



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:10 AM UTC

PDB ID : 7XSH / pdb_00007xsh
Title : Crystal structure of ClAgl29B bound with L-glucose
Authors : Shishiuchi, R.; Kang, H.; Tagami, T.; Okuyama, M.
Deposited on : 2022-05-14
Resolution : 1.71 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

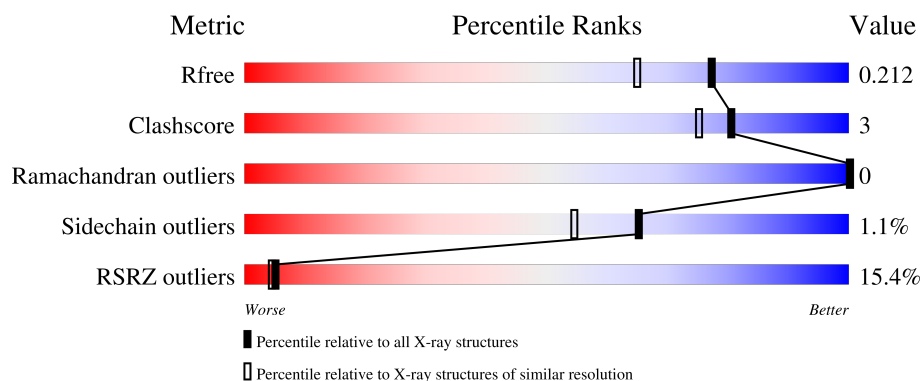
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	587	21% 86% 6% • 7%
1	B	587	8% 87% 6% • 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
4	GOL	B	605	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9706 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 Alpha-L-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	2	0
			4455	2865	723	851	16			
1	B	548	Total	C	N	O	S	0	6	0
			4483	2881	727	859	16			

There are 42 discrepancies between the modelled and reference sequences:

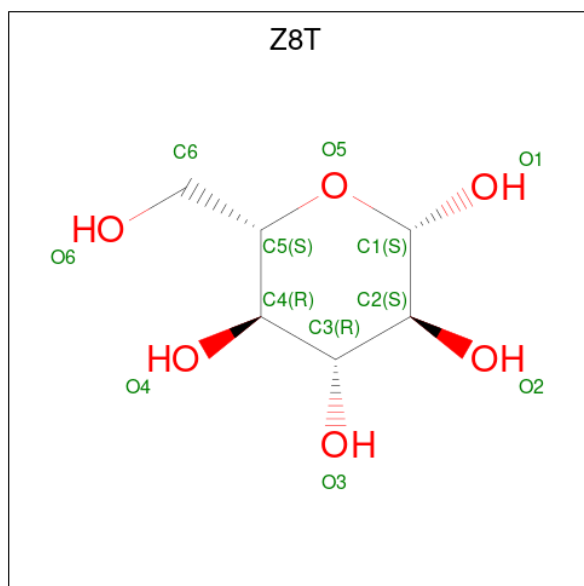
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP K1KV82
A	1	GLY	-	expression tag	UNP K1KV82
A	2	SER	-	expression tag	UNP K1KV82
A	3	SER	-	expression tag	UNP K1KV82
A	4	HIS	-	expression tag	UNP K1KV82
A	5	HIS	-	expression tag	UNP K1KV82
A	6	HIS	-	expression tag	UNP K1KV82
A	7	HIS	-	expression tag	UNP K1KV82
A	8	HIS	-	expression tag	UNP K1KV82
A	9	HIS	-	expression tag	UNP K1KV82
A	10	SER	-	expression tag	UNP K1KV82
A	11	SER	-	expression tag	UNP K1KV82
A	12	GLY	-	expression tag	UNP K1KV82
A	13	LEU	-	expression tag	UNP K1KV82
A	14	VAL	-	expression tag	UNP K1KV82
A	15	PRO	-	expression tag	UNP K1KV82
A	16	ARG	-	expression tag	UNP K1KV82
A	17	GLY	-	expression tag	UNP K1KV82
A	18	SER	-	expression tag	UNP K1KV82
A	19	HIS	-	expression tag	UNP K1KV82
A	20	MET	-	expression tag	UNP K1KV82
B	0	MET	-	initiating methionine	UNP K1KV82
B	1	GLY	-	expression tag	UNP K1KV82
B	2	SER	-	expression tag	UNP K1KV82
B	3	SER	-	expression tag	UNP K1KV82

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	expression tag	UNP K1KV82
B	5	HIS	-	expression tag	UNP K1KV82
B	6	HIS	-	expression tag	UNP K1KV82
B	7	HIS	-	expression tag	UNP K1KV82
B	8	HIS	-	expression tag	UNP K1KV82
B	9	HIS	-	expression tag	UNP K1KV82
B	10	SER	-	expression tag	UNP K1KV82
B	11	SER	-	expression tag	UNP K1KV82
B	12	GLY	-	expression tag	UNP K1KV82
B	13	LEU	-	expression tag	UNP K1KV82
B	14	VAL	-	expression tag	UNP K1KV82
B	15	PRO	-	expression tag	UNP K1KV82
B	16	ARG	-	expression tag	UNP K1KV82
B	17	GLY	-	expression tag	UNP K1KV82
B	18	SER	-	expression tag	UNP K1KV82
B	19	HIS	-	expression tag	UNP K1KV82
B	20	MET	-	expression tag	UNP K1KV82

- Molecule 2 is beta-L-glucopyranose (CCD ID: Z8T) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).

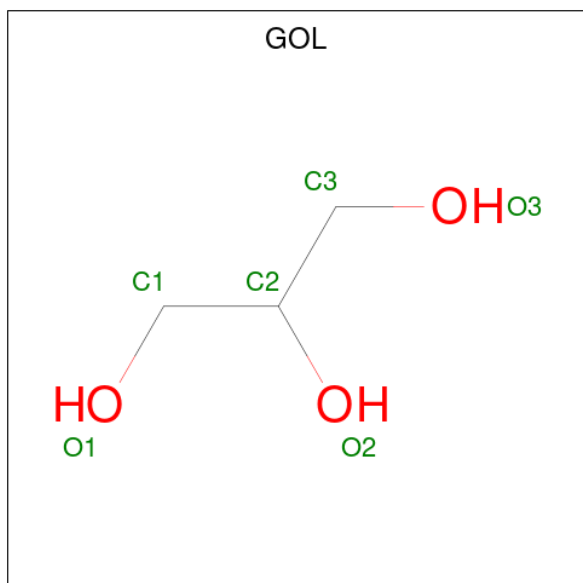


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

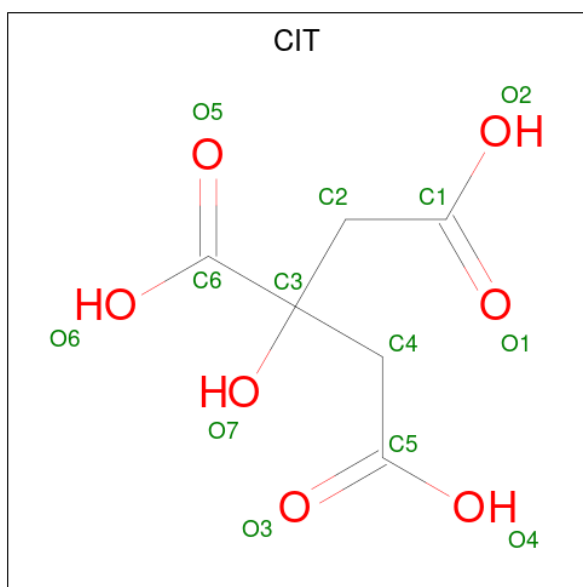
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



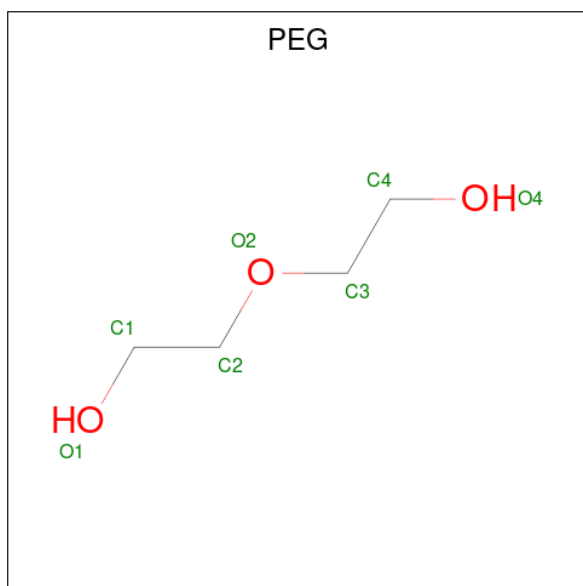
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		

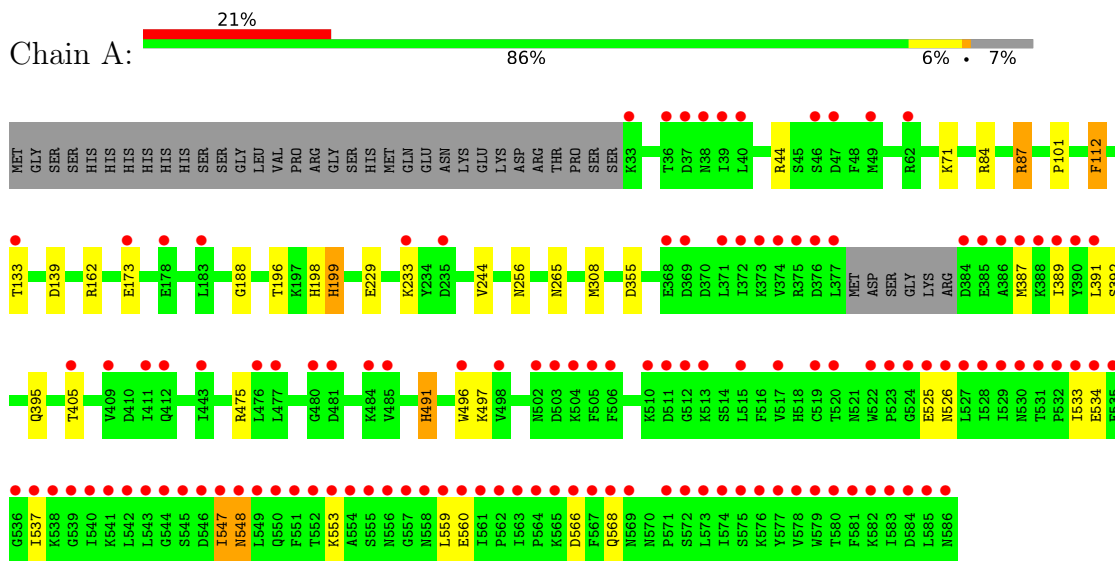
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	281	Total 281	O 281	0	0
7	B	411	Total 411	O 411	0	0

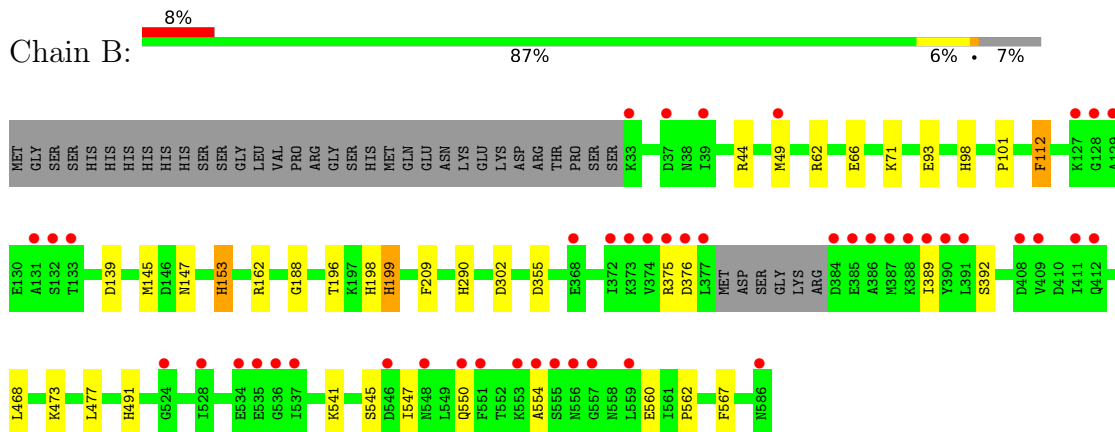
3 Residue-property plots [i](#)

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: Alpha-L-fucosidase



• Molecule 1: Alpha-L-fucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.39Å 121.58Å 166.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.60 – 1.71 46.60 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.60-1.71) 99.8 (46.60-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.8.0349	Depositor
R, R_{free}	0.179 , 0.202 0.190 , 0.212	Depositor DCC
R_{free} test set	7948 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 32.4	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	0.96	EDS
Total number of atoms	9706	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: PEG, GOL, NA, Z8T, CIT

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	0.55	2/4578 (0.0%)	0.85	2/6204 (0.0%)
1	B	0.56	4/4606 (0.1%)	0.84	3/6242 (0.0%)
All	All	0.56	6/9184 (0.1%)	0.85	5/12446 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	290	HIS	CE1-NE2	6.75	1.39	1.32
1	B	199	HIS	CE1-NE2	5.73	1.38	1.32
1	B	153	HIS	CE1-NE2	5.32	1.37	1.32
1	A	199	HIS	CE1-NE2	5.13	1.37	1.32
1	A	491	HIS	CE1-NE2	5.10	1.37	1.32
1	B	98	HIS	CE1-NE2	5.06	1.37	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	PHE	CA-CB-CG	5.85	119.65	113.80
1	B	139	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	139	ASP	CA-CB-CG	5.28	117.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	112	PHE	CA-CB-CG	5.16	118.96	113.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162[A]	ARG	Sidechain
1	A	44	ARG	Sidechain
1	A	475	ARG	Sidechain
1	A	84	ARG	Sidechain
1	A	87	ARG	Sidechain
1	B	162[A]	ARG	Sidechain
1	B	44	ARG	Sidechain
1	B	62	ARG	Sidechain

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	4455	0	4288	24	0
1	B	4483	0	4309	22	0
2	A	12	0	0	0	0
2	B	12	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	16	0	0
4	B	18	0	24	5	0
5	A	13	0	5	0	0
6	B	7	0	10	0	0
7	A	281	0	0	2	0
7	B	411	0	0	3	0
All	All	9706	0	8652	46	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 (46) 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:256:ASN:HD21	1:A:265:ASN:H	1.18	0.87
1:A:547:ILE:HD12	1:A:548:ASN:O	1.87	0.74
1:A:537:ILE:HD11	1:A:559:LEU:HD21	1.70	0.72
1:B:147:ASN:HD22	4:B:605:GOL:C1	2.03	0.71
1:A:533:ILE:HD12	1:A:559:LEU:HD22	1.71	0.70
1:B:147:ASN:HD22	4:B:605:GOL:H12	1.57	0.70
1:A:525:GLU:HG2	1:A:526:ASN:ND2	2.07	0.69
1:A:229:GLU:O	1:A:233:LYS:HE3	1.93	0.68
1:A:387:MET:HE3	1:A:391:LEU:HD11	1.78	0.64
1:B:468:LEU:O	1:B:473:LYS:HE3	2.00	0.61
1:B:93:GLU:HG2	7:B:1010:HOH:O	2.02	0.59
1:B:550:GLN:HE21	1:B:562:PRO:HG2	1.68	0.59
1:A:244:VAL:HG13	1:A:308[B]:MET:SD	2.44	0.57
1:A:537:ILE:CD1	1:A:559:LEU:HD21	2.33	0.57
1:A:87:ARG:HH11	1:A:87:ARG:HG2	1.71	0.56
1:B:554:ALA:HB2	1:B:560:GLU:OE2	2.06	0.54
1:A:525:GLU:HA	1:A:568:GLN:HE22	1.73	0.54
1:B:188:GLY:O	1:B:491:HIS:HE1	1.90	0.53
1:B:147:ASN:ND2	4:B:605:GOL:H12	2.22	0.53
1:B:66:GLU:CD	7:B:912:HOH:O	2.53	0.52
1:B:477[B]:LEU:C	1:B:477[B]:LEU:HD23	2.35	0.51
1:B:541:LYS:HE3	1:B:545[B]:SER:O	2.10	0.51
1:A:188:GLY:O	1:A:491:HIS:HE1	1.94	0.51
1:A:392:SER:O	1:A:395:GLN:NE2	2.27	0.50
1:B:491:HIS:HD2	7:B:1067:HOH:O	1.94	0.49
1:B:71:LYS:HD3	1:B:209:PHE:CZ	2.49	0.48
1:A:387:MET:HE3	1:A:391:LEU:CD1	2.44	0.48
1:B:375:ARG:NH1	1:B:376:ASP:OD1	2.47	0.47
1:B:147:ASN:ND2	4:B:605:GOL:C1	2.73	0.47
1:B:547:ILE:HD12	1:B:567:PHE:CZ	2.49	0.46
1:A:229:GLU:C	1:A:233:LYS:HE3	2.40	0.46
1:B:147:ASN:HD22	4:B:605:GOL:H11	1.80	0.45
1:A:87:ARG:HH11	1:A:87:ARG:CG	2.30	0.45
1:B:389:ILE:O	1:B:392:SER:OG	2.34	0.43
1:A:496:TRP:CZ2	1:A:497:LYS:HE2	2.54	0.43
1:A:198:HIS:CG	1:A:199:HIS:H	2.36	0.42
1:B:198:HIS:CG	1:B:199:HIS:H	2.37	0.42
1:A:133:THR:O	1:A:405:THR:HG23	2.20	0.42
1:A:525:GLU:HA	1:A:568:GLN:NE2	2.34	0.42
1:A:534:GLU:HG2	7:A:924:HOH:O	2.19	0.42
1:A:101:PRO:HB3	1:A:355:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:MET:HE3	1:B:153:HIS:CE1	2.55	0.41
1:B:554:ALA:HB2	1:B:560:GLU:CD	2.45	0.41
1:A:173:GLU:CD	7:A:736:HOH:O	2.63	0.41
1:A:389:ILE:O	1:A:392:SER:OG	2.36	0.40
1:B:101:PRO:HB3	1:B:355[B]:ASP:CG	2.46	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	546/587 (93%)	529 (97%)	17 (3%)	0	100	100
1	B	550/587 (94%)	533 (97%)	17 (3%)	0	100	100
All	All	1096/1174 (93%)	1062 (97%)	34 (3%)	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	484/517 (94%)	476 (98%)	8 (2%)	53	38
1	B	488/517 (94%)	485 (99%)	3 (1%)	78	72
All	All	972/1034 (94%)	961 (99%)	11 (1%)	65	54

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LYS
1	A	112	PHE
1	A	196	THR
1	A	547	ILE
1	A	548	ASN
1	A	553	LYS
1	A	560	GLU
1	A	566	ASP
1	B	49	MET
1	B	112	PHE
1	B	196	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	256	ASN
1	A	265	ASN
1	A	412	GLN
1	A	430	GLN
1	A	491	HIS
1	A	499	GLN
1	A	518	HIS
1	A	526	ASN
1	A	548	ASN
1	A	568	GLN
1	B	186	ASN
1	B	255	GLN
1	B	259	GLN
1	B	270	GLN
1	B	275	GLN
1	B	491	HIS
1	B	518	HIS
1	B	526	ASN
1	B	548	ASN
1	B	550	GLN

5.3.3 RNA ⓘ

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](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\# Z > 2$
4	GOL	A	603	-	5,5,5	0.11	0	5,5,5	0.21	0
2	Z8T	B	601	-	12,12,12	0.43	0	17,17,17	1.33	4 (23%)
2	Z8T	A	601	-	12,12,12	0.68	0	17,17,17	1.20	1 (5%)
4	GOL	B	604	-	5,5,5	0.19	0	5,5,5	0.42	0
4	GOL	A	604	-	5,5,5	0.09	0	5,5,5	0.24	0
5	CIT	A	605	-	12,12,12	1.35	1 (8%)	17,17,17	1.22	2 (11%)
4	GOL	B	603	-	5,5,5	0.25	0	5,5,5	0.63	0
6	PEG	B	606	-	6,6,6	0.14	0	5,5,5	0.07	0
4	GOL	B	605	-	5,5,5	0.25	0	5,5,5	0.84	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
4	GOL	A	603	-	-	0/4/4/4	-
2	Z8T	B	601	-	-	2/2/22/22	0/1/1/1
2	Z8T	A	601	-	-	2/2/22/22	0/1/1/1
4	GOL	B	604	-	-	1/4/4/4	-
4	GOL	A	604	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CIT	A	605	-	-	2/16/16/16	-
4	GOL	B	603	-	-	4/4/4/4	-
6	PEG	B	606	-	-	3/4/4/4	-
4	GOL	B	605	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	CIT	C3-C6	2.97	1.56	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	Z8T	O2-C2-C3	2.87	117.14	110.38
5	A	605	CIT	O6-C6-C3	2.75	118.41	113.14
5	A	605	CIT	O5-C6-C3	-2.61	117.04	122.09
2	B	601	Z8T	O1-C1-C2	2.56	116.40	108.98
2	B	601	Z8T	O2-C2-C3	2.26	115.72	110.38
2	B	601	Z8T	O5-C5-C4	2.23	113.71	109.70
2	B	601	Z8T	O4-C4-C5	-2.01	104.38	109.32

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	GOL	O1-C1-C2-C3
4	B	603	GOL	O1-C1-C2-C3
4	B	603	GOL	C1-C2-C3-O3
4	B	603	GOL	O2-C2-C3-O3
2	A	601	Z8T	C4-C5-C6-O6
2	A	601	Z8T	O5-C5-C6-O6
6	B	606	PEG	O1-C1-C2-O2
6	B	606	PEG	O2-C3-C4-O4
2	B	601	Z8T	C4-C5-C6-O6
4	B	605	GOL	C1-C2-C3-O3
4	A	604	GOL	O1-C1-C2-O2
4	B	603	GOL	O1-C1-C2-O2
2	B	601	Z8T	O5-C5-C6-O6
6	B	606	PEG	C1-C2-O2-C3
5	A	605	CIT	C2-C3-C6-O6

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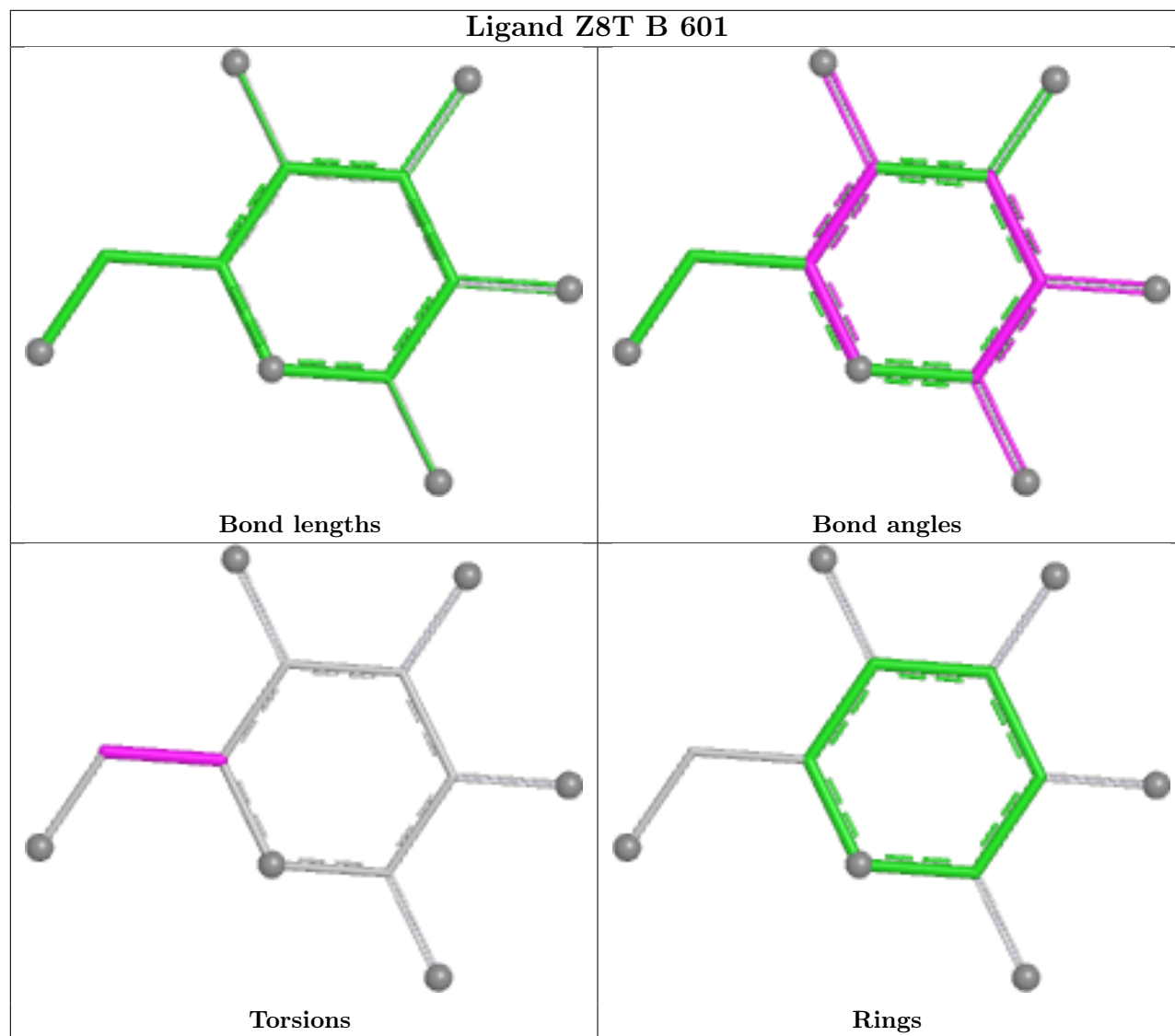
Mol	Chain	Res	Type	Atoms
4	B	604	GOL	O1-C1-C2-O2
5	A	605	CIT	O7-C3-C6-O6

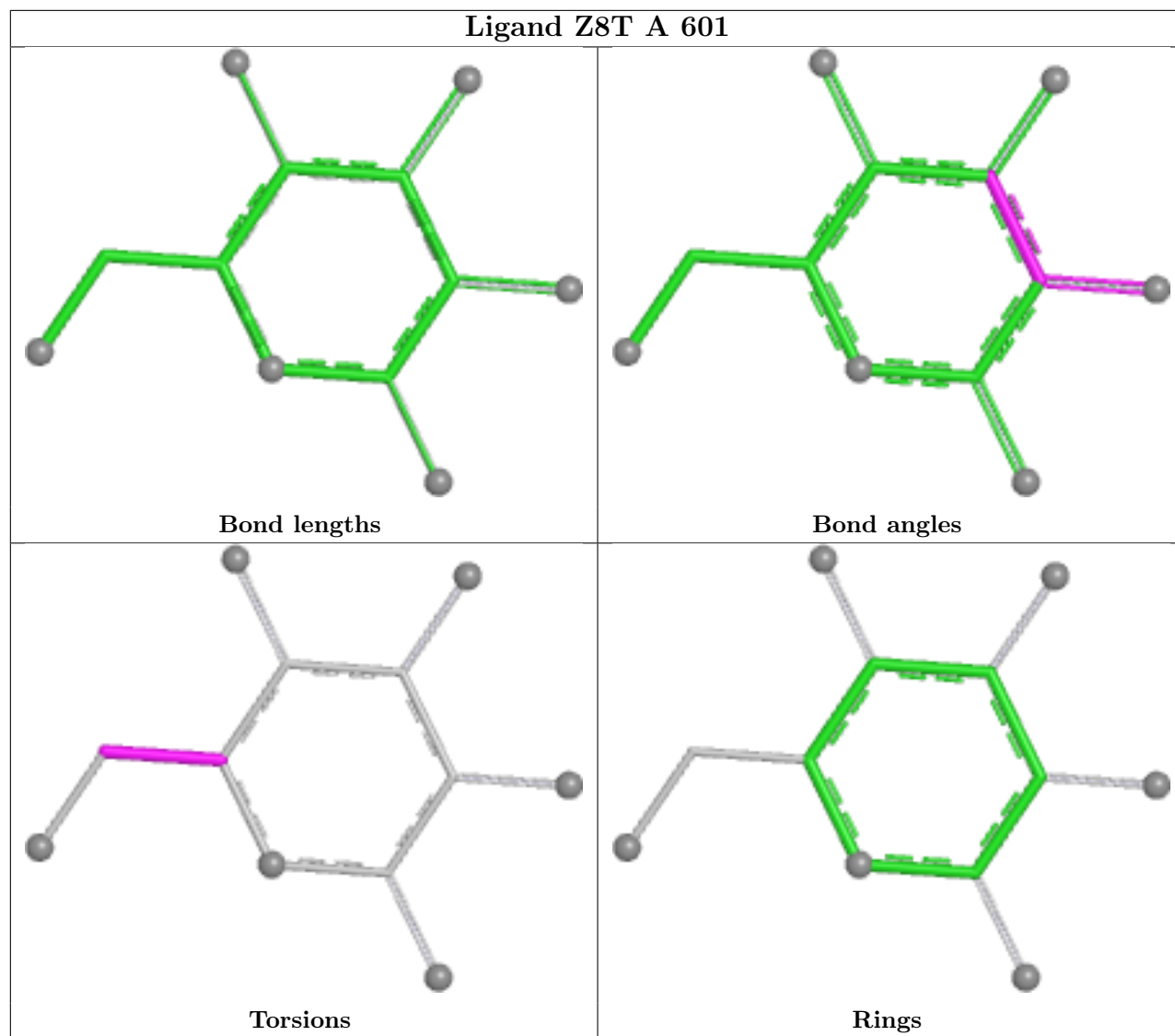
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	605	GOL	5	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	548/587 (93%)	1.03	123 (22%) 2 2	8, 25, 65, 97	2 (0%)
1	B	548/587 (93%)	0.03	46 (8%) 17 18	8, 17, 47, 77	6 (1%)
All	All	1096/1174 (93%)	0.53	169 (15%) 5 4	8, 21, 60, 97	8 (0%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	549	LEU	9.7
1	A	567	PHE	9.4
1	A	559	LEU	8.7
1	A	547	ILE	8.5
1	B	377	LEU	8.2
1	A	554	ALA	8.2
1	A	522	TRP	8.1
1	A	561	ILE	8.0
1	A	386	ALA	7.8
1	A	377	LEU	6.0
1	A	542	LEU	6.0
1	A	571	PRO	5.9
1	A	529	ILE	5.7
1	A	581	PHE	5.6
1	A	552	THR	5.5
1	B	386	ALA	5.4
1	A	573	LEU	5.4
1	A	557	GLY	5.3
1	A	568	GLN	5.1
1	A	527	LEU	5.1
1	A	528	ILE	5.0
1	A	563	ILE	5.0
1	A	374	VAL	5.0
1	A	578	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	565	LYS	4.9
1	A	564	PRO	4.8
1	A	551	PHE	4.7
1	A	560	GLU	4.7
1	A	372	ILE	4.7
1	A	389	ILE	4.7
1	A	574	ILE	4.6
1	A	553	LYS	4.6
1	A	525	GLU	4.5
1	A	562	PRO	4.5
1	B	374	VAL	4.5
1	A	526	ASN	4.4
1	A	579	TRP	4.3
1	A	572	SER	4.3
1	A	524	GLY	4.3
1	A	537	ILE	4.3
1	A	550	GLN	4.3
1	B	555	SER	4.3
1	A	546	ASP	4.2
1	A	33	LYS	4.2
1	A	569	ASN	4.2
1	A	533	ILE	4.1
1	A	548	ASN	4.1
1	A	540	ILE	4.0
1	A	583	ILE	4.0
1	A	532	PRO	4.0
1	A	558	ASN	4.0
1	A	519	CYS	3.9
1	A	515	LEU	3.9
1	A	566	ASP	3.9
1	B	586	ASN	3.9
1	B	372	ILE	3.8
1	A	555	SER	3.8
1	A	543	LEU	3.8
1	A	390	TYR	3.8
1	A	531	THR	3.8
1	A	517	VAL	3.8
1	A	556	ASN	3.8
1	A	575	SER	3.7
1	B	39	ILE	3.6
1	B	384	ASP	3.6
1	B	409	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	544	GLY	3.6
1	B	33	LYS	3.6
1	A	586	ASN	3.6
1	A	523	PRO	3.5
1	A	411	ILE	3.5
1	B	131	ALA	3.5
1	A	545	SER	3.5
1	A	40	LEU	3.4
1	A	534	GLU	3.4
1	A	387	MET	3.3
1	B	556	ASN	3.3
1	A	498	VAL	3.3
1	A	506	PHE	3.3
1	A	371	LEU	3.2
1	A	502	ASN	3.2
1	B	554	ALA	3.2
1	A	580	THR	3.2
1	B	391	LEU	3.2
1	A	503	ASP	3.2
1	A	39	ILE	3.2
1	A	585	LEU	3.2
1	A	584	ASP	3.2
1	A	530	ASN	3.1
1	B	553	LYS	3.1
1	A	577	TYR	3.1
1	A	511	ASP	3.1
1	A	476	LEU	3.1
1	A	538	LYS	3.1
1	A	485	VAL	3.1
1	B	389	ILE	3.1
1	B	557	GLY	3.0
1	A	391	LEU	3.0
1	A	405	THR	3.0
1	B	129	ALA	3.0
1	B	537	ILE	3.0
1	A	375	ARG	3.0
1	A	477	LEU	3.0
1	B	411	ILE	3.0
1	B	388	LYS	2.9
1	B	551	PHE	2.9
1	A	409	VAL	2.9
1	A	539	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	376	ASP	2.9
1	A	384	ASP	2.9
1	A	233	LYS	2.9
1	A	388	LYS	2.9
1	A	505	PHE	2.9
1	A	520	THR	2.9
1	B	408	ASP	2.8
1	A	510	LYS	2.8
1	A	47	ASP	2.8
1	A	512	GLY	2.8
1	B	128	GLY	2.8
1	A	484	LYS	2.8
1	A	536	GLY	2.8
1	B	132	SER	2.8
1	A	373	LYS	2.7
1	A	46	SER	2.7
1	A	496	TRP	2.7
1	A	183	LEU	2.7
1	A	368	GLU	2.6
1	B	385	GLU	2.6
1	B	550	GLN	2.6
1	A	412	GLN	2.6
1	A	513	LYS	2.6
1	A	36	THR	2.5
1	A	49	MET	2.5
1	B	387	MET	2.5
1	B	535	GLU	2.5
1	A	481	ASP	2.5
1	A	576	LYS	2.5
1	B	373	LYS	2.5
1	B	528	ILE	2.5
1	A	133	THR	2.5
1	B	375	ARG	2.4
1	B	524	GLY	2.4
1	A	535	GLU	2.4
1	B	127	LYS	2.4
1	A	582	LYS	2.4
1	A	37	ASP	2.3
1	A	541	LYS	2.3
1	B	37	ASP	2.3
1	A	173	GLU	2.3
1	A	369	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	49	MET	2.2
1	B	536	GLY	2.2
1	A	504	LYS	2.2
1	A	235	ASP	2.2
1	B	376	ASP	2.2
1	B	368	GLU	2.2
1	A	62	ARG	2.2
1	B	133	THR	2.2
1	A	385	GLU	2.1
1	A	38	ASN	2.1
1	B	534	GLU	2.1
1	A	480	GLY	2.1
1	B	559	LEU	2.1
1	A	178	GLU	2.1
1	B	390	TYR	2.1
1	B	548	ASN	2.1
1	B	412	GLN	2.0
1	B	546	ASP	2.0
1	A	443	ILE	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
4	GOL	B	605	6/6	0.71	0.23	37,46,47,50	0
4	GOL	A	604	6/6	0.79	0.24	44,52,55,63	0
4	GOL	B	604	6/6	0.82	0.16	27,37,41,46	0
5	CIT	A	605	13/13	0.85	0.11	34,42,51,53	0

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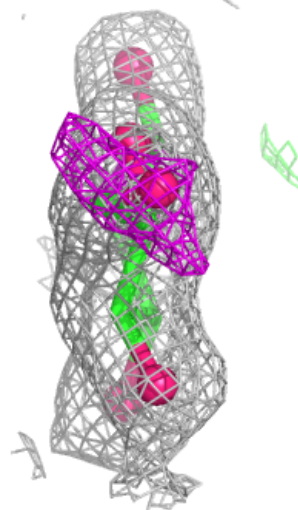
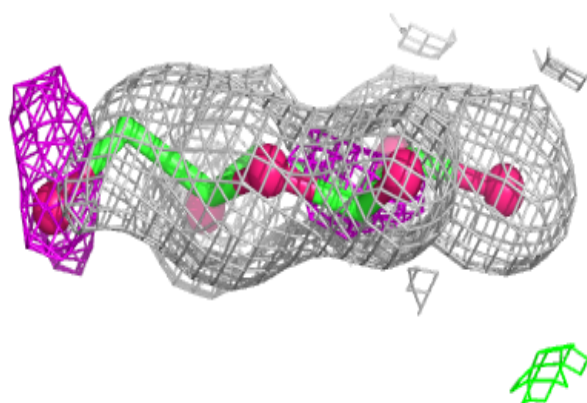
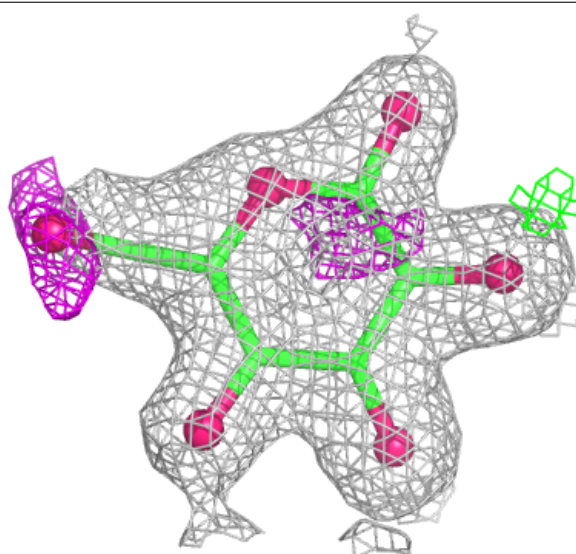
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	603	6/6	0.86	0.14	28,29,34,34	0
6	PEG	B	606	7/7	0.88	0.16	47,48,50,53	0
2	Z8T	A	601	12/12	0.92	0.11	24,30,39,44	0
2	Z8T	B	601	12/12	0.94	0.08	18,24,31,41	0
4	GOL	A	603	6/6	0.94	0.09	26,28,29,30	0
3	NA	A	602	1/1	0.95	0.12	34,34,34,34	0
3	NA	B	602	1/1	0.99	0.10	23,23,23,23	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.

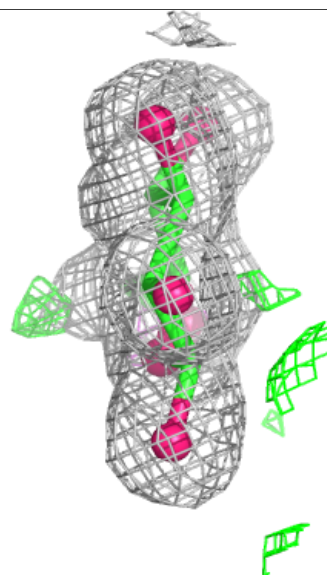
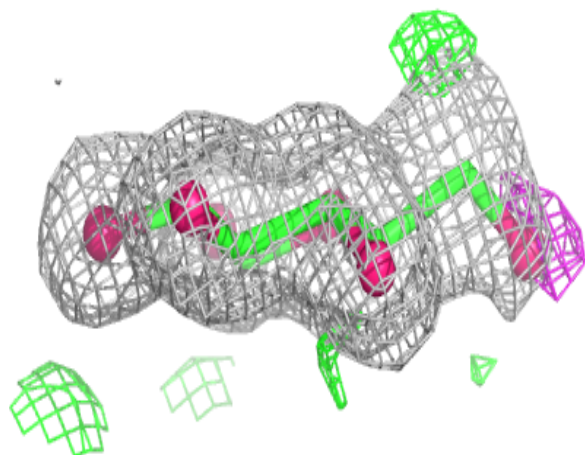
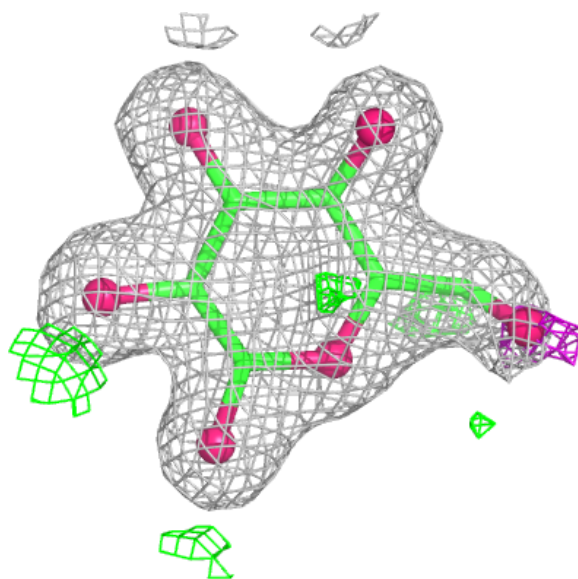
Electron density around Z8T A 601:

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



Electron density around Z8T B 601:

$2mF_o-DF_c$ (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.