



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 10:35 AM UTC

PDB ID : 1W0P / pdb_00001w0p
Title : Vibrio cholerae sialidase with alpha-2,6-sialyllactose
Authors : Moustafa, I.; Connaris, H.; Taylor, M.; Zaitsev, V.; Wilson, J.C.; Kiefel, M.J.;
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Deposited on : 2004-06-09
Resolution : 1.60 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

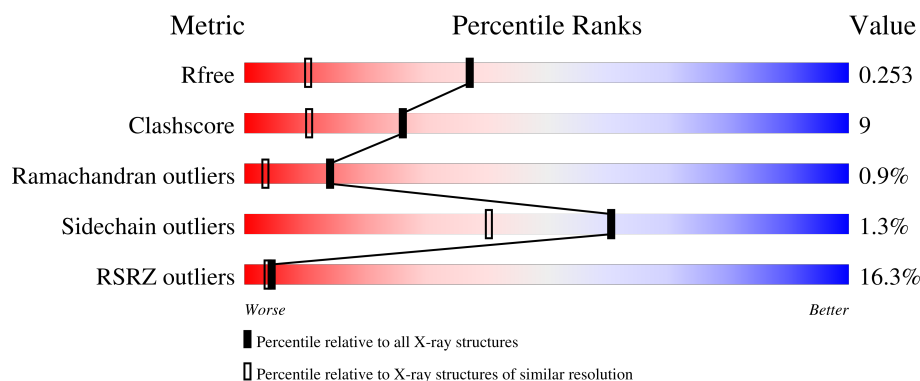
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	781	16% 80% 15% ...

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
2	GOL	A	1778	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6452 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 SIALIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	753	Total	C	N	O	S	0	0	0
			5827	3651	1006	1158	12			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



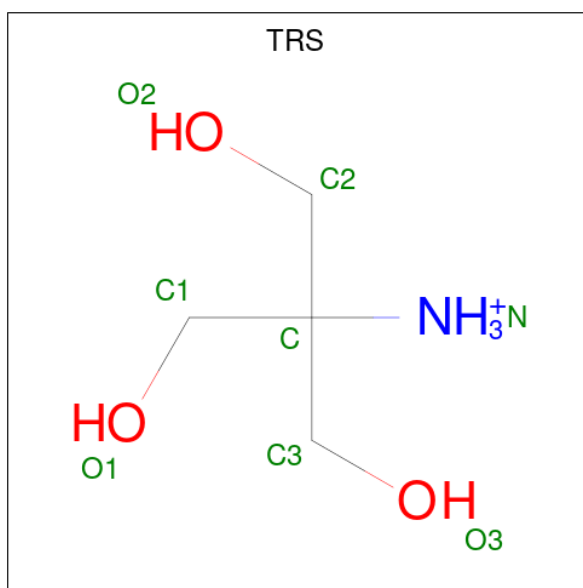
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		

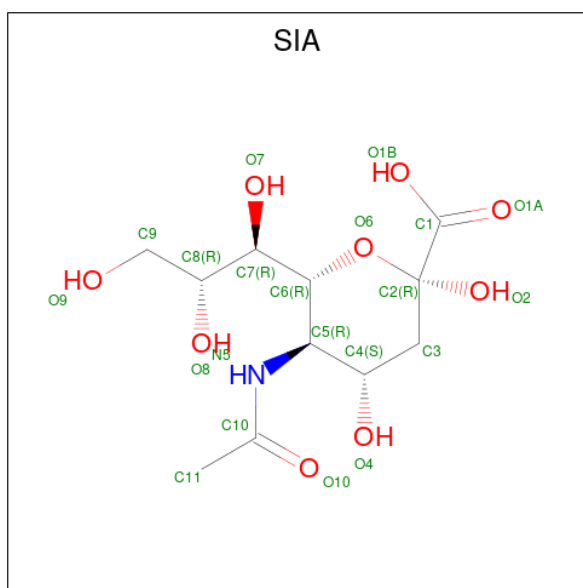
- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS)

(formula: $\text{C}_4\text{H}_{12}\text{NO}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	11	1	9		

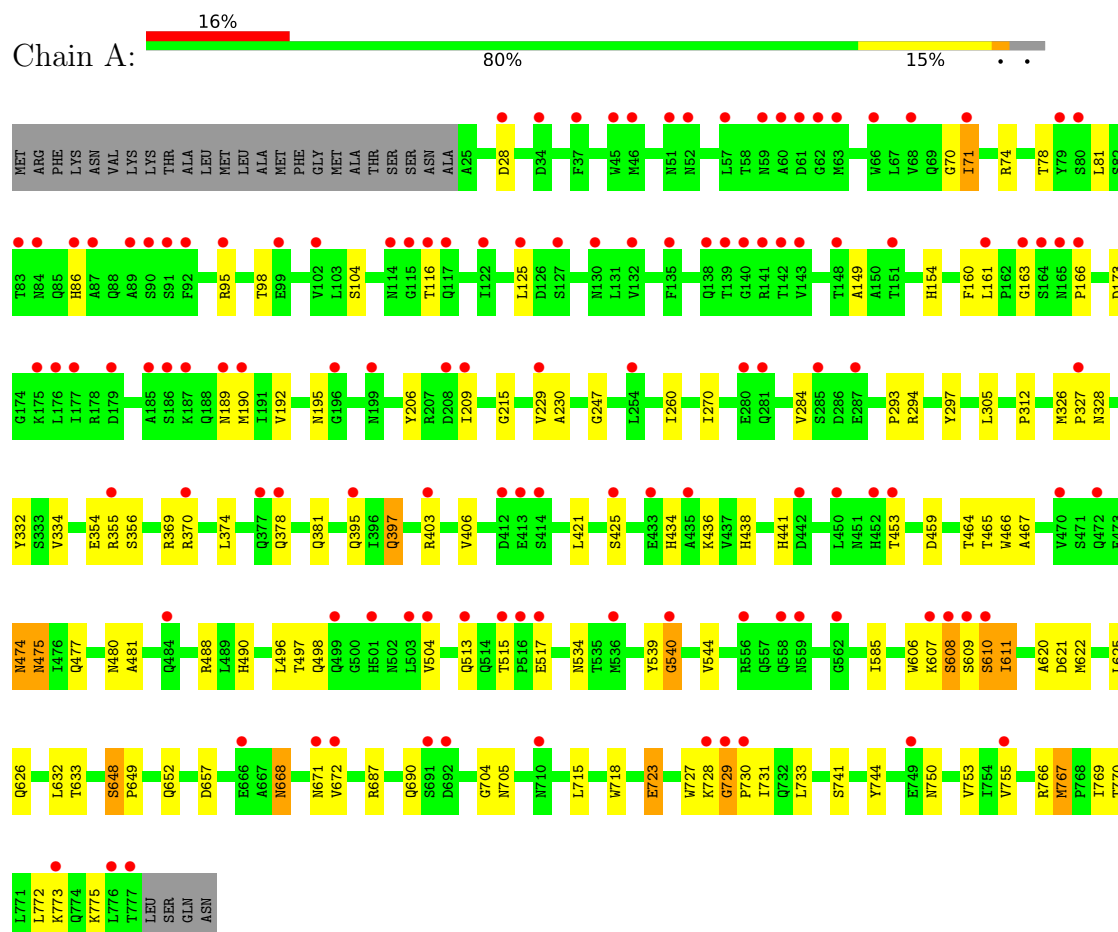
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	586	Total 586	O 586	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: SIALIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.31Å 74.91Å 151.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60 50.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.60) 99.8 (50.00-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.59Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , (Not available) 0.238 , 0.253	Depositor DCC
R_{free} test set	10692 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.3	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	0.92	EDS
Total number of atoms	6452	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, TRS, CA, SIA

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	0.34	0/5955	0.89	16/8109 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	ALA	N-CA-C	7.86	123.08	113.17
1	A	312	PRO	N-CA-C	-7.29	99.78	111.38
1	A	395	GLN	N-CA-C	7.17	119.82	109.14
1	A	585	ILE	N-CA-C	-6.59	98.89	108.11
1	A	284	VAL	N-CA-C	6.16	118.75	111.05
1	A	767	MET	N-CA-C	6.10	118.46	109.62
1	A	731	ILE	N-CA-C	-5.83	99.48	107.99
1	A	28	ASP	N-CA-C	5.73	117.49	108.96
1	A	326	MET	CA-C-N	5.70	126.96	119.84
1	A	326	MET	C-N-CA	5.70	126.96	119.84
1	A	611	ILE	N-CA-C	5.61	115.88	107.51
1	A	247	GLY	N-CA-C	-5.22	107.33	114.64
1	A	215	GLY	N-CA-C	5.07	122.83	115.32
1	A	704	GLY	N-CA-C	-5.07	105.31	112.81
1	A	425	SER	N-CA-C	5.02	116.45	110.97
1	A	769	ILE	N-CA-C	5.02	115.74	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	5827	0	5589	108	0
2	A	6	0	4	0	0
3	A	4	0	0	0	0
4	A	8	0	9	0	0
5	A	21	0	18	1	0
6	A	586	0	0	7	0
All	All	6452	0	5620	108	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 9.

All (108) 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:71:ILE:H	1:A:71:ILE:HD13	1.27	1.00
1:A:305:LEU:HD21	1:A:332:TYR:CD1	2.01	0.95
1:A:626:GLN:HE21	1:A:687:ARG:HH22	1.16	0.93
1:A:496:LEU:HB3	1:A:504:VAL:HG22	1.51	0.92
1:A:305:LEU:HD23	1:A:334:VAL:HG22	1.52	0.89
1:A:715:LEU:HD22	1:A:755:VAL:HG11	1.57	0.86
1:A:534:ASN:HD21	1:A:609:SER:HA	1.42	0.84
1:A:95:ARG:HH12	1:A:750:ASN:HD21	1.24	0.83
1:A:626:GLN:NE2	1:A:687:ARG:HH22	1.76	0.81
1:A:633:THR:HG22	1:A:652:GLN:HG3	1.62	0.80
1:A:488:ARG:HE	1:A:490:HIS:HE1	1.29	0.78
1:A:652:GLN:HE21	1:A:668:ASN:HD22	1.32	0.74
1:A:741:SER:HB2	1:A:755:VAL:HG12	1.69	0.74
1:A:356:SER:O	1:A:540:GLY:N	2.21	0.72
1:A:260:ILE:HD12	1:A:293:PRO:HG3	1.70	0.72
1:A:229:VAL:HG21	1:A:297:TYR:HB2	1.72	0.71
1:A:733:LEU:HD22	1:A:767:MET:HE2	1.73	0.71
1:A:753:VAL:HG12	1:A:755:VAL:HG13	1.72	0.71
1:A:741:SER:CB	1:A:755:VAL:HG12	2.22	0.70
1:A:229:VAL:HG23	1:A:744:TYR:CZ	2.28	0.69
1:A:71:ILE:HD13	1:A:71:ILE:N	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:HH12	1:A:750:ASN:ND2	1.92	0.65
1:A:480:ASN:ND2	6:A:2343:HOH:O	2.29	0.64
1:A:149:ALA:O	1:A:154:HIS:HE1	1.82	0.63
1:A:539:TYR:O	1:A:540:GLY:O	2.17	0.63
1:A:270:ILE:HD11	1:A:766:ARG:CZ	2.29	0.62
1:A:767:MET:HE3	1:A:772:LEU:HD11	1.82	0.62
1:A:328:ASN:HD21	1:A:544:VAL:H	1.48	0.62
1:A:441:HIS:HD2	1:A:459:ASP:OD2	1.84	0.60
1:A:70:GLY:HA3	1:A:195:ASN:HD22	1.65	0.60
1:A:648:SER:HB2	1:A:649:PRO:HD2	1.83	0.60
1:A:374:LEU:H	1:A:474:ASN:HD21	1.47	0.60
1:A:475:ASN:C	1:A:475:ASN:HD22	2.08	0.60
1:A:690:GLN:NE2	1:A:770:THR:HG22	2.17	0.60
1:A:98:THR:HG23	1:A:209:ILE:HD13	1.84	0.60
1:A:206:TYR:CD2	1:A:209:ILE:HD11	2.37	0.59
1:A:652:GLN:HE21	1:A:668:ASN:ND2	2.00	0.58
1:A:369:ARG:HB2	1:A:477:GLN:HE21	1.68	0.58
1:A:496:LEU:CB	1:A:504:VAL:HG22	2.29	0.58
1:A:534:ASN:ND2	1:A:609:SER:HA	2.16	0.58
1:A:728:LYS:O	1:A:729:GLY:O	2.21	0.58
1:A:71:ILE:H	1:A:71:ILE:CD1	2.08	0.57
1:A:715:LEU:CD2	1:A:755:VAL:HG11	2.33	0.57
1:A:671:ASN:HB2	6:A:2499:HOH:O	2.03	0.57
1:A:270:ILE:HD11	1:A:766:ARG:NH2	2.20	0.57
1:A:305:LEU:HD23	1:A:334:VAL:CG2	2.32	0.56
1:A:621:ASP:O	1:A:632:LEU:HD22	2.06	0.56
1:A:160:PHE:CZ	1:A:166:PRO:HB2	2.41	0.56
1:A:98:THR:HG23	1:A:209:ILE:CD1	2.35	0.56
1:A:620:ALA:HB1	1:A:632:LEU:HD21	1.88	0.56
1:A:397:GLN:HB2	1:A:406:VAL:HG22	1.89	0.55
1:A:718:TRP:CE2	1:A:730:PRO:HB3	2.42	0.55
1:A:81:LEU:HB2	1:A:86:HIS:CE1	2.42	0.54
1:A:354:GLU:C	1:A:355:ARG:HD3	2.32	0.54
1:A:606:TRP:HB3	1:A:608:SER:O	2.07	0.54
1:A:606:TRP:C	1:A:608:SER:H	2.15	0.54
1:A:436:LYS:O	1:A:441:HIS:HE1	1.91	0.53
1:A:229:VAL:CG2	1:A:297:TYR:HB2	2.37	0.52
1:A:381:GLN:OE1	1:A:497:THR:HG23	2.10	0.52
1:A:453:THR:OG1	1:A:465:THR:HG22	2.10	0.52
1:A:354:GLU:OE2	1:A:490:HIS:HD2	1.93	0.52
1:A:690:GLN:HE21	1:A:770:THR:HG22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:LYS:HD2	1:A:611:ILE:HD12	1.90	0.51
1:A:154:HIS:HD2	1:A:173:ASP:OD2	1.94	0.51
1:A:608:SER:OG	1:A:609:SER:N	2.43	0.51
1:A:438:HIS:HE1	6:A:2291:HOH:O	1.94	0.51
1:A:206:TYR:HD2	1:A:209:ILE:HD11	1.76	0.51
1:A:163:GLY:O	1:A:166:PRO:HD3	2.12	0.50
1:A:397:GLN:HG2	1:A:477:GLN:HB3	1.94	0.49
1:A:378:GLN:HG3	1:A:498:GLN:NE2	2.27	0.49
1:A:475:ASN:C	1:A:475:ASN:ND2	2.69	0.49
1:A:355:ARG:HD3	1:A:355:ARG:N	2.28	0.49
1:A:608:SER:C	1:A:610:SER:H	2.19	0.49
1:A:78:THR:HG22	1:A:192:VAL:HG22	1.94	0.49
1:A:513:GLN:NE2	6:A:2364:HOH:O	2.41	0.48
1:A:229:VAL:HG21	1:A:297:TYR:CB	2.43	0.48
1:A:434:HIS:HD2	1:A:657:ASP:OD2	1.95	0.48
1:A:104:SER:HA	1:A:125:LEU:HD12	1.94	0.48
1:A:370:ARG:HG2	1:A:370:ARG:HH11	1.78	0.47
1:A:190:MET:HG3	1:A:192:VAL:HG23	1.95	0.47
1:A:305:LEU:HD21	1:A:332:TYR:HD1	1.70	0.47
1:A:229:VAL:HG22	1:A:230:ALA:N	2.29	0.47
1:A:71:ILE:HG12	1:A:71:ILE:O	2.15	0.47
1:A:70:GLY:HA3	1:A:195:ASN:ND2	2.29	0.46
1:A:515:THR:OG1	1:A:517:GLU:HG2	2.16	0.45
1:A:625:LEU:HD22	1:A:723:GLU:HG3	1.98	0.45
1:A:672:VAL:HG22	1:A:727:TRP:HD1	1.81	0.45
1:A:190:MET:HG3	1:A:192:VAL:CG2	2.47	0.45
1:A:95:ARG:NH1	1:A:750:ASN:HD21	2.02	0.45
1:A:74:ARG:HD3	5:A:1784:SIA:O1A	2.15	0.45
1:A:622:MET:HB3	1:A:632:LEU:HD23	1.98	0.45
1:A:705:ASN:HD22	1:A:705:ASN:C	2.24	0.45
1:A:606:TRP:C	1:A:608:SER:N	2.75	0.44
1:A:189:ASN:O	1:A:190:MET:HB3	2.18	0.44
1:A:71:ILE:N	1:A:71:ILE:CD1	2.77	0.44
1:A:421:LEU:HD11	1:A:464:THR:HG21	2.00	0.44
1:A:403:ARG:HG2	1:A:467:ALA:O	2.18	0.43
1:A:305:LEU:C	1:A:305:LEU:HD13	2.44	0.43
1:A:687:ARG:NE	6:A:2518:HOH:O	2.42	0.42
1:A:657:ASP:HB2	6:A:2408:HOH:O	2.19	0.42
1:A:161:LEU:HD12	1:A:775:LYS:HE2	2.02	0.42
1:A:608:SER:C	1:A:610:SER:N	2.79	0.41
1:A:632:LEU:C	1:A:632:LEU:HD13	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:SER:H	1:A:540:GLY:HA2	1.85	0.41
1:A:453:THR:OG1	1:A:465:THR:CG2	2.69	0.41
1:A:488:ARG:HE	1:A:490:HIS:CE1	2.20	0.40
1:A:773:LYS:HD3	6:A:2581:HOH:O	2.22	0.40
1:A:728:LYS:O	1:A:729:GLY:C	2.64	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	A	751/781 (96%)	717 (96%)	27 (4%)	7 (1%)	14 3

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	GLY
1	A	729	GLY
1	A	608	SER
1	A	116	THR
1	A	610	SER
1	A	327	PRO
1	A	648	SER

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	633/656 (96%)	625 (99%)	8 (1%)	61 40

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ILE
1	A	294	ARG
1	A	397	GLN
1	A	466	TRP
1	A	474	ASN
1	A	475	ASN
1	A	668	ASN
1	A	723	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	69	GLN
1	A	76	GLN
1	A	86	HIS
1	A	117	GLN
1	A	154	HIS
1	A	165	ASN
1	A	180	ASN
1	A	182	GLN
1	A	195	ASN
1	A	317	GLN
1	A	328	ASN
1	A	377	GLN
1	A	378	GLN
1	A	395	GLN
1	A	397	GLN
1	A	434	HIS
1	A	438	HIS
1	A	441	HIS
1	A	462	GLN
1	A	474	ASN
1	A	475	ASN
1	A	477	GLN
1	A	490	HIS
1	A	502	ASN

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Mol	Chain	Res	Type
1	A	513	GLN
1	A	550	HIS
1	A	557	GLN
1	A	559	ASN
1	A	626	GLN
1	A	668	ASN
1	A	690	GLN
1	A	703	GLN
1	A	705	ASN
1	A	750	ASN

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 ⓘ

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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
5	SIA	A	1784	-	21,21,21	0.71	0	24,31,31	1.03	2 (8%)
4	TRS	A	1783	3	7,7,7	1.18	2 (28%)	9,9,9	1.89	3 (33%)
2	GOL	A	1778	-	5,5,5	4.79	5 (100%)	5,5,5	6.09	3 (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
5	SIA	A	1784	-	-	1/20/38/38	0/1/1/1
4	TRS	A	1783	3	-	3/9/9/9	-
2	GOL	A	1778	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1778	GOL	C3-C2	-8.03	1.21	1.51
2	A	1778	GOL	O1-C1	4.59	1.61	1.42
2	A	1778	GOL	O3-C3	3.42	1.56	1.42
2	A	1778	GOL	C1-C2	-3.02	1.40	1.51
2	A	1778	GOL	O2-C2	-2.91	1.34	1.43
4	A	1783	TRS	O2-C2	2.17	1.49	1.42
4	A	1783	TRS	O1-C1	2.02	1.48	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1778	GOL	O3-C3-C2	11.01	159.94	110.38
2	A	1778	GOL	O2-C2-C3	7.20	138.99	109.18
4	A	1783	TRS	C1-C-N	3.66	117.49	108.17
2	A	1778	GOL	O1-C1-C2	3.40	125.70	110.38
5	A	1784	SIA	O1A-C1-C2	-3.05	118.77	123.85
4	A	1783	TRS	C3-C-C1	-2.55	103.87	110.66
4	A	1783	TRS	C3-C-C2	2.20	116.51	110.66
5	A	1784	SIA	O6-C6-C7	2.19	110.07	106.65

There are no chirality outliers.

All (6) torsion outliers are listed below:

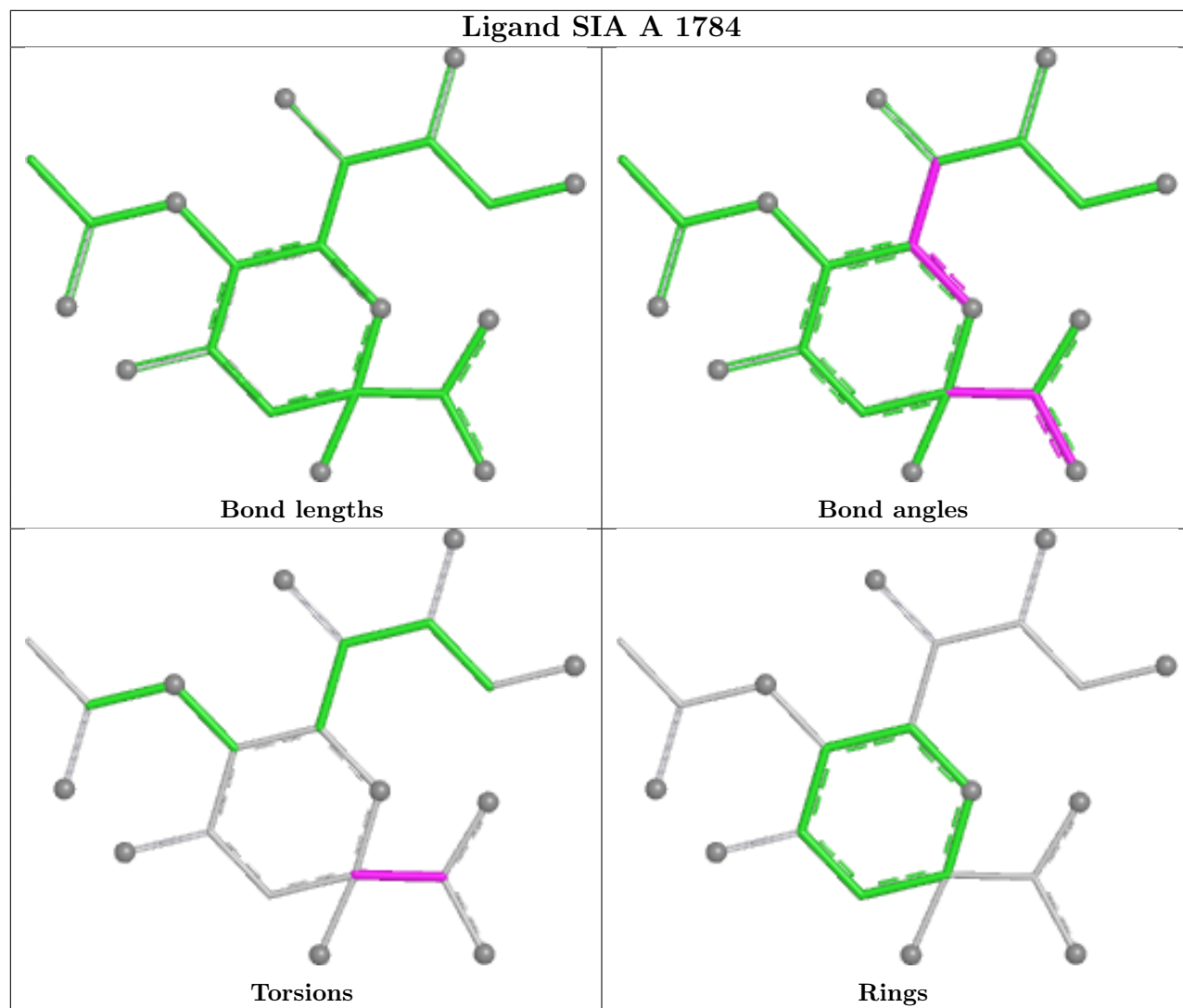
Mol	Chain	Res	Type	Atoms
2	A	1778	GOL	O1-C1-C2-C3
2	A	1778	GOL	C1-C2-C3-O3
4	A	1783	TRS	C2-C-C1-O1
4	A	1783	TRS	C3-C-C1-O1
4	A	1783	TRS	N-C-C1-O1
5	A	1784	SIA	O1B-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1784	SIA	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	753/781 (96%)	1.13	123 (16%) 4 4	4, 12, 25, 38	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	609	SER	10.7
1	A	540	GLY	9.9
1	A	115	GLY	9.8
1	A	777	THR	8.8
1	A	729	GLY	8.8
1	A	608	SER	8.3
1	A	610	SER	6.7
1	A	60	ALA	6.6
1	A	189	ASN	5.1
1	A	61	ASP	5.0
1	A	62	GLY	4.9
1	A	90	SER	4.6
1	A	139	THR	4.5
1	A	63	MET	4.1
1	A	46	MET	4.0
1	A	501	HIS	3.9
1	A	190	MET	3.8
1	A	34	ASP	3.7
1	A	165	ASN	3.6
1	A	281	GLN	3.6
1	A	499	GLN	3.6
1	A	442	ASP	3.6
1	A	71	ILE	3.5
1	A	114	ASN	3.5
1	A	414	SER	3.4
1	A	710	ASN	3.4
1	A	287	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	776	LEU	3.3
1	A	472	GLN	3.2
1	A	559	ASN	3.2
1	A	517	GLU	3.2
1	A	209	ILE	3.2
1	A	452	HIS	3.1
1	A	141	ARG	3.1
1	A	92	PHE	3.1
1	A	138	GLN	3.0
1	A	556	ARG	3.0
1	A	95	ARG	3.0
1	A	164	SER	3.0
1	A	86	HIS	3.0
1	A	163	GLY	3.0
1	A	166	PRO	3.0
1	A	196	GLY	3.0
1	A	773	LYS	2.9
1	A	513	GLN	2.9
1	A	413	GLU	2.8
1	A	117	GLN	2.8
1	A	116	THR	2.8
1	A	185	ALA	2.7
1	A	83	THR	2.7
1	A	691	SER	2.7
1	A	403	ARG	2.7
1	A	52	ASN	2.7
1	A	177	ILE	2.7
1	A	87	ALA	2.7
1	A	175	LYS	2.6
1	A	562	GLY	2.6
1	A	692	ASP	2.6
1	A	84	ASN	2.6
1	A	199	ASN	2.6
1	A	450	LEU	2.6
1	A	91	SER	2.6
1	A	127	SER	2.6
1	A	484	GLN	2.6
1	A	161	LEU	2.6
1	A	51	ASN	2.6
1	A	377	GLN	2.5
1	A	57	LEU	2.5
1	A	503	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	140	GLY	2.5
1	A	125	LEU	2.5
1	A	412	ASP	2.5
1	A	516	PRO	2.5
1	A	728	LYS	2.4
1	A	186	SER	2.4
1	A	378	GLN	2.4
1	A	66	TRP	2.4
1	A	285	SER	2.4
1	A	558	GLN	2.4
1	A	89	ALA	2.4
1	A	671	ASN	2.3
1	A	176	LEU	2.3
1	A	122	ILE	2.3
1	A	151	THR	2.3
1	A	80	SER	2.3
1	A	470	VAL	2.3
1	A	515	THR	2.3
1	A	148	THR	2.2
1	A	355	ARG	2.2
1	A	28	ASP	2.2
1	A	37	PHE	2.2
1	A	102	VAL	2.2
1	A	672	VAL	2.2
1	A	755	VAL	2.2
1	A	435	ALA	2.2
1	A	79	TYR	2.2
1	A	187	LYS	2.2
1	A	327	PRO	2.2
1	A	143	VAL	2.1
1	A	179	ASP	2.1
1	A	370	ARG	2.1
1	A	229	VAL	2.1
1	A	504	VAL	2.1
1	A	45	TRP	2.1
1	A	433	GLU	2.1
1	A	749	GLU	2.1
1	A	453	THR	2.1
1	A	607	LYS	2.1
1	A	132	VAL	2.1
1	A	59	ASN	2.1
1	A	99	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	536	MET	2.1
1	A	254	LEU	2.1
1	A	142	THR	2.1
1	A	730	PRO	2.1
1	A	280	GLU	2.0
1	A	666	GLU	2.0
1	A	425	SER	2.0
1	A	130	ASN	2.0
1	A	395	GLN	2.0
1	A	135	PHE	2.0
1	A	208	ASP	2.0
1	A	68	VAL	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](#)

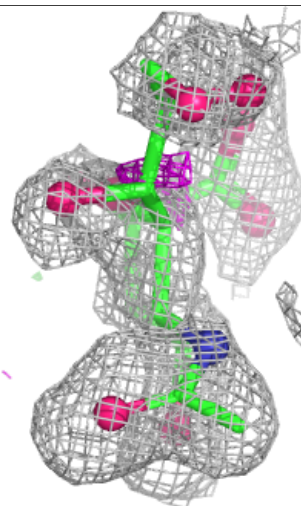
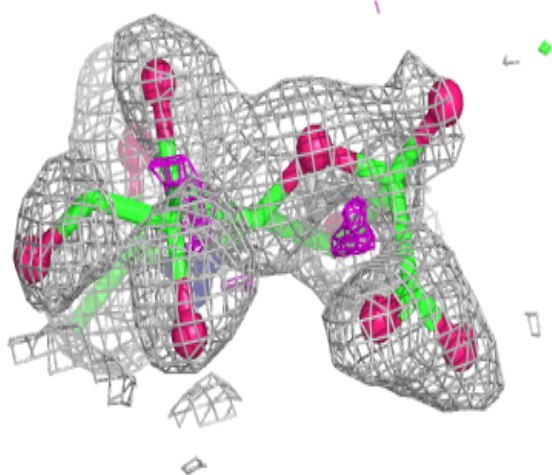
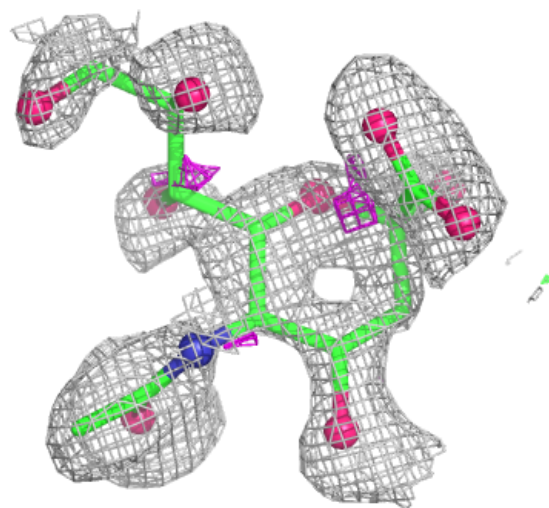
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	1778	6/6	0.59	0.19	32,32,33,33	0
5	SIA	A	1784	21/21	0.71	0.18	28,33,35,37	0
4	TRS	A	1783	8/8	0.72	0.22	21,27,29,29	0
3	CA	A	1782	1/1	0.90	0.08	10,10,10,10	0
3	CA	A	1780	1/1	0.94	0.07	5,5,5,5	0
3	CA	A	1781	1/1	0.97	0.04	9,9,9,9	0
3	CA	A	1779	1/1	0.97	0.04	6,6,6,6	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 SIA A 1784:

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.