2
3	AAA	902	PG4	O2-C3-C4-O3
5	AAA	905	56I	C5-C4-N10-S15
2	AAA	901	EDO	O1-C1-C2-O2
4	AAA	903	OXL	O3-C1-C2-O4
4	AAA	903	OXL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	902	PG4	1	0
2	AAA	901	EDO	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	AAA	780/836 (93%)	0.34	72 (9%) 14 14	15, 36, 72, 115	5 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	137	VAL	9.8
1	AAA	43	LEU	5.0
1	AAA	117	PHE	4.4
1	AAA	101	LEU	4.4
1	AAA	112	ILE	4.1
1	AAA	118	ALA	4.0
1	AAA	94	LEU	3.7
1	AAA	769	HIS	3.6
1	AAA	141	LYS	3.6
1	AAA	35	ALA	3.5
1	AAA	142	ILE	3.5
1	AAA	37	PHE	3.5
1	AAA	57	ILE	3.4
1	AAA	38	TYR	3.4
1	AAA	369	GLN	3.4
1	AAA	52	THR	3.3
1	AAA	106	GLY	3.3
1	AAA	116	PRO	3.2
1	AAA	69	VAL	3.1
1	AAA	233	ALA	3.1
1	AAA	54	GLN	3.1
1	AAA	93	GLN	3.1
1	AAA	50	ILE	3.0
1	AAA	147	TYR	3.0
1	AAA	136	GLN	3.0
1	AAA	229	SER	3.0
1	AAA	234	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AAA	790	LEU	2.9
1	AAA	95	THR	2.8
1	AAA	49	VAL	2.8
1	AAA	39	LYS	2.8
1	AAA	376	TYR	2.7
1	AAA	130	ALA	2.7
1	AAA	98	GLU	2.7
1	AAA	48	LEU	2.6
1	AAA	59	LEU	2.6
1	AAA	367	GLN	2.6
1	AAA	228	LYS	2.6
1	AAA	150	PRO	2.6
1	AAA	40	GLU	2.5
1	AAA	127	LEU	2.5
1	AAA	56	ASN	2.5
1	AAA	135	PHE	2.5
1	AAA	51	THR	2.5
1	AAA	99	ASN	2.4
1	AAA	104	SER	2.4
1	AAA	55	GLY	2.4
1	AAA	97	THR	2.3
1	AAA	89	ALA	2.3
1	AAA	660	HIS	2.3
1	AAA	74	ASP	2.3
1	AAA	107	THR	2.3
1	AAA	785	ALA	2.3
1	AAA	76	LYS	2.3
1	AAA	808	ARG	2.3
1	AAA	120	SER	2.3
1	AAA	42	LYS	2.3
1	AAA	451[A]	ASP	2.2
1	AAA	36	VAL	2.2
1	AAA	215	ILE	2.2
1	AAA	75	SER	2.2
1	AAA	105	GLY	2.2
1	AAA	115	ARG	2.2
1	AAA	129	LEU	2.1
1	AAA	67	ILE	2.1
1	AAA	151	GLY	2.1
1	AAA	768	GLN	2.1
1	AAA	91	LYS	2.0
1	AAA	124	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AAA	392	ARG	2.0
1	AAA	240	ASN	2.0
1	AAA	86	PRO	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](#)

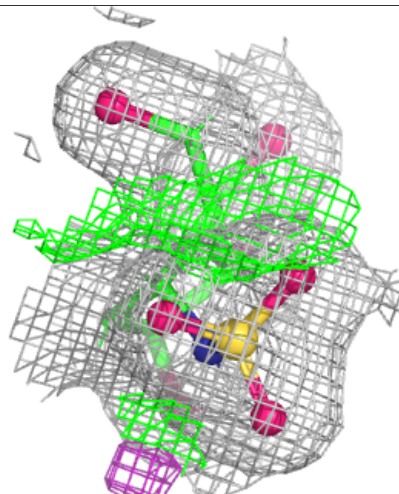
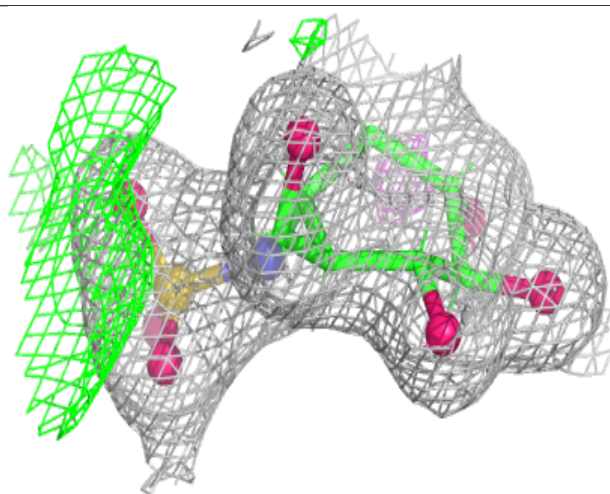
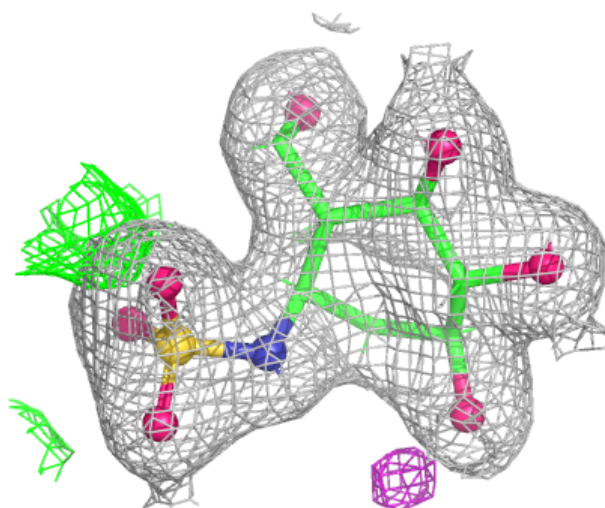
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	AAA	912	5/5	0.58	0.14	117,124,129,137	0
6	SO4	AAA	913	5/5	0.68	0.14	69,89,100,102	0
2	EDO	AAA	904	4/4	0.79	0.20	66,66,67,67	1
4	OXL	AAA	903	6/6	0.80	0.18	44,55,61,61	0
6	SO4	AAA	911	5/5	0.80	0.11	71,77,81,83	5
6	SO4	AAA	910	5/5	0.81	0.14	56,57,65,69	5
2	EDO	AAA	901	4/4	0.81	0.18	55,58,64,64	1
6	SO4	AAA	908	5/5	0.87	0.10	66,78,79,87	0
3	PG4	AAA	902	13/13	0.88	0.17	55,64,66,72	1
6	SO4	AAA	909	5/5	0.89	0.10	70,76,90,93	0
6	SO4	AAA	907	5/5	0.93	0.09	57,59,74,85	0
5	56I	AAA	905	16/16	0.97	0.05	24,26,33,36	4
6	SO4	AAA	906	5/5	0.99	0.04	41,43,46,53	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 56I AAA 905:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.