



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:06 AM UTC

PDB ID : 9LTB / pdb_00009ltb
Title : Crystal structure of Altererythrobacter sp. S1-5 Tryptophan halogenase putative
Authors : Arold, S.T.; Hameed, U.F.S.
Deposited on : 2025-02-05
Resolution : 1.49 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

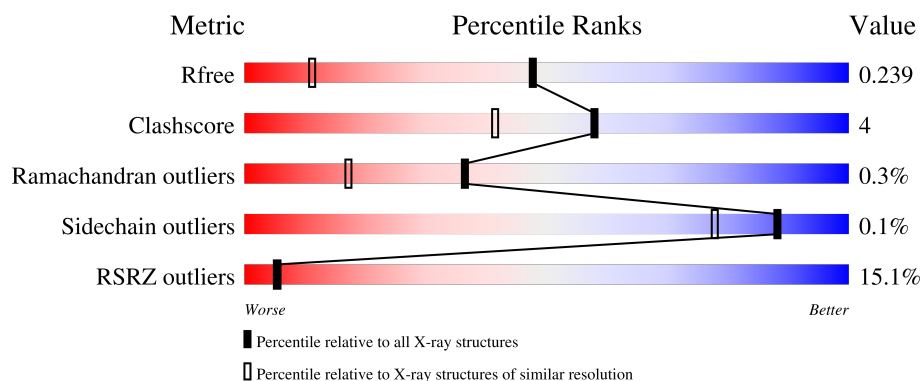
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	515	14% 85% 6% • 8%
1	B	515	14% 84% 9% 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
3	CL	B	602	-	-	X	-

2 Entry composition [i](#)

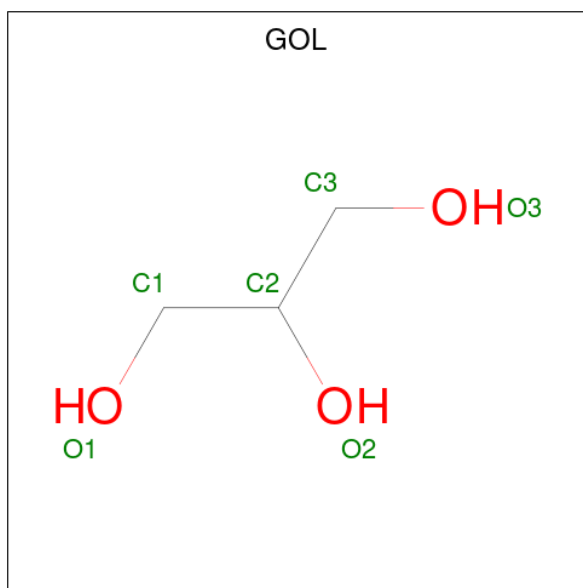
There are 5 unique types of molecules in this entry. The entry contains 7948 atoms, of which 37 are hydrogens and 0 are deuteriums.

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 Tryptophan halogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	476	Total	C	H	N	O	S	0	0	0
			3684	2337	5	650	681	11			
1	B	479	Total	C	H	N	O	S	0	2	0
			3738	2376	5	657	689	11			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



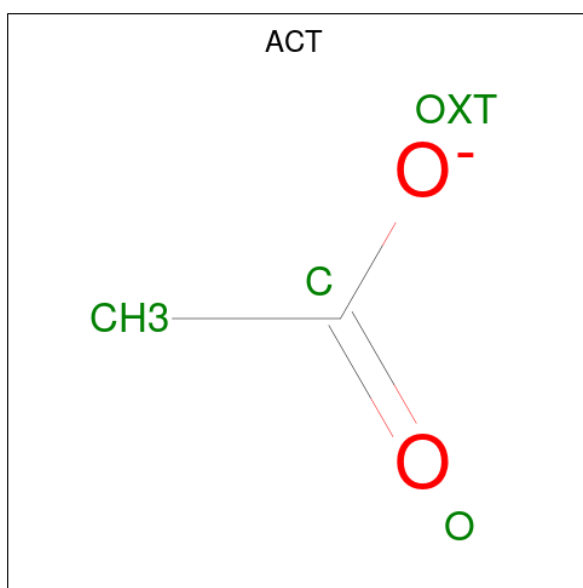
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest")

by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	2	Total	Cl	0	0
			2	2		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			7	2	3	2		

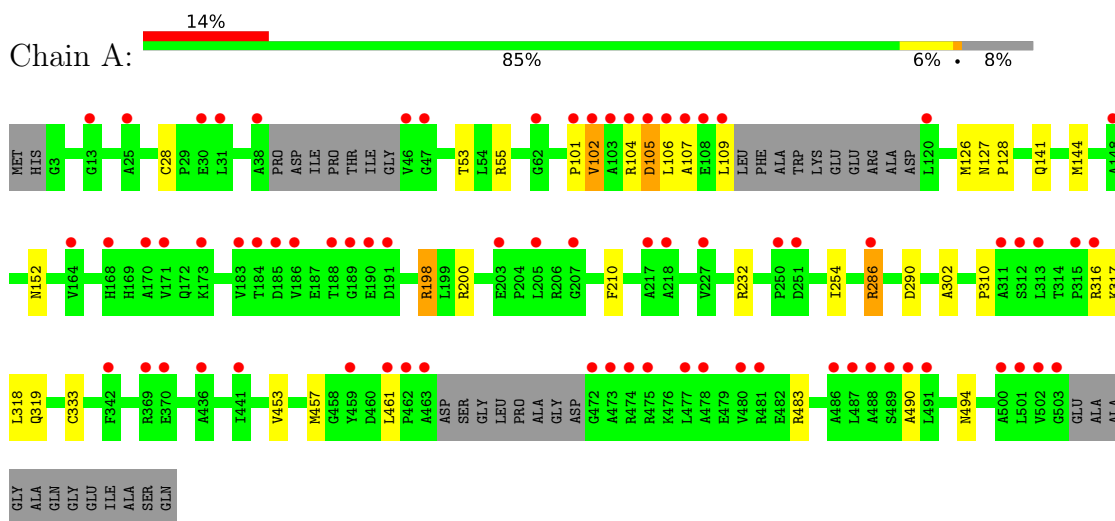
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	234	Total	O	0	0
			234	234		
5	B	240	Total	O	0	0
			240	240		

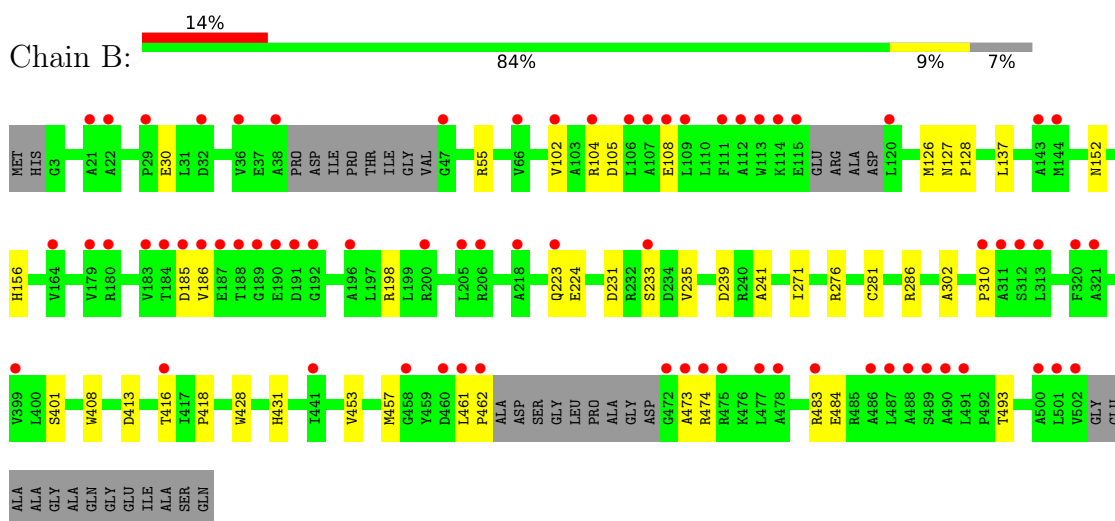
3 Residue-property plots [i](#)

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: Tryptophan halogenase



• Molecule 1: Tryptophan halogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.02Å 65.50Å 81.93Å 104.46° 107.61° 92.79°	Depositor
Resolution (Å)	47.24 – 1.49 47.24 – 1.49	Depositor EDS
% Data completeness (in resolution range)	94.5 (47.24-1.49) 94.5 (47.24-1.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.49Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.209 , 0.234 0.214 , 0.239	Depositor DCC
R_{free} test set	1989 reflections (1.28%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7948	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 6.31% 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: CL, GOL, ACT

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	0.32	0/3770	0.55	0/5134
1	B	0.30	0/3827	0.54	0/5212
All	All	0.31	0/7597	0.54	0/10346

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	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	ARG	Sidechain
1	A	200	ARG	Sidechain
1	A	286	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	3679	5	3583	35	0
1	B	3733	5	3634	30	0
2	A	12	16	16	1	0
2	B	6	8	7	0	0
3	A	1	0	0	0	0
3	B	2	0	0	3	0
4	B	4	3	3	0	0
5	A	234	0	0	3	0
5	B	240	0	0	2	0
All	All	7911	37	7243	66	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 4.

All (66) 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:141:GLN:OE1	1:A:144:MET:HE3	1.75	0.87
1:A:317:LYS:HE2	1:A:319:GLN:HE21	1.42	0.83
1:A:28:CYS:SG	5:A:918:HOH:O	2.41	0.78
1:A:104:ARG:NH1	1:A:106:LEU:HB2	2.00	0.77
3:B:601:CL:CL	5:B:925:HOH:O	2.39	0.76
1:A:109:LEU:HD21	1:A:461:LEU:HD11	1.76	0.67
1:B:55:ARG:NH2	1:B:152:ASN:OD1	2.27	0.66
1:A:104:ARG:NH2	1:A:109:LEU:HD21	2.11	0.64
1:B:231:ASP:OD1	1:B:233:SER:HB2	1.99	0.63
1:B:185:ASP:HB3	1:B:198:ARG:HB2	1.81	0.62
1:A:104:ARG:HH22	1:A:109:LEU:HD11	1.67	0.58
1:A:127:ASN:HB2	1:A:128:PRO:CD	2.34	0.57
1:B:474:ARG:HE	1:B:474:ARG:H	1.52	0.57
1:B:102:VAL:CG1	1:B:104:ARG:HG2	2.35	0.56
1:B:286:ARG:HH11	1:B:286:ARG:HG3	1.71	0.55
1:A:232:ARG:NH1	5:A:702:HOH:O	2.36	0.55
1:A:109:LEU:CD2	1:A:461:LEU:HD11	2.36	0.55
1:A:55:ARG:NH2	1:A:152:ASN:OD1	2.41	0.54
1:A:127:ASN:HB2	1:A:128:PRO:HD3	1.90	0.53
1:B:156:HIS:CD2	1:B:271:ILE:HG23	2.42	0.53
1:B:108:GLU:HB3	1:B:473:ALA:HA	1.90	0.53
1:A:101:PRO:O	1:A:102:VAL:HB	2.09	0.51
1:A:316:ARG:HG2	1:A:318:LEU:HD21	1.92	0.51
1:A:104:ARG:O	1:A:105:ASP:C	2.53	0.51
1:B:453:VAL:O	1:B:457:MET:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ARG:HG3	1:B:286:ARG:NH1	2.26	0.50
1:B:128:PRO:HB3	1:B:484:GLU:HG3	1.93	0.49
1:A:104:ARG:HH12	1:A:106:LEU:CB	2.24	0.49
1:A:302:ALA:HB2	1:A:310:PRO:HG3	1.96	0.48
1:A:254:ILE:HB	1:A:494:ASN:HB2	1.95	0.48
1:A:286:ARG:HG3	5:A:736:HOH:O	2.13	0.48
1:A:101:PRO:HB3	1:A:126:MET:HB3	1.96	0.48
1:B:401:SER:HB3	3:B:602:CL:CL	2.51	0.48
1:A:106:LEU:HD22	1:A:126:MET:HE1	1.96	0.47
1:A:141:GLN:NE2	1:A:490:ALA:O	2.41	0.47
1:A:101:PRO:HB3	1:A:126:MET:SD	2.54	0.47
1:A:316:ARG:HG2	1:A:318:LEU:CD2	2.45	0.47
1:A:210:PHE:O	1:A:333:CYS:HA	2.16	0.46
1:B:408:TRP:O	3:B:602:CL:CL	2.70	0.46
1:B:483:ARG:HD3	1:B:483:ARG:HA	1.72	0.46
1:B:186:VAL:HB	1:B:224:GLU:HG2	1.98	0.46
1:B:413:ASP:O	1:B:416[A]:THR:HG22	2.16	0.46
1:B:104:ARG:HG3	1:B:105:ASP:OD1	2.16	0.45
1:B:128:PRO:HB3	1:B:484:GLU:CG	2.47	0.45
1:A:104:ARG:HH22	1:A:109:LEU:HD21	1.80	0.44
1:B:302:ALA:HB2	1:B:310:PRO:HG3	2.00	0.43
1:B:241:ALA:HA	1:B:281:CYS:O	2.19	0.43
1:A:104:ARG:NH1	1:A:106:LEU:CB	2.76	0.43
1:B:126:MET:O	1:B:127:ASN:HB3	2.19	0.42
1:A:453:VAL:O	1:A:457:MET:HG3	2.19	0.42
1:B:30:GLU:H	1:B:30:GLU:CD	2.27	0.42
1:A:104:ARG:HH22	1:A:109:LEU:CG	2.33	0.42
1:A:53:THR:HB	2:A:603:GOL:H2	2.00	0.42
1:B:239:ASP:CG	1:B:286:ARG:HH12	2.27	0.42
1:A:105:ASP:O	1:A:105:ASP:OD1	2.38	0.42
1:B:223:GLN:HE21	1:B:223:GLN:HB3	1.66	0.41
1:A:104:ARG:HH22	1:A:109:LEU:CD1	2.32	0.41
1:B:428:TRP:HA	1:B:431:HIS:O	2.20	0.41
1:A:290:ASP:OD2	1:A:317:LYS:NZ	2.49	0.41
1:B:137:LEU:HA	1:B:493:THR:HA	2.02	0.41
1:A:109:LEU:CD2	1:A:461:LEU:CD1	2.98	0.41
1:B:461:LEU:HD12	1:B:462:PRO:CD	2.51	0.41
1:B:235:VAL:HG21	1:B:418:PRO:HG3	2.02	0.41
1:B:102:VAL:HG12	1:B:104:ARG:HG2	2.03	0.41
1:B:276:ARG:NH1	5:B:711:HOH:O	2.52	0.41
1:A:483:ARG:HA	1:A:483:ARG:HD2	1.44	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	468/515 (91%)	450 (96%)	15 (3%)	3 (1%)	21	6
1	B	473/515 (92%)	463 (98%)	10 (2%)	0	100	100
All	All	941/1030 (91%)	913 (97%)	25 (3%)	3 (0%)	36	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ALA
1	A	105	ASP
1	A	102	VAL

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	371/398 (93%)	370 (100%)	1 (0%)	86	75
1	B	377/398 (95%)	377 (100%)	0	100	100
All	All	748/796 (94%)	747 (100%)	1 (0%)	88	78

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	223	GLN
1	A	319	GLN
1	A	440	GLN
1	A	442	ASN
1	B	168	HIS
1	B	223	GLN
1	B	440	GLN
1	B	442	ASN

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](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	GOL	A	601	-	5,5,5	0.82	0	5,5,5	1.10	1 (20%)
2	GOL	A	603	-	5,5,5	0.92	0	5,5,5	1.20	0
2	GOL	B	603	-	5,5,5	1.22	0	5,5,5	1.34	2 (40%)
4	ACT	B	604	-	3,3,3	1.14	0	3,3,3	1.44	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	GOL	A	601	-	-	2/4/4/4	-
2	GOL	A	603	-	-	3/4/4/4	-
2	GOL	B	603	-	-	2/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	GOL	C3-C2-C1	-2.14	103.95	111.80
2	B	603	GOL	O2-C2-C1	2.10	117.88	109.18
2	B	603	GOL	C3-C2-C1	-2.00	104.45	111.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

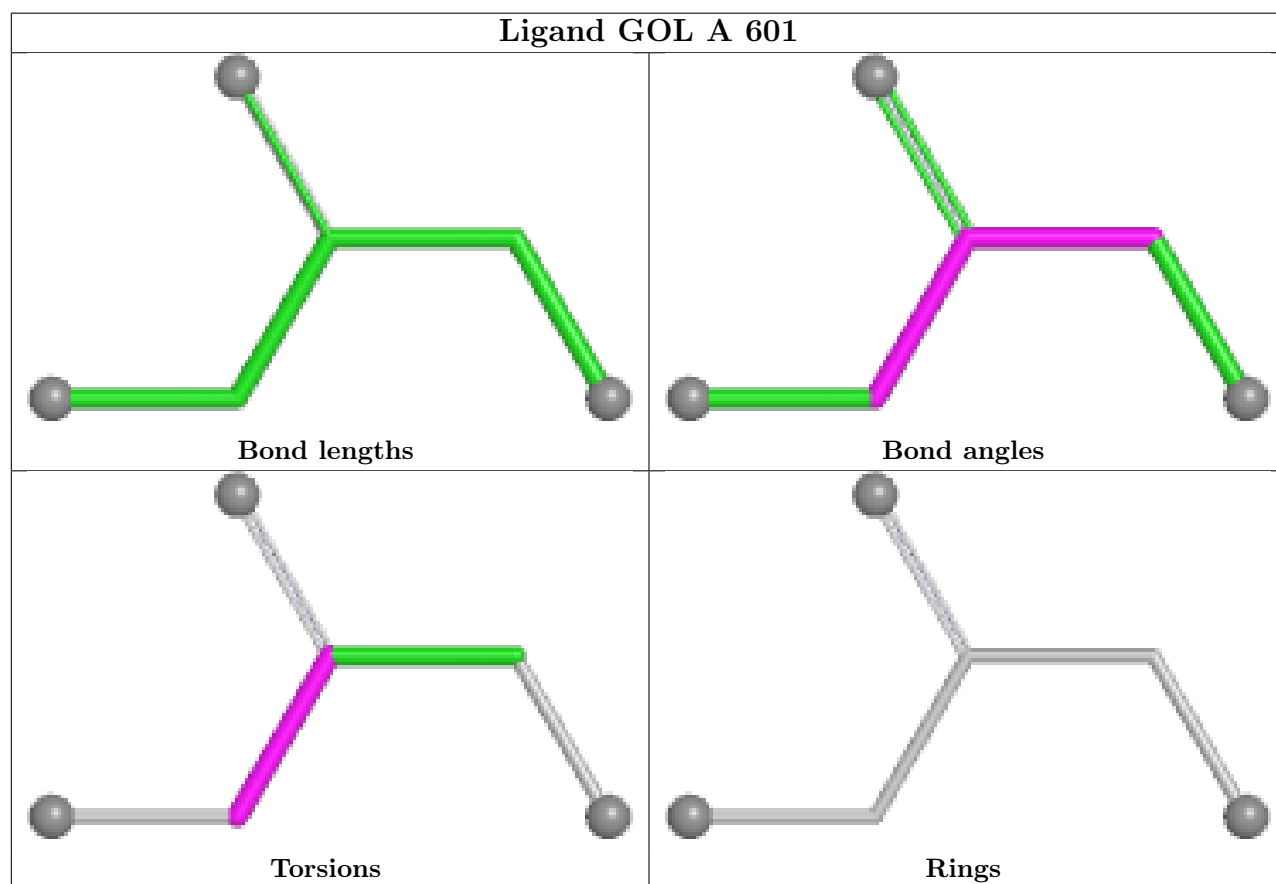
Mol	Chain	Res	Type	Atoms
2	B	603	GOL	O1-C1-C2-C3
2	A	601	GOL	C1-C2-C3-O3
2	A	603	GOL	O1-C1-C2-C3
2	B	603	GOL	O1-C1-C2-O2
2	A	601	GOL	O2-C2-C3-O3
2	A	603	GOL	O1-C1-C2-O2
2	A	603	GOL	O2-C2-C3-O3

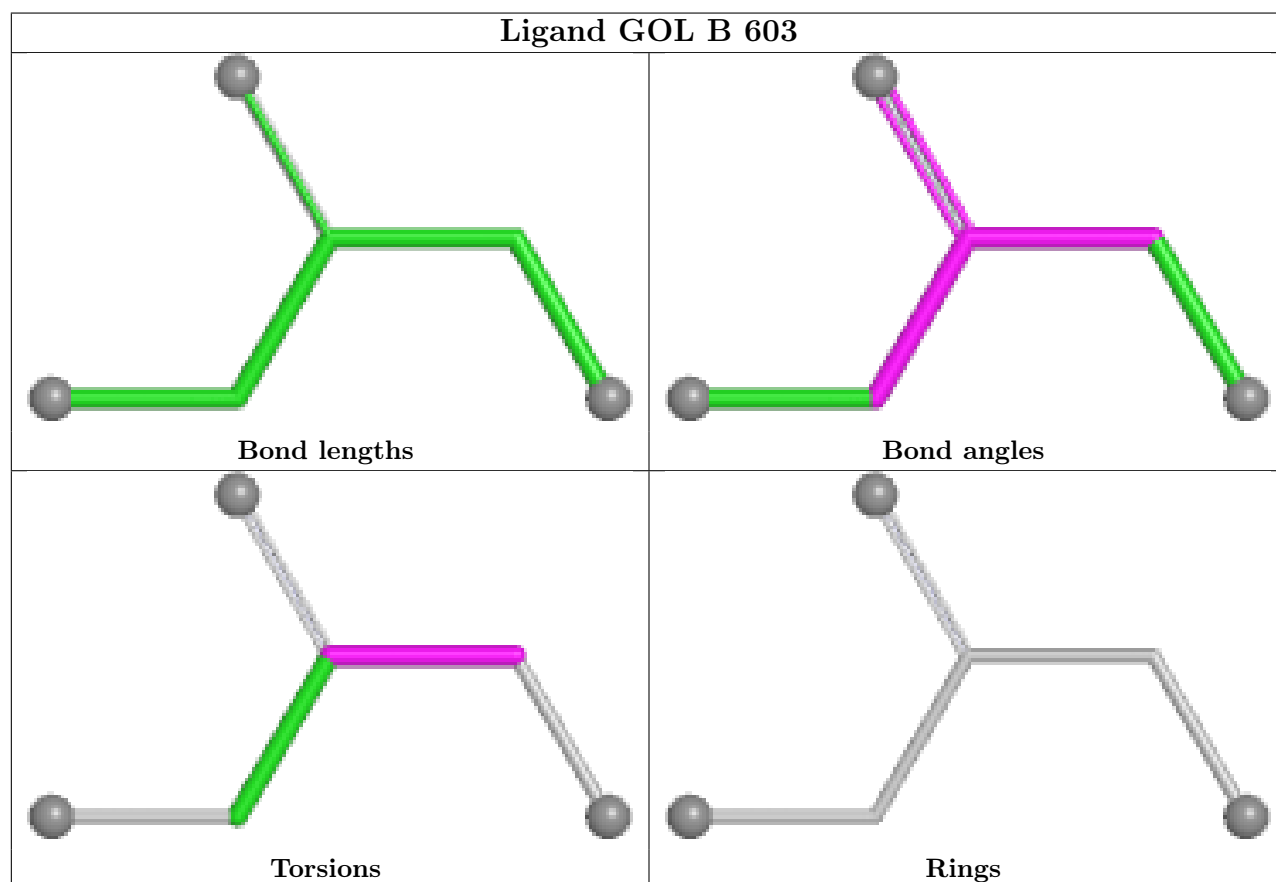
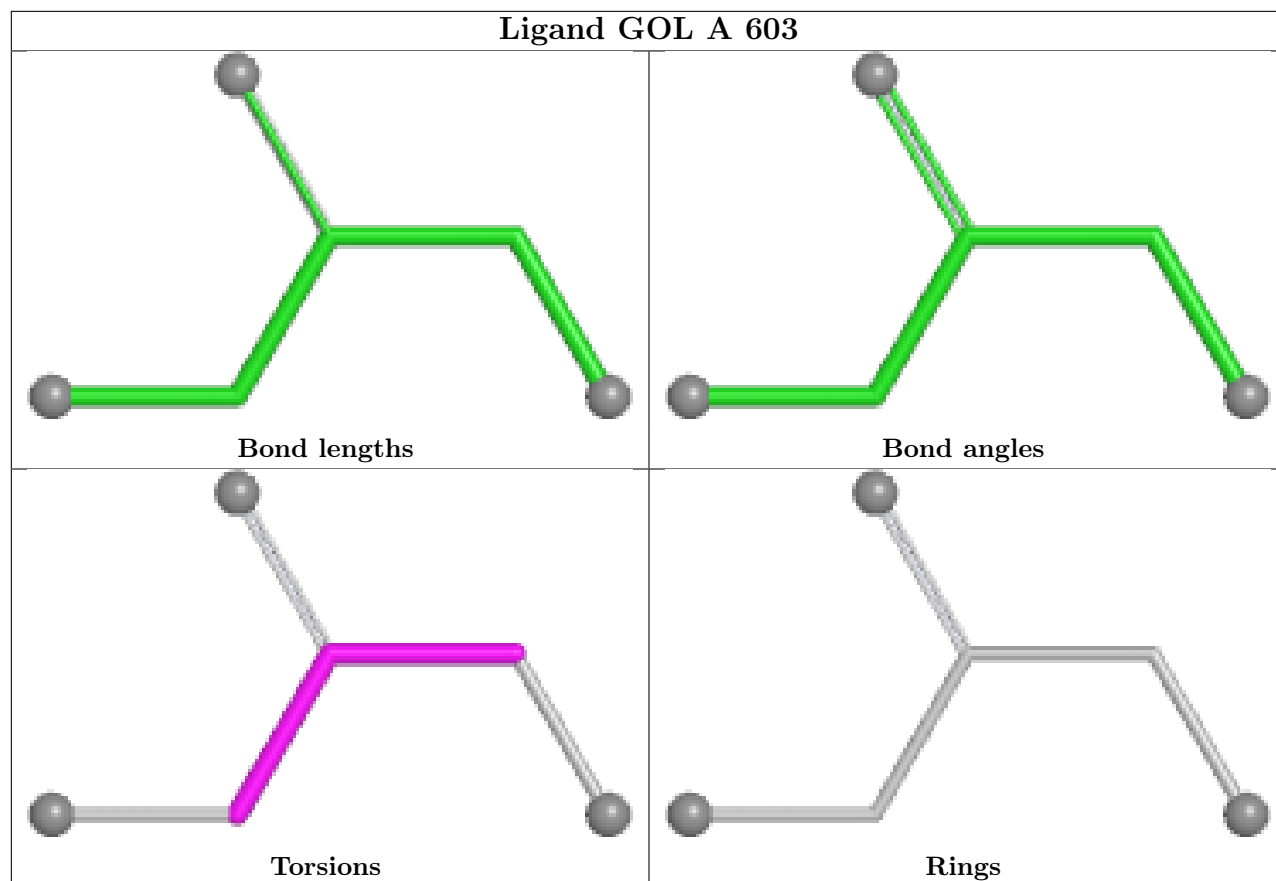
There are no ring outliers.

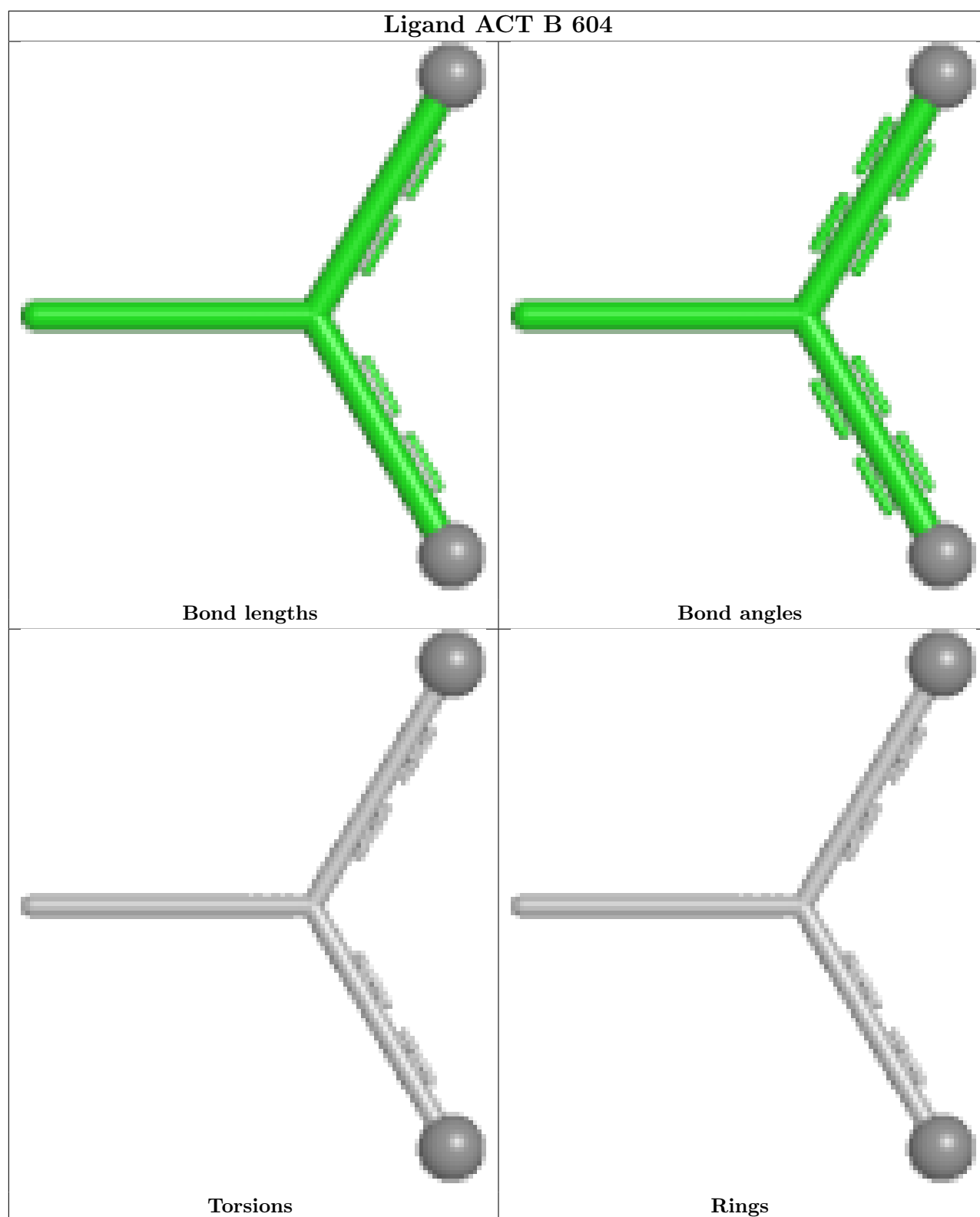
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	GOL	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 ⓘ

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	476/515 (92%)	1.20	73 (15%) 5 5	16, 24, 44, 104	0
1	B	479/515 (93%)	1.05	71 (14%) 5 6	10, 24, 43, 81	2 (0%)
All	All	955/1030 (92%)	1.12	144 (15%) 5 5	10, 24, 43, 104	2 (0%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	LEU	11.0
1	A	106	LEU	10.8
1	A	107	ALA	8.9
1	A	102	VAL	7.7
1	A	103	ALA	7.4
1	A	463	ALA	7.0
1	A	489	SER	6.8
1	B	502	VAL	6.2
1	A	108	GLU	5.9
1	B	490	ALA	5.7
1	A	46	VAL	5.6
1	B	489	SER	5.3
1	A	38	ALA	5.2
1	A	101	PRO	5.2
1	B	488	ALA	5.0
1	B	472	GLY	4.9
1	A	105	ASP	4.8
1	A	488	ALA	4.7
1	B	311	ALA	4.7
1	A	312	SER	4.6
1	B	38	ALA	4.6
1	A	104	ARG	4.5
1	A	189	GLY	4.2
1	B	47	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	502	VAL	3.9
1	B	441	ILE	3.9
1	A	13	GLY	3.9
1	A	473	ALA	3.9
1	A	472	GLY	3.9
1	B	111	PHE	3.8
1	B	416[A]	THR	3.8
1	B	486	ALA	3.8
1	B	461	LEU	3.7
1	A	478	ALA	3.7
1	B	501	LEU	3.6
1	A	186	VAL	3.6
1	A	190	GLU	3.6
1	A	191	ASP	3.6
1	B	313	LEU	3.5
1	B	114	LYS	3.5
1	B	190	GLU	3.4
1	A	120	LEU	3.3
1	A	503	GLY	3.3
1	B	460	ASP	3.2
1	A	188	THR	3.2
1	A	31	LEU	3.1
1	B	186	VAL	3.0
1	A	490	ALA	3.0
1	B	473	ALA	3.0
1	B	113	TRP	3.0
1	A	170	ALA	2.9
1	A	171	VAL	2.9
1	B	185	ASP	2.9
1	A	441	ILE	2.9
1	A	474	ARG	2.8
1	A	461	LEU	2.8
1	B	109	LEU	2.8
1	B	115	GLU	2.8
1	A	459	TYR	2.8
1	B	106	LEU	2.8
1	B	477	LEU	2.8
1	B	399[A]	VAL	2.7
1	B	478	ALA	2.7
1	A	185	ASP	2.7
1	A	436	ALA	2.7
1	B	183	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	102	VAL	2.6
1	B	112	ALA	2.6
1	A	184	THR	2.6
1	A	477	LEU	2.6
1	A	218	ALA	2.6
1	A	369	ARG	2.6
1	B	462	PRO	2.6
1	B	144	MET	2.6
1	B	474	ARG	2.6
1	B	475	ARG	2.6
1	A	203	GLU	2.5
1	A	164	VAL	2.5
1	A	250	PRO	2.5
1	A	462	PRO	2.5
1	B	184	THR	2.5
1	B	188	THR	2.5
1	B	107	ALA	2.5
1	B	189	GLY	2.5
1	A	217	ALA	2.4
1	B	192	GLY	2.4
1	A	491	LEU	2.4
1	B	108	GLU	2.4
1	A	286	ARG	2.4
1	A	475	ARG	2.4
1	B	483	ARG	2.4
1	B	321	ALA	2.4
1	A	183	VAL	2.4
1	B	180	ARG	2.4
1	B	487	LEU	2.4
1	A	30	GLU	2.4
1	A	370	GLU	2.3
1	B	120	LEU	2.3
1	B	200	ARG	2.3
1	A	315	PRO	2.3
1	B	310	PRO	2.3
1	A	251	ASP	2.3
1	B	21	ALA	2.3
1	B	187	GLU	2.3
1	A	342	PHE	2.3
1	B	164	VAL	2.3
1	B	191	ASP	2.2
1	A	316	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	206	ARG	2.2
1	B	320	PHE	2.2
1	A	207	GLY	2.2
1	A	501	LEU	2.2
1	B	491	LEU	2.2
1	A	148	ALA	2.2
1	B	104	ARG	2.2
1	A	62	GLY	2.2
1	B	312	SER	2.2
1	B	36	VAL	2.2
1	A	25	ALA	2.2
1	B	143	ALA	2.2
1	B	500	ALA	2.2
1	A	227	VAL	2.2
1	A	168	HIS	2.2
1	A	311	ALA	2.1
1	A	480	VAL	2.1
1	B	458	GLY	2.1
1	B	205	LEU	2.1
1	A	481	ARG	2.1
1	B	179	VAL	2.1
1	A	486	ALA	2.1
1	B	22	ALA	2.1
1	A	205	LEU	2.1
1	A	47	GLY	2.1
1	B	32	ASP	2.0
1	A	173	LYS	2.0
1	B	29	PRO	2.0
1	B	223	GLN	2.0
1	A	500	ALA	2.0
1	B	196	ALA	2.0
1	B	218	ALA	2.0
1	B	66	VAL	2.0
1	A	313	LEU	2.0
1	A	487	LEU	2.0
1	B	233	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

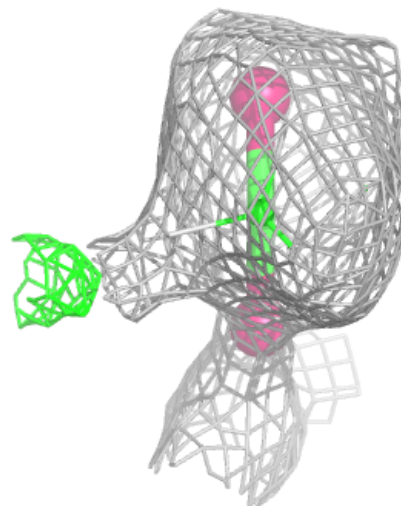
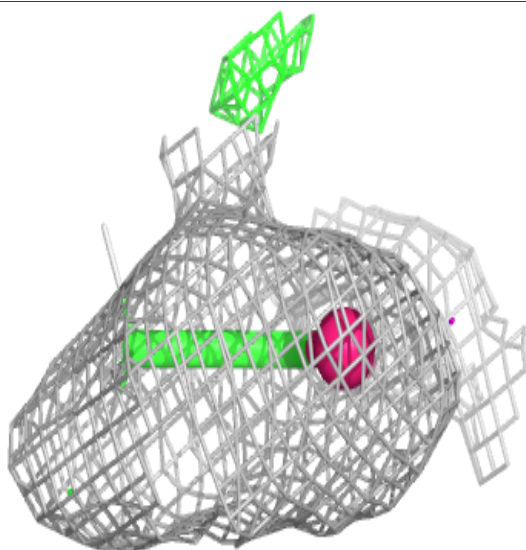
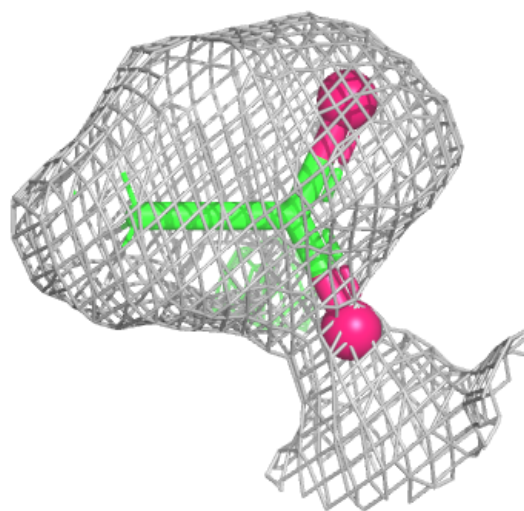
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACT	B	604	4/4	0.78	0.20	46,57,64,74	0
3	CL	A	602	1/1	0.84	0.20	45,45,45,45	0
2	GOL	A	603	6/6	0.88	0.11	28,34,35,42	0
2	GOL	B	603	6/6	0.89	0.14	24,29,60,60	0
2	GOL	A	601	6/6	0.96	0.07	22,26,37,37	0
3	CL	B	602	1/1	0.97	0.37	31,31,31,31	0
3	CL	B	601	1/1	0.97	0.11	38,38,38,38	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.

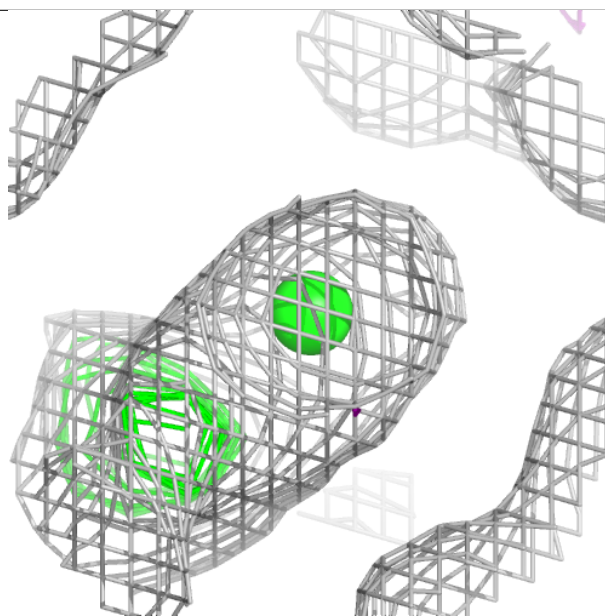
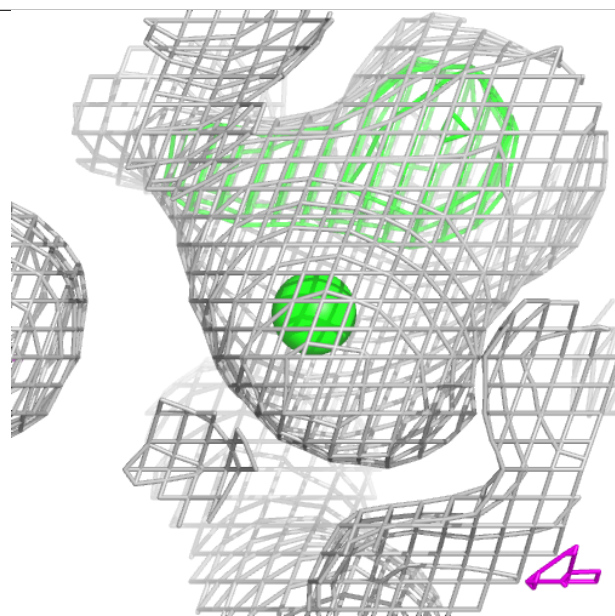
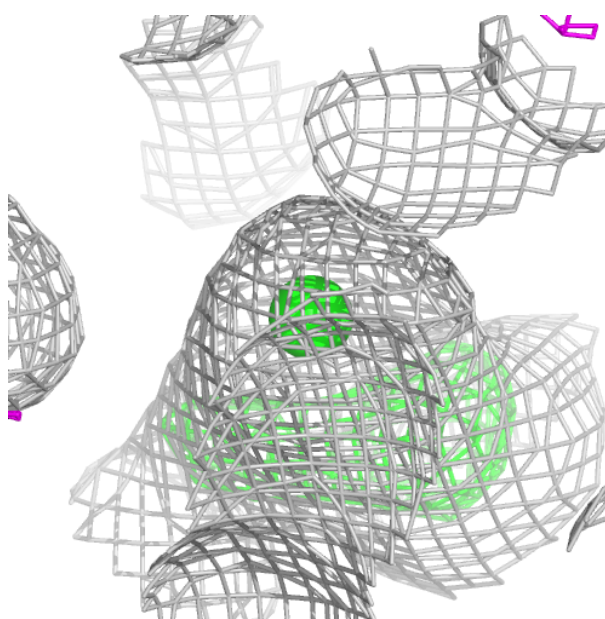
Electron density around ACT B 604:

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



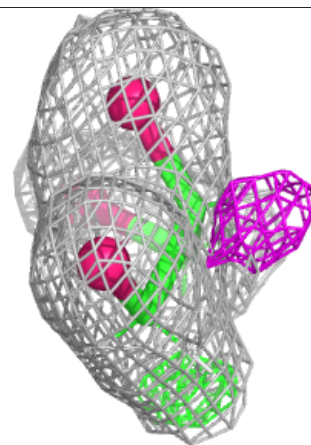
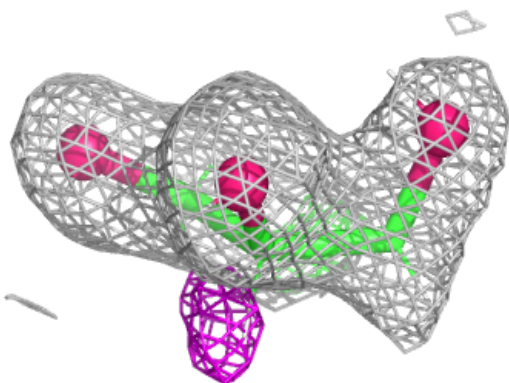
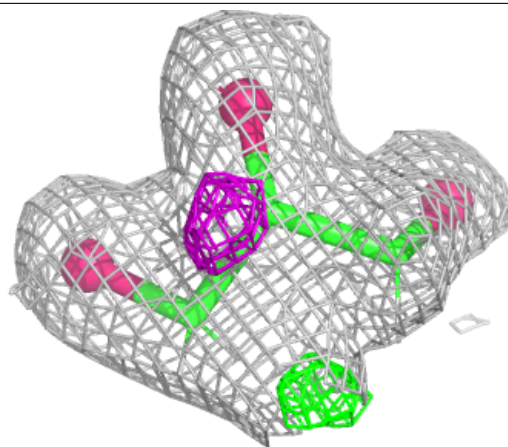
Electron density around CL A 602:

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



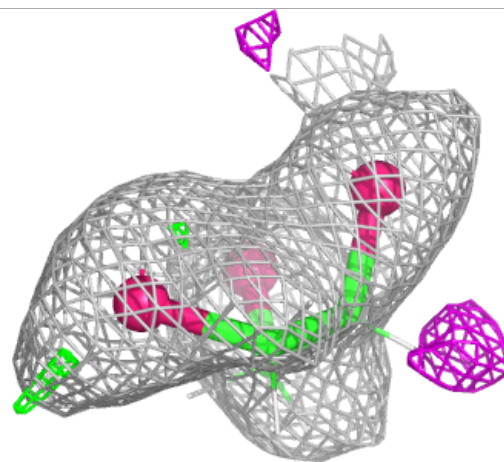
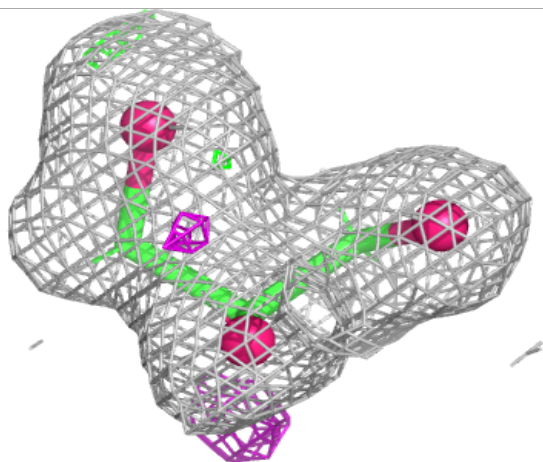
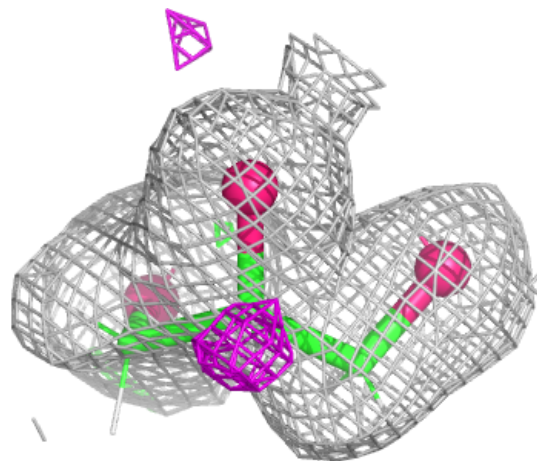
Electron density around GOL A 603:

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



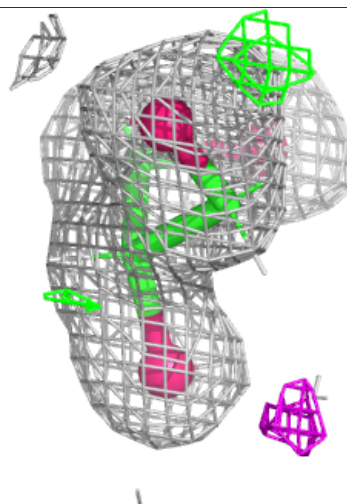
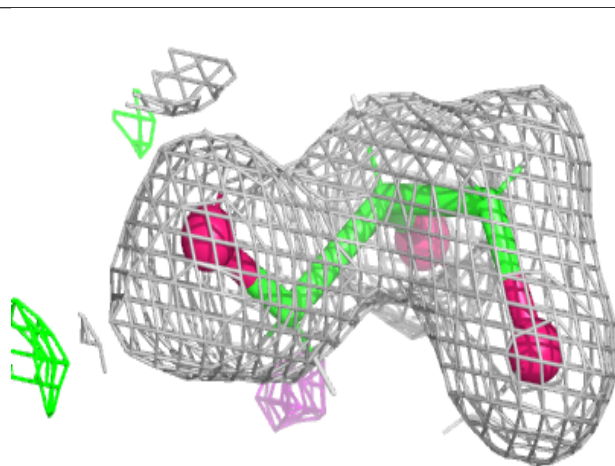
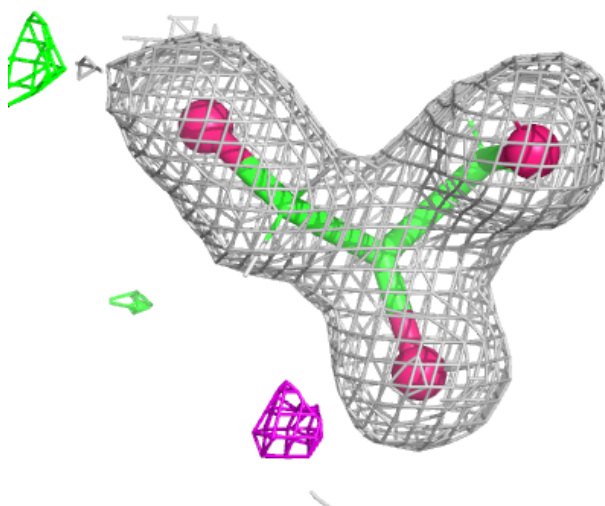
Electron density around GOL B 603:

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and green (positive)



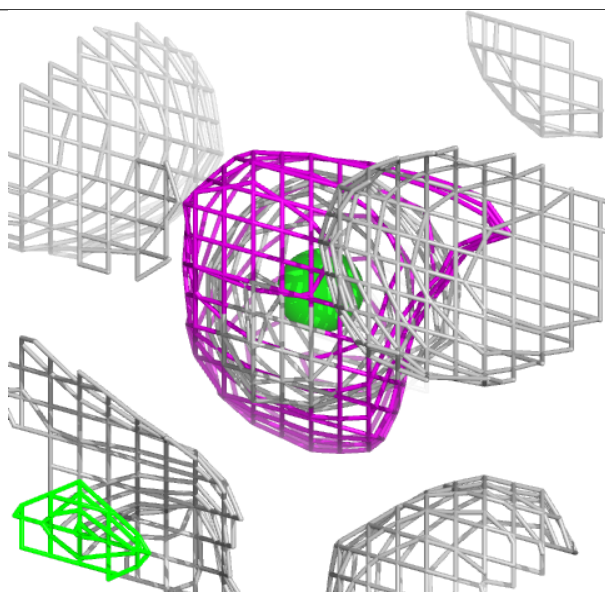
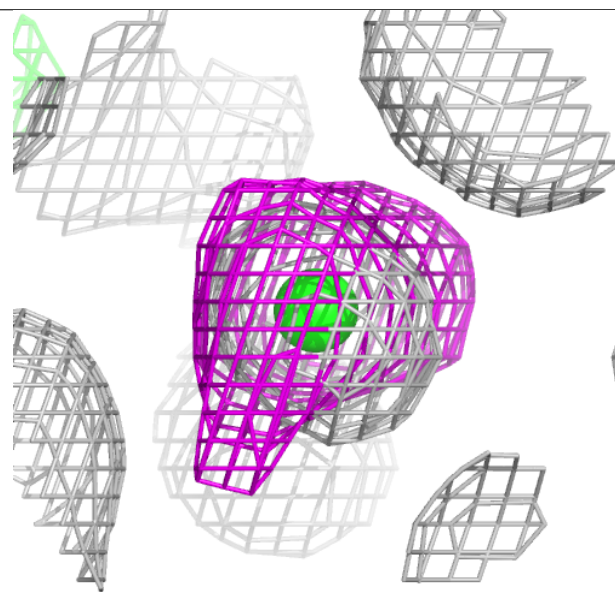
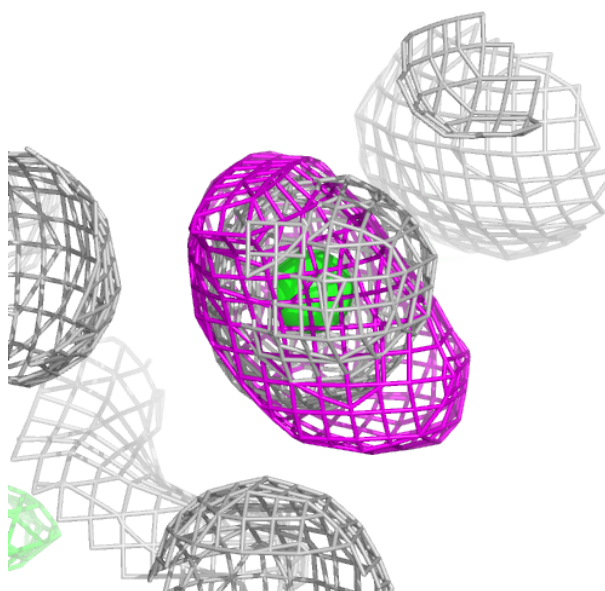
Electron density around GOL A 601:

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



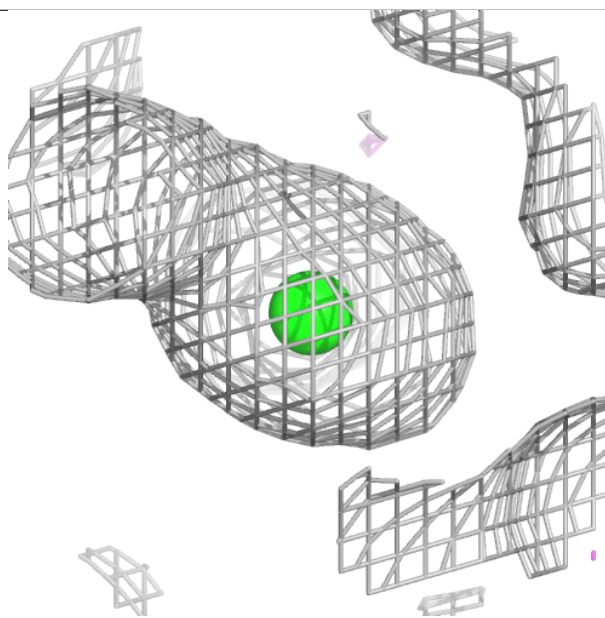
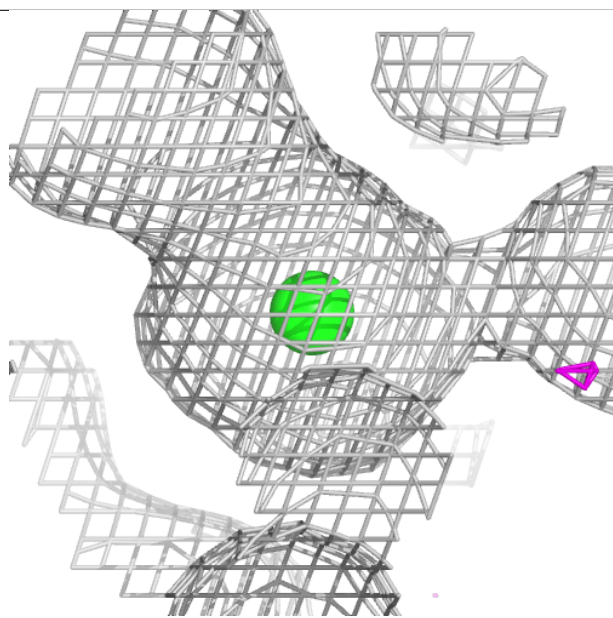
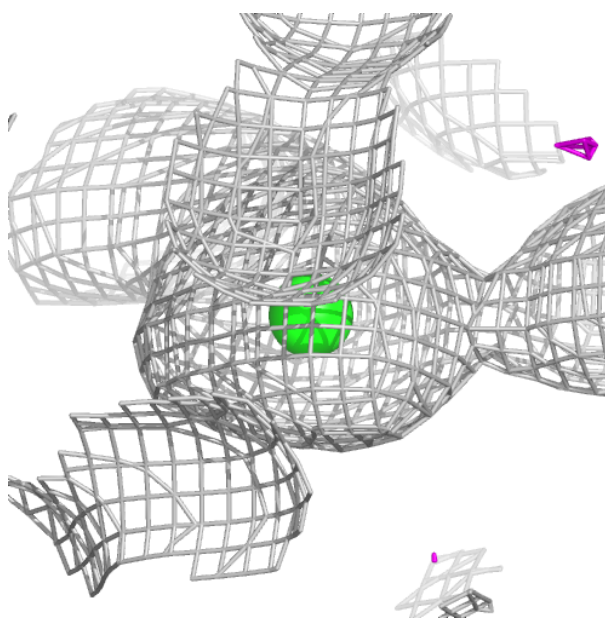
Electron density around CL B 602:

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



Electron density around CL 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.