Full wwPDB X-ray Structure Validation Report (i)

Jan 10, 2023 – 12:11 PM JST

PDB ID	:	7XSH
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 (i) 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 (i)) were used in the production of this report:

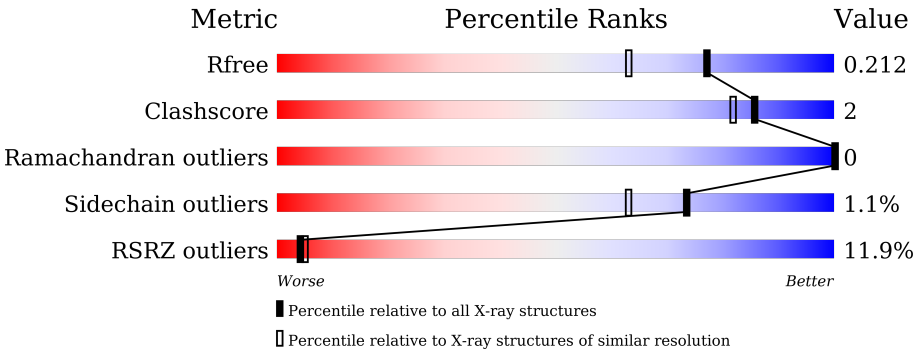
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 <=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	16% 87% 6% • 7%
1	B	587	6% 88% 5% 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 (i)

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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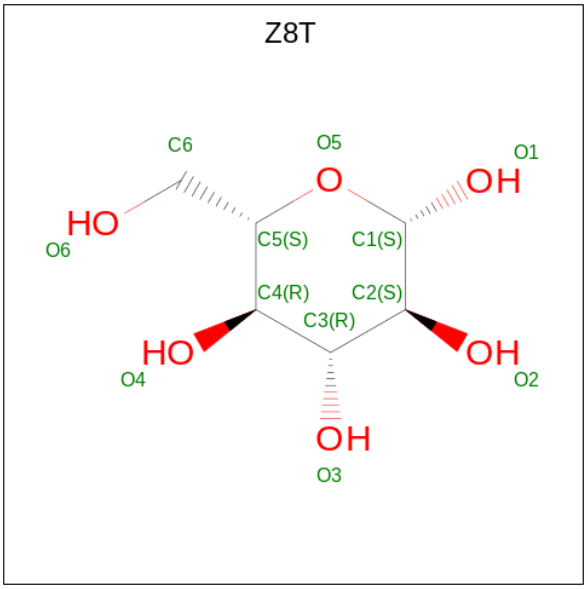
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	expression tag	UNP K1KV82
B	5	HIS	-	expression tag	UNP K1KV82
B	6	HIS	-	expression tag	UNP K1KV82
B	7	HIS	-	expression tag	UNP K1KV82
B	8	HIS	-	expression tag	UNP K1KV82
B	9	HIS	-	expression tag	UNP K1KV82
B	10	SER	-	expression tag	UNP K1KV82
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 (three-letter code: Z8T) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).

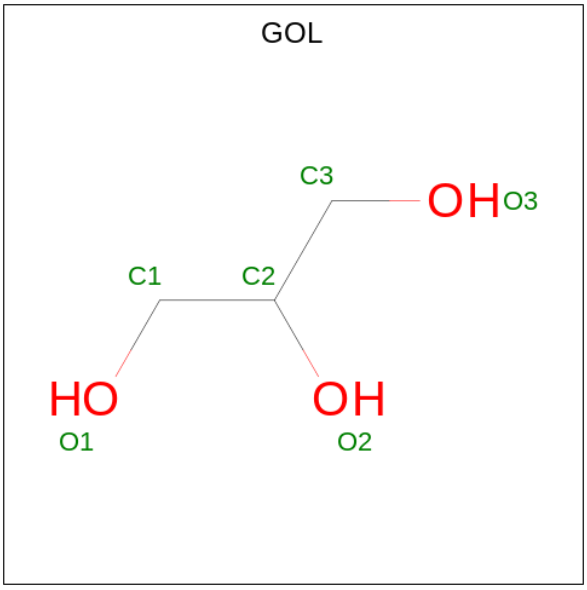


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

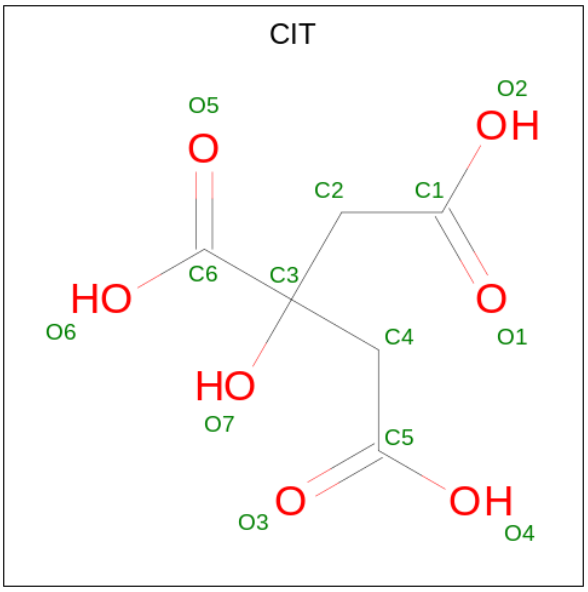
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



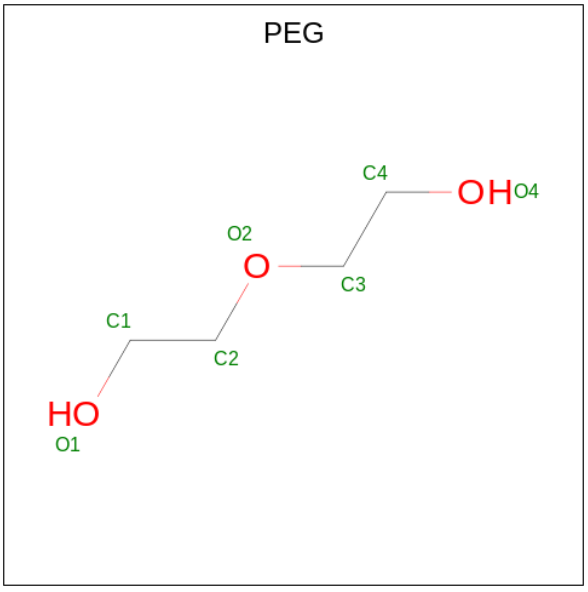
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is water.

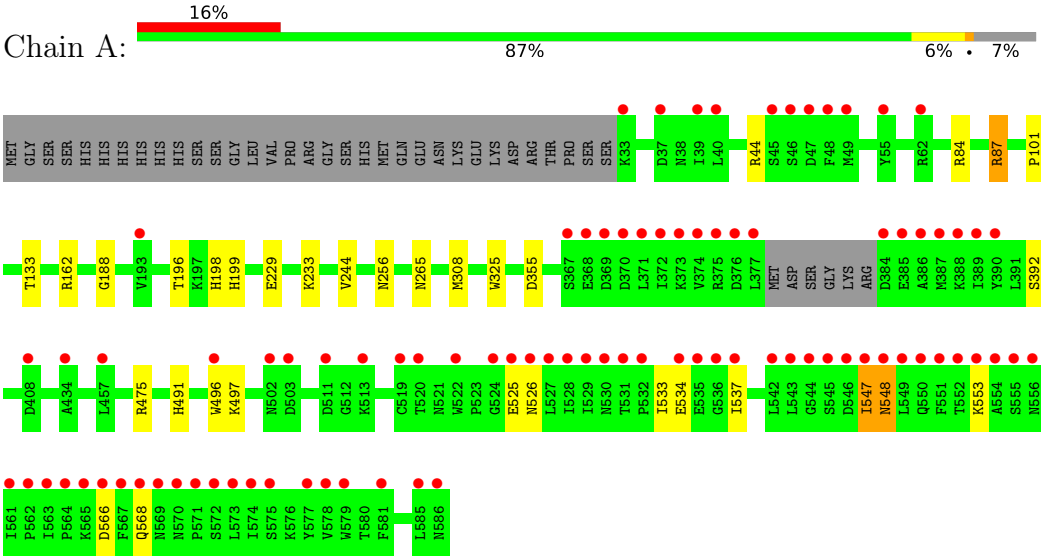
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	281	Total O 281 281	0	0
7	B	411	Total O 411 411	0	0

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.

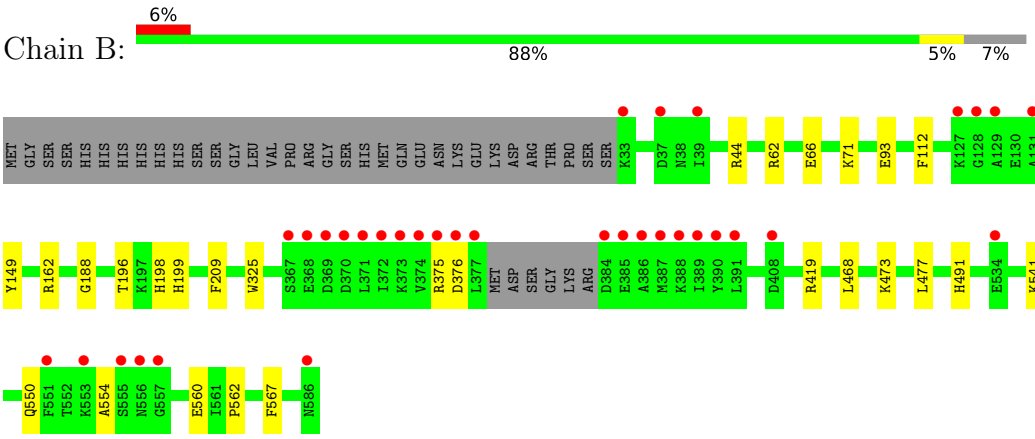
• Molecule 1: Alpha-L-fucosidase

Chain A:



• Molecule 1: Alpha-L-fucosidase

Chain B:



4 Data and refinement statistics (i)

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 46.55 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.60-1.71) 99.8 (46.55-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [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 (5.00%)	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)	0.39 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, PEG, NA, CIT, Z8T

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	0.38	0/4578	0.64	0/6204
1	B	0.42	0/4606	0.67	2/6242 (0.0%)
All	All	0.40	0/9184	0.66	2/12446 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	419	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	B	149	TYR	CB-CG-CD1	5.34	124.20	121.00

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

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Mol	Chain	Res	Type	Group
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 (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	4455	0	4288	20	0
1	B	4483	0	4309	18	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	1	0
7	B	411	0	0	3	0
All	All	9706	0	8652	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 2.

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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLU:O	1:A:233:LYS:HE3	1.93	0.68
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: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:B:66:GLU:CD	7:B:912:HOH:O	2.53	0.47
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:477[B]:LEU:C	1:B:477[B]:LEU:HD23	2.35	0.47
1:B:547:ILE:HD12	1:B:567:PHE:CZ	2.49	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: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
1:A:229:GLU:C	1:A:233:LYS:HE3	2.40	0.41

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%)	60	46
1	B	488/517 (94%)	485 (99%)	3 (1%)	86	80
All	All	972/1034 (94%)	961 (99%)	11 (1%)	73	63

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

Mol	Chain	Res	Type
1	A	112	PHE
1	A	196	THR
1	A	325	TRP
1	A	547	ILE
1	A	548	ASN
1	A	553	LYS
1	A	560	GLU
1	A	566	ASP
1	B	112	PHE
1	B	196	THR
1	B	325	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	A	430	GLN
1	A	491	HIS
1	A	518	HIS
1	A	526	ASN
1	A	548	ASN
1	B	186	ASN
1	B	255	GLN
1	B	259	GLN
1	B	275	GLN
1	B	491	HIS
1	B	518	HIS
1	B	530	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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
2	Z8T	A	601	-	12,12,12	0.68	0	17,17,17	1.21	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	A	604	-	5,5,5	0.09	0	5,5,5	0.25	0
4	GOL	B	604	-	5,5,5	0.19	0	5,5,5	0.41	0
4	GOL	A	603	-	5,5,5	0.09	0	5,5,5	0.21	0
2	Z8T	B	601	-	12,12,12	0.44	0	17,17,17	1.34	3 (17%)
6	PEG	B	606	-	6,6,6	0.15	0	5,5,5	0.07	0
5	CIT	A	605	-	12,12,12	1.34	1 (8%)	17,17,17	1.41	2 (11%)
4	GOL	B	605	-	5,5,5	0.25	0	5,5,5	0.81	0
4	GOL	B	603	-	5,5,5	0.23	0	5,5,5	0.59	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
2	Z8T	A	601	-	-	2/2/22/22	0/1/1/1
4	GOL	A	604	-	-	2/4/4/4	-
4	GOL	B	604	-	-	1/4/4/4	-
4	GOL	A	603	-	-	0/4/4/4	-
2	Z8T	B	601	-	-	2/2/22/22	0/1/1/1
6	PEG	B	606	-	-	3/4/4/4	-
5	CIT	A	605	-	-	1/16/16/16	-
4	GOL	B	605	-	-	1/4/4/4	-
4	GOL	B	603	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	CIT	C3-C6	3.03	1.56	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	605	CIT	O5-C6-C3	-3.68	117.04	122.25
5	A	605	CIT	O6-C6-C3	3.09	118.41	113.05
2	A	601	Z8T	O2-C2-C3	2.94	117.14	110.35
2	B	601	Z8T	O1-C1-C2	2.62	116.40	109.03
2	B	601	Z8T	O2-C2-C3	2.32	115.72	110.35
2	B	601	Z8T	O5-C5-C4	2.21	113.71	109.69

There are no chirality outliers.

All (16) 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
4	B	605	GOL	C1-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
2	B	601	Z8T	C4-C5-C6-O6
6	B	606	PEG	O2-C3-C4-O4
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
4	B	604	GOL	O1-C1-C2-O2

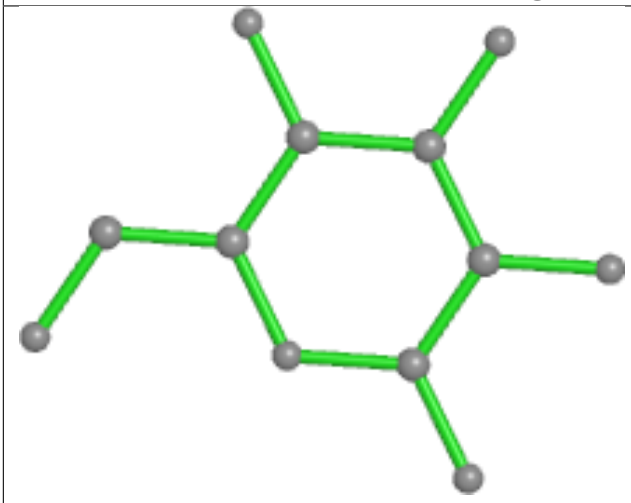
There are no ring outliers.

1 monomer is involved in 5 short contacts:

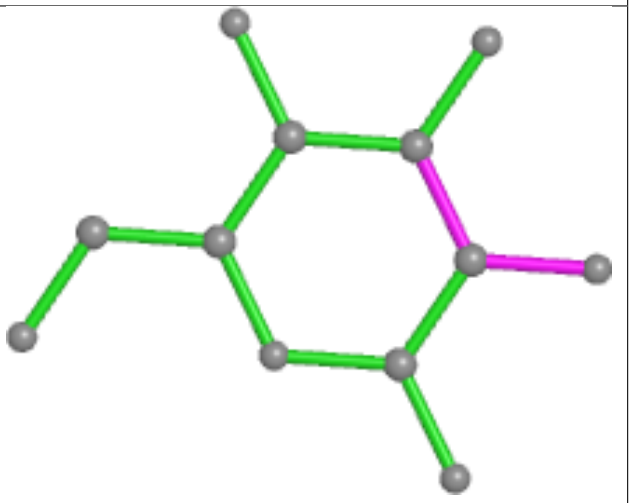
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	605	GOL	5	0

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 then 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.

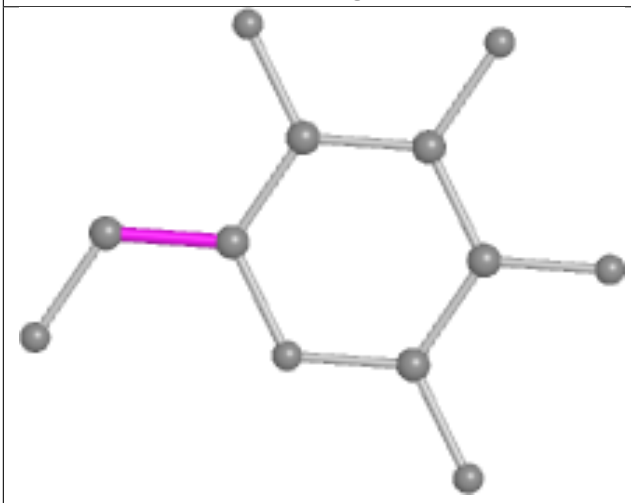
Ligand Z8T A 601



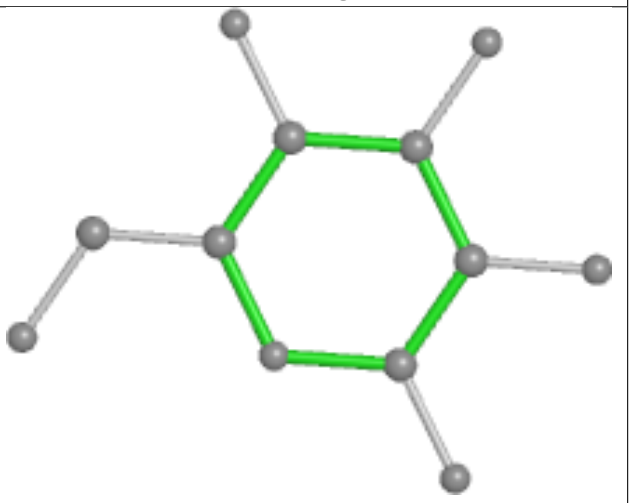
Bond lengths



Bond angles

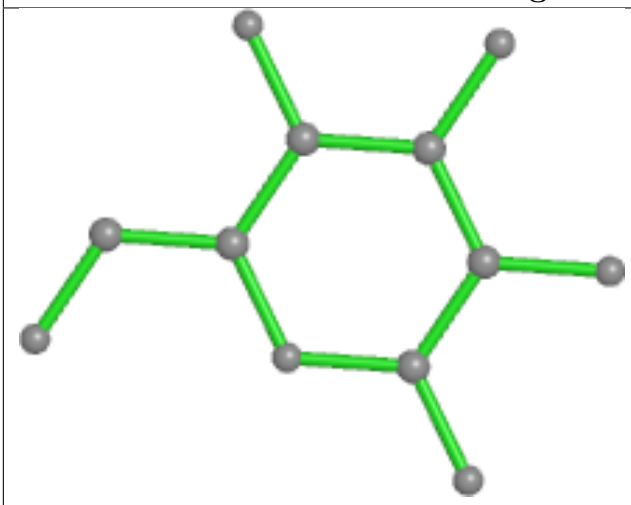


Torsions

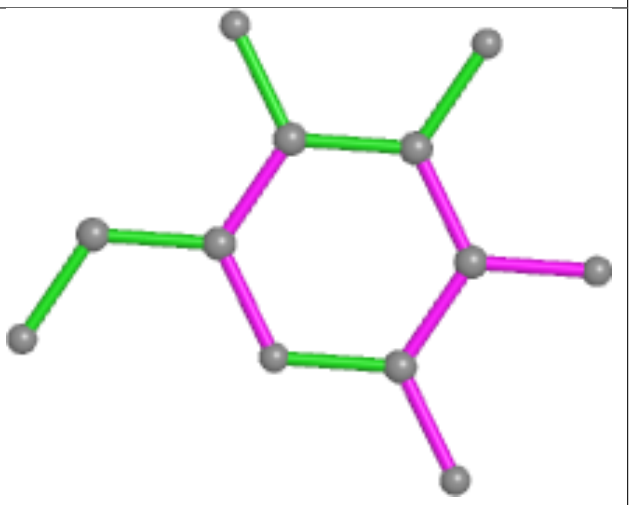


Rings

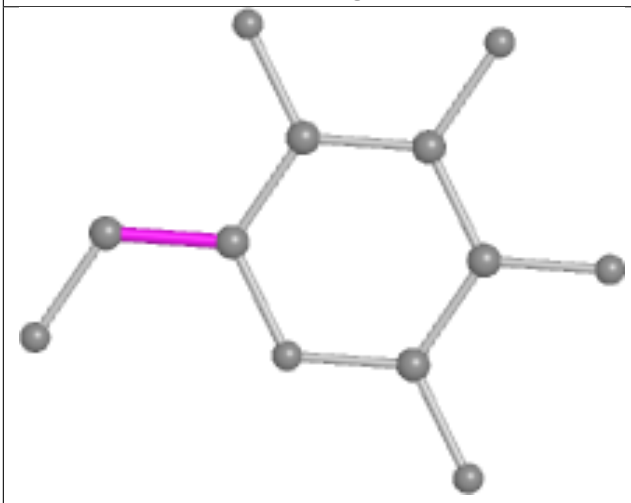
Ligand Z8T B 601



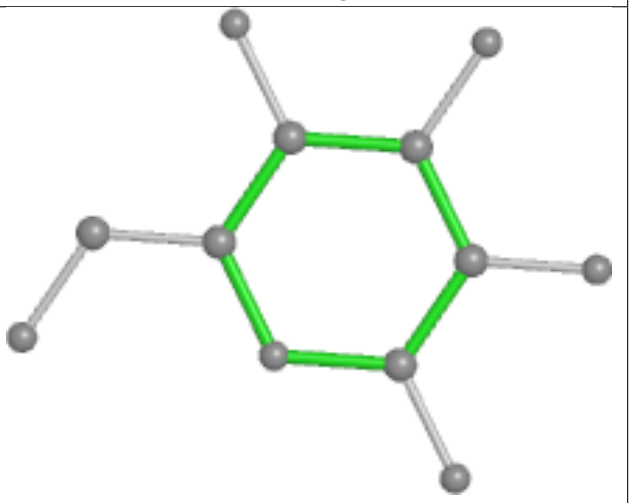
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.90	95 (17%) 1 1	14, 25, 65, 97	0
1	B	548/587 (93%)	0.28	35 (6%) 19 21	12, 17, 47, 77	0
All	All	1096/1174 (93%)	0.59	130 (11%) 4 5	12, 21, 60, 97	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	555	SER	8.9
1	A	549	LEU	8.7
1	A	522	TRP	8.7
1	A	386	ALA	8.4
1	A	554	ALA	8.4
1	A	567	PHE	8.3
1	A	546	ASP	6.7
1	A	384	ASP	6.5
1	B	384	ASP	6.4
1	A	573	LEU	6.3
1	A	569	ASN	6.2
1	A	561	ILE	5.8
1	B	375	ARG	5.8
1	B	372	ILE	5.8
1	B	374	VAL	5.8
1	A	559	LEU	5.8
1	A	389	ILE	5.7
1	B	586	ASN	5.6
1	B	377	LEU	5.6
1	A	547	ILE	5.6
1	A	376	ASP	5.6
1	A	372	ILE	5.5
1	A	385	GLU	5.4
1	A	47	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	557	GLY	5.4
1	A	553	LYS	5.3
1	A	534	GLU	5.2
1	A	528	ILE	5.2
1	A	375	ARG	5.1
1	A	564	PRO	5.1
1	A	572	SER	5.0
1	A	527	LEU	5.0
1	B	555	SER	4.8
1	A	374	VAL	4.8
1	B	557	GLY	4.7
1	A	552	THR	4.7
1	B	387	MET	4.7
1	A	563	ILE	4.6
1	A	368	GLU	4.6
1	A	525	GLU	4.6
1	A	39	ILE	4.5
1	B	389	ILE	4.5
1	A	387	MET	4.4
1	A	371	LEU	4.3
1	A	524	GLY	4.3
1	A	369	ASP	4.2
1	A	558	ASN	4.1
1	B	128	GLY	4.1
1	A	556	ASN	4.1
1	A	377	LEU	4.0
1	A	37	ASP	4.0
1	B	386	ALA	3.9
1	A	579	TRP	3.9
1	A	566	ASP	3.9
1	B	388	LYS	3.9
1	B	376	ASP	3.9
1	B	385	GLU	3.9
1	A	388	LYS	3.8
1	B	37	ASP	3.7
1	B	391	LEU	3.6
1	A	574	ILE	3.4
1	A	536	GLY	3.4
1	B	408	ASP	3.4
1	B	129	ALA	3.3
1	A	535	GLU	3.3
1	A	49	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	33	LYS	3.3
1	B	534	GLU	3.3
1	B	369	ASP	3.2
1	A	40	LEU	3.2
1	B	131	ALA	3.2
1	B	370	ASP	3.1
1	A	565	LYS	3.1
1	B	553	LYS	3.1
1	A	530	ASN	3.1
1	A	578	VAL	3.0
1	A	537	ILE	3.0
1	A	390	TYR	2.9
1	A	128	GLY	2.9
1	A	520	THR	2.9
1	A	502	ASN	2.9
1	B	390	TYR	2.9
1	A	586	ASN	2.9
1	A	526	ASN	2.9
1	B	551	PHE	2.8
1	B	373	LYS	2.8
1	A	560	GLU	2.8
1	A	542	LEU	2.8
1	A	373	LYS	2.8
1	A	496	TRP	2.8
1	B	127	LYS	2.8
1	A	581	PHE	2.7
1	A	568	GLN	2.7
1	B	367	SER	2.7
1	B	132	SER	2.7
1	A	577	TYR	2.7
1	A	46	SER	2.7
1	B	368	GLU	2.6
1	A	544	GLY	2.6
1	A	511	ASP	2.6
1	A	575	SER	2.6
1	A	370	ASP	2.5
1	A	519	CYS	2.5
1	A	408	ASP	2.5
1	A	529	ILE	2.5
1	A	543	LEU	2.5
1	A	367	SER	2.4
1	A	548	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	434	ALA	2.4
1	A	513	LYS	2.4
1	A	503	ASP	2.4
1	B	556	ASN	2.3
1	A	550	GLN	2.3
1	A	33	LYS	2.3
1	A	585	LEU	2.3
1	A	457	LEU	2.2
1	A	551	PHE	2.2
1	A	570	ASN	2.2
1	A	193	VAL	2.1
1	A	571	PRO	2.1
1	A	55	TYR	2.1
1	A	48	PHE	2.1
1	A	562	PRO	2.1
1	A	45	SER	2.1
1	B	371	LEU	2.1
1	B	39	ILE	2.1
1	A	62	ARG	2.1
1	A	532	PRO	2.1
1	A	545	SER	2.0
1	A	531	THR	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	605	6/6	0.70	0.26	37,46,47,50	0

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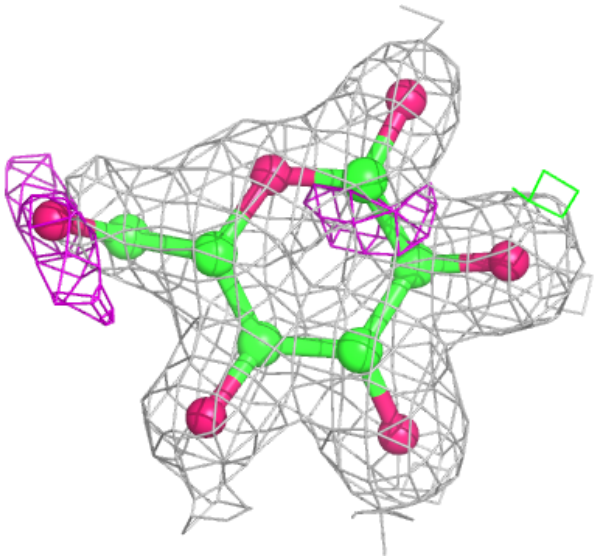
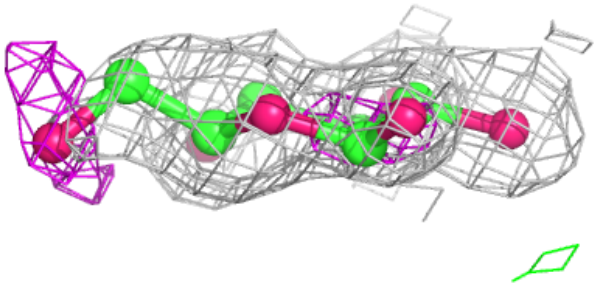
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CIT	A	605	13/13	0.82	0.28	34,42,51,53	0
4	GOL	A	604	6/6	0.85	0.18	44,52,55,63	0
4	GOL	B	604	6/6	0.85	0.17	27,37,41,46	0
6	PEG	B	606	7/7	0.85	0.19	47,48,50,53	0
4	GOL	B	603	6/6	0.88	0.15	28,29,34,34	0
2	Z8T	A	601	12/12	0.89	0.15	24,30,39,44	0
2	Z8T	B	601	12/12	0.92	0.12	18,24,31,41	0
4	GOL	A	603	6/6	0.94	0.08	26,28,29,30	0
3	NA	A	602	1/1	0.97	0.13	34,34,34,34	0
3	NA	B	602	1/1	0.98	0.08	23,23,23,23	0

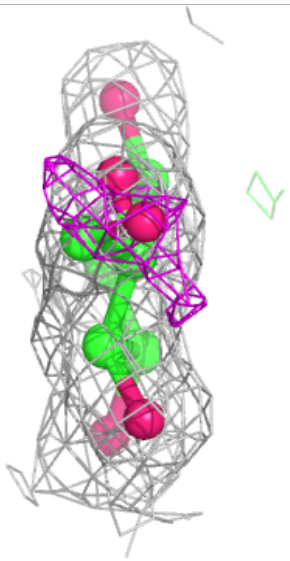
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

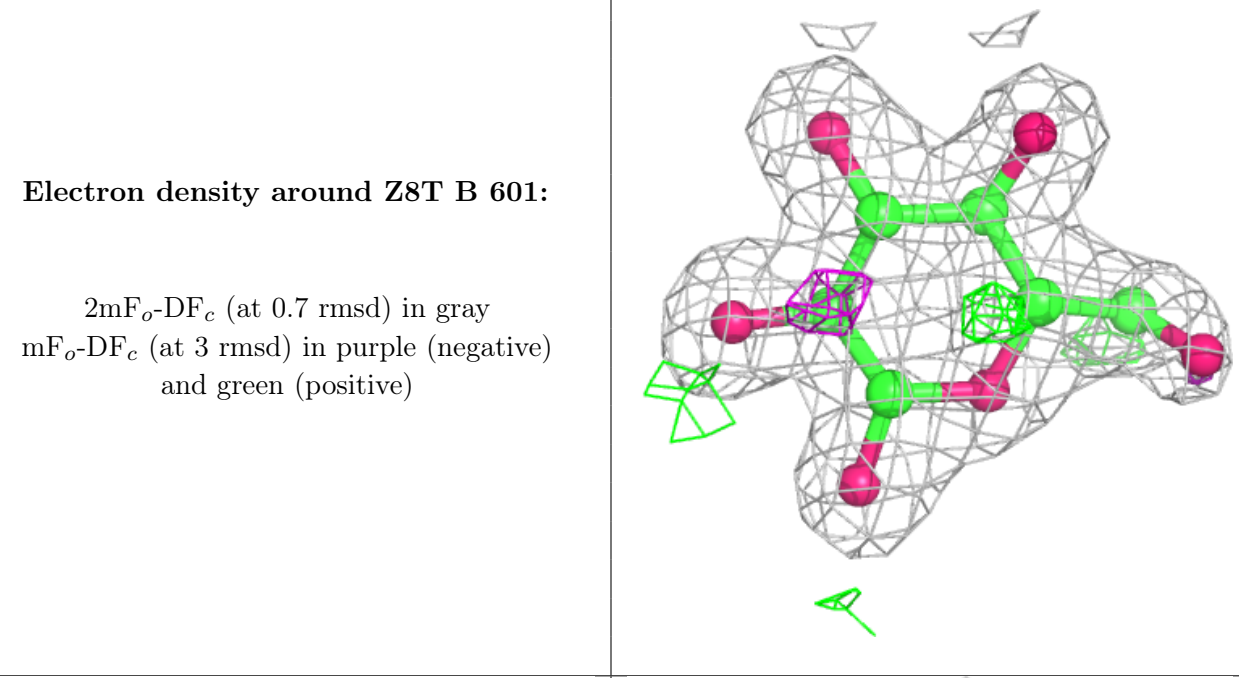


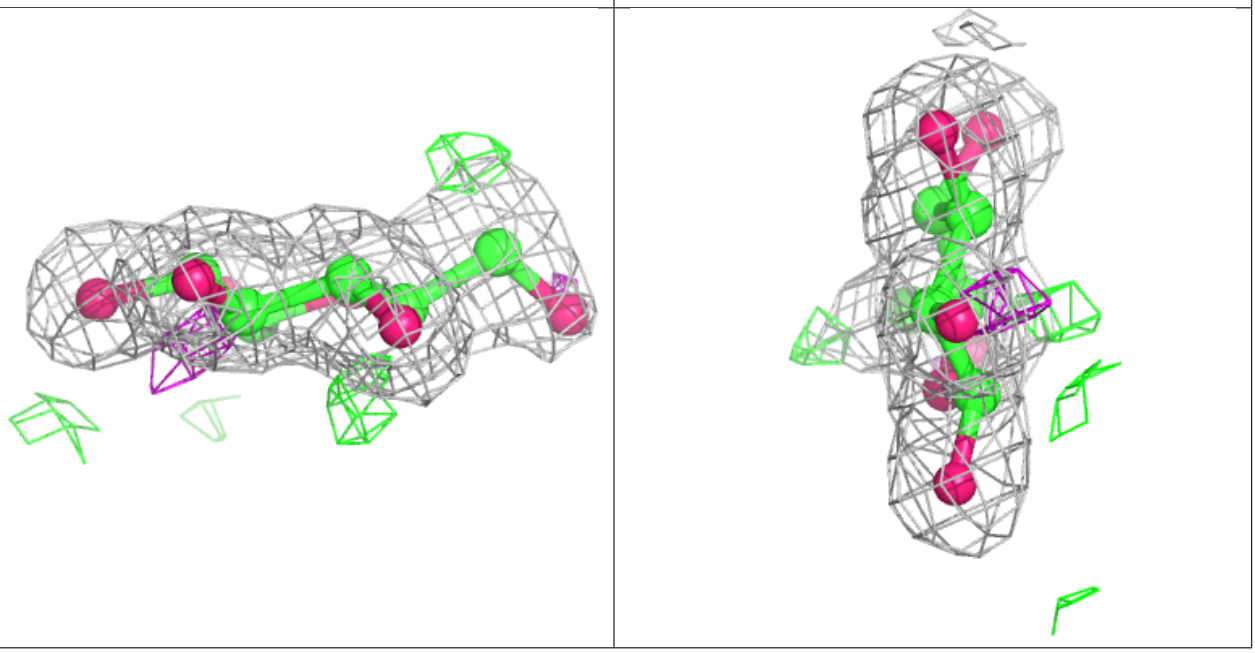




Electron density around Z8T B 601:

$2mF_o$-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.