



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:07 PM UTC

PDB ID : 9LB7 / pdb_00009lb7
Title : Crystal structure of trehalose-6-phosphate phosphorylase from *Weissella ceti* in complex with beta-Glc1P
Authors : Feng, Y.; Xue, S.
Deposited on : 2025-01-03
Resolution : 2.35 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

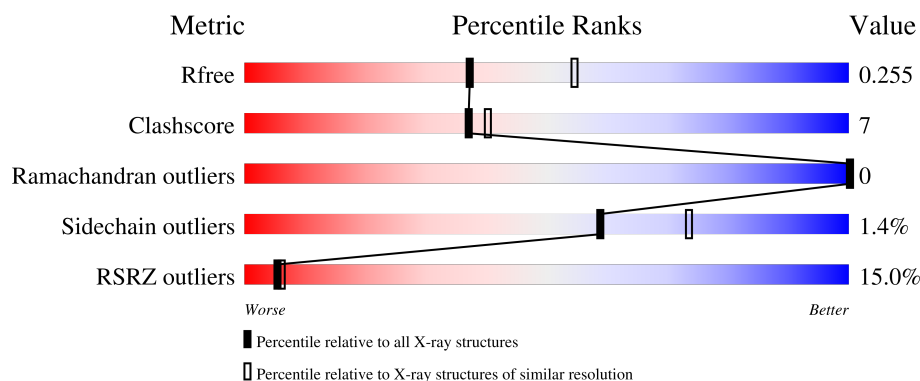
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	777	

2 Entry composition [i](#)

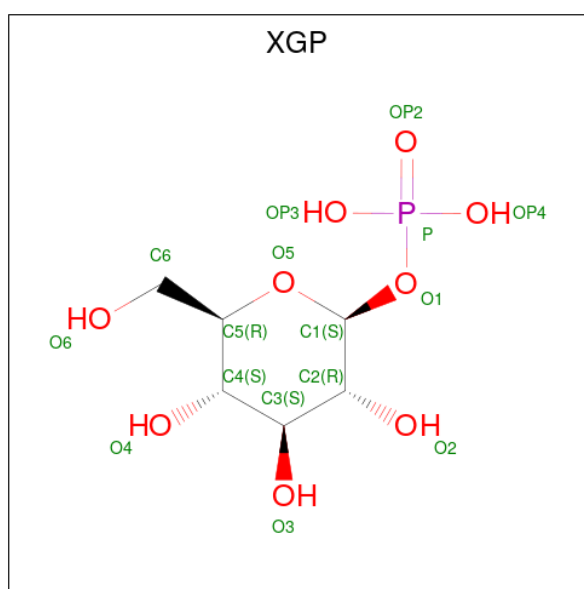
There are 4 unique types of molecules in this entry. The entry contains 6438 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Trehalose-6-phosphate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	775	Total	C	N	O	S	0	0	0
			6090	3847	1016	1206	21			

- Molecule 2 is 1-O-phosphono-beta-D-glucopyranose (CCD ID: XGP) (formula: $C_6H_{13}O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	331	Total 331	O 331	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: Trehalose-6-phosphate hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.38Å 62.16Å 77.27Å 90.00° 106.09° 90.00°	Depositor
Resolution (Å)	48.21 – 2.35 48.21 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.21-2.35) 97.0 (48.21-2.35)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.224 , 0.255 0.237 , 0.255	Depositor DCC
R_{free} test set	1719 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6438	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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: XGP, MG

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	0.11	0/6219	0.29	0/8471

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6090	0	5859	85	0
2	A	16	0	10	0	0
3	A	1	0	0	0	0
4	A	331	0	0	33	0
All	All	6438	0	5869	85	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 7.

All (85) 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:558:GLN:NE2	4:A:906:HOH:O	2.06	0.83
1:A:7:ARG:HB3	1:A:9:MET:HE3	1.61	0.83
1:A:286:TRP:O	4:A:902:HOH:O	2.01	0.79
1:A:516:GLU:OE1	4:A:901:HOH:O	2.01	0.77
1:A:219:ASN:OD1	4:A:903:HOH:O	2.05	0.74
1:A:284:GLU:OE2	4:A:905:HOH:O	2.06	0.73
1:A:610:TYR:O	4:A:908:HOH:O	2.08	0.71
1:A:664:ASN:OD1	4:A:907:HOH:O	2.08	0.71
1:A:736:LYS:HE2	1:A:741:MET:HE1	1.71	0.71
1:A:17:LYS:HB3	1:A:686:GLY:HA3	1.71	0.71
1:A:209:GLU:OE1	4:A:909:HOH:O	2.09	0.70
1:A:604:ASP:OD2	4:A:911:HOH:O	2.11	0.69
1:A:530:ASP:OD1	4:A:910:HOH:O	2.10	0.68
1:A:144:GLY:N	4:A:918:HOH:O	2.27	0.67
1:A:21:GLY:HA3	4:A:1019:HOH:O	1.97	0.65
1:A:196:LYS:NZ	1:A:203:ASP:OD1	2.31	0.64
1:A:87:THR:HG21	4:A:954:HOH:O	1.99	0.62
1:A:62:ARG:NE	4:A:904:HOH:O	2.06	0.62
1:A:5:ALA:N	4:A:933:HOH:O	2.32	0.61
1:A:276:GLU:OE1	4:A:912:HOH:O	2.16	0.61
1:A:126:GLN:O	1:A:126:GLN:NE2	2.35	0.60
1:A:615:ARG:NH2	4:A:925:HOH:O	2.28	0.59
1:A:427:ILE:O	1:A:431:ILE:HG13	2.04	0.58
1:A:462:LYS:O	4:A:913:HOH:O	2.17	0.57
1:A:407:THR:O	4:A:914:HOH:O	2.18	0.56
1:A:403:ILE:HD13	1:A:414:PRO:HA	1.86	0.56
1:A:136:ASP:O	1:A:140:TYR:HA	2.05	0.56
1:A:330:ARG:NH2	4:A:952:HOH:O	2.39	0.55
1:A:746:MET:HG2	1:A:751:VAL:HG23	1.88	0.55
1:A:340:HIS:ND1	1:A:391:GLN:OE1	2.35	0.55
1:A:62:ARG:HB2	4:A:904:HOH:O	2.07	0.55
1:A:115:THR:OG1	4:A:915:HOH:O	2.18	0.55
1:A:349:VAL:HG22	1:A:363:ILE:HD11	1.89	0.54
1:A:126:GLN:HG3	1:A:152:ASP:CG	2.32	0.54
1:A:711:VAL:HG22	1:A:720:ILE:HD12	1.90	0.54
1:A:429:TYR:HA	1:A:506:TRP:CH2	2.43	0.53
1:A:579:ASP:OD1	1:A:581:HIS:ND1	2.42	0.53
1:A:46:GLU:HG3	1:A:47:HIS:CE1	2.44	0.52
1:A:65:VAL:HG12	4:A:931:HOH:O	2.11	0.51
1:A:9:MET:HE2	1:A:106:GLY:HA3	1.93	0.51
1:A:684:GLN:H	1:A:684:GLN:CD	2.19	0.51
1:A:550:ILE:HG12	1:A:556:ILE:HG12	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:HG21	1:A:178:PHE:HA	1.95	0.49
1:A:137:PRO:HB2	1:A:138:LYS:HZ3	1.77	0.49
1:A:394:MET:HA	4:A:1082:HOH:O	2.11	0.49
1:A:403:ILE:HG22	1:A:412:TRP:CE3	2.49	0.48
1:A:291:ILE:HD12	1:A:308:ILE:HD11	1.96	0.47
1:A:181:ARG:HA	4:A:961:HOH:O	2.12	0.47
1:A:684:GLN:OE1	1:A:684:GLN:N	2.41	0.47
1:A:49:TYR:CE2	1:A:171:ASN:HB2	2.49	0.47
1:A:110:GLN:HG3	4:A:1130:HOH:O	2.14	0.47
1:A:15:THR:HB	1:A:47:HIS:CE1	2.49	0.46
1:A:349:VAL:HG11	1:A:430:ASN:HB3	1.97	0.46
1:A:160:GLU:HG3	4:A:963:HOH:O	2.15	0.46
1:A:713:LEU:O	4:A:916:HOH:O	2.21	0.46
1:A:682:ASP:CG	1:A:686:GLY:H	2.21	0.46
1:A:181:ARG:HD2	4:A:961:HOH:O	2.17	0.45
1:A:58:PHE:HB3	1:A:73:GLU:HG2	1.99	0.45
1:A:449:LEU:HD21	1:A:522:PHE:HA	1.99	0.45
1:A:656:ALA:O	1:A:660:VAL:HG23	2.17	0.45
1:A:49:TYR:OH	1:A:335:GLU:OE2	2.35	0.44
1:A:143:LEU:HB2	1:A:247:ILE:HB	1.98	0.44
1:A:274:VAL:HG11	4:A:918:HOH:O	2.16	0.44
1:A:142:MET:HE1	1:A:248:ALA:HB2	1.99	0.44
1:A:254:GLU:HG2	1:A:255:LEU:HG	2.00	0.44
1:A:36:ARG:HD3	1:A:51:GLY:HA3	2.00	0.43
1:A:445:ARG:HB2	1:A:521:MET:HE2	1.99	0.43
1:A:132:VAL:HB	1:A:146:GLN:HB2	2.00	0.43
1:A:666:ASP:HB2	4:A:907:HOH:O	2.17	0.43
1:A:582:ARG:HH21	1:A:584:ASP:CG	2.26	0.42
1:A:483:HIS:NE2	1:A:597:TYR:O	2.51	0.42
1:A:317:HIS:CE1	1:A:321:LYS:HB3	2.55	0.42
1:A:404:HIS:HB2	4:A:1093:HOH:O	2.19	0.42
1:A:311:ILE:O	1:A:352:TYR:OH	2.30	0.42
1:A:115:THR:HA	1:A:131:THR:O	2.20	0.41
1:A:209:GLU:CD	4:A:909:HOH:O	2.61	0.41
1:A:744:PHE:HB3	1:A:746:MET:HE3	2.02	0.41
1:A:381:ASP:HB2	1:A:387:MET:HE1	2.02	0.41
1:A:579:ASP:CG	1:A:581:HIS:HD1	2.29	0.40
1:A:68:LYS:HD2	1:A:412:TRP:CD1	2.56	0.40
1:A:720:ILE:HG22	1:A:722:PRO:HD3	2.04	0.40
1:A:27:THR:HG23	1:A:35:TRP:C	2.46	0.40
1:A:303:MET:HE3	1:A:303:MET:HB2	1.83	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:MET:HE1	1:A:680:TYR:HB2	2.04	0.40
1:A:724:LEU:HB2	1:A:748:PRO:HA	2.02	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	773/777 (100%)	752 (97%)	21 (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	647/648 (100%)	638 (99%)	9 (1%)	59	73

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	THR
1	A	150	THR
1	A	216	THR
1	A	239	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	256	SER
1	A	426	THR
1	A	494	ILE
1	A	648	SER
1	A	717	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	139	GLN
1	A	146	GLN
1	A	236	GLN
1	A	263	GLN
1	A	409	ASN
1	A	461	ASN
1	A	537	ASN
1	A	663	ASN
1	A	773	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	XGP	A	801	-	15,16,16	1.50	2 (13%)	24,24,24	0.94	1 (4%)

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	XGP	A	801	-	-	4/7/27/27	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	XGP	O5-C1	3.69	1.51	1.41
2	A	801	XGP	P-O1	3.58	1.65	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	XGP	O5-C1-O1	-2.16	108.55	111.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

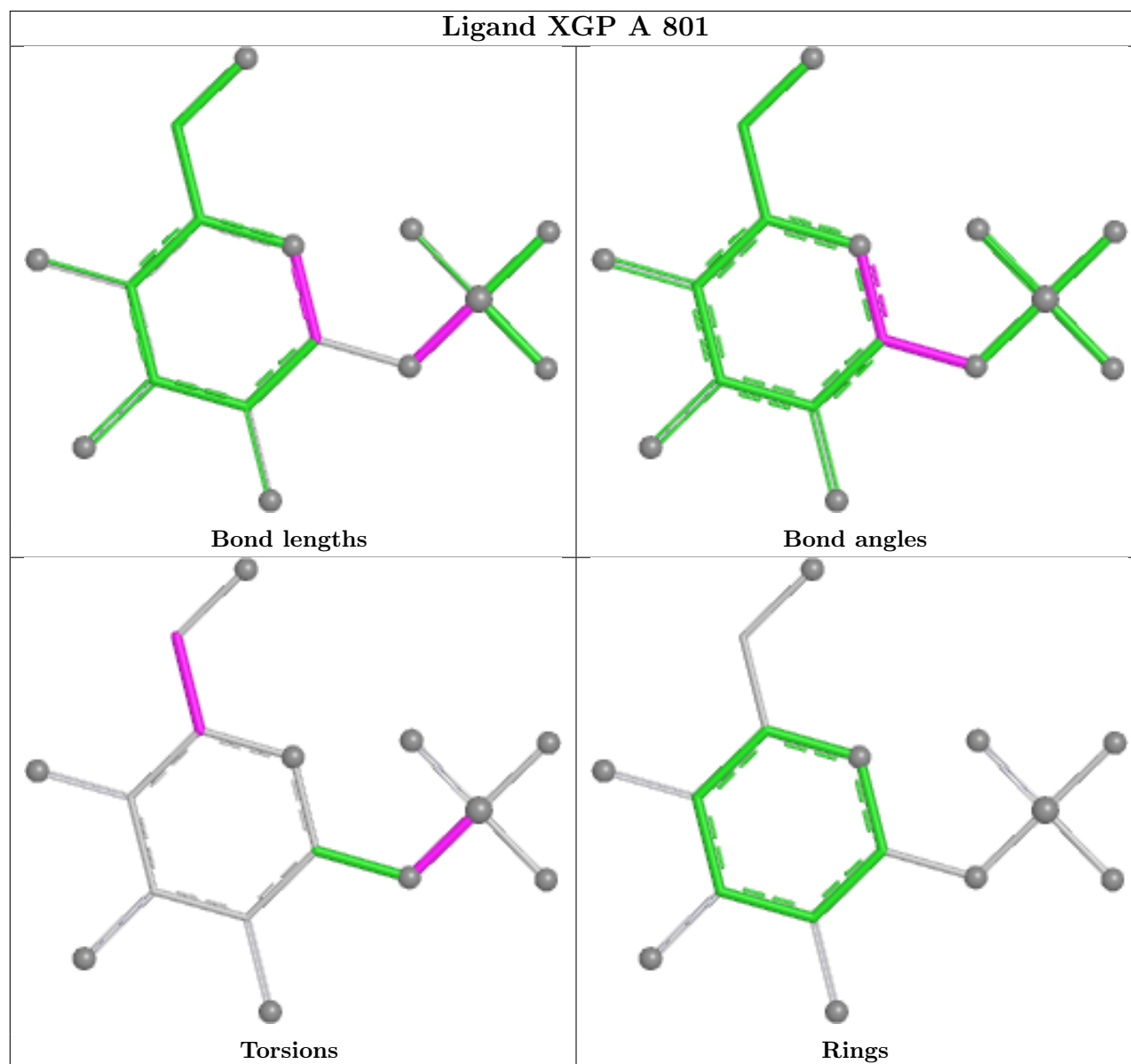
Mol	Chain	Res	Type	Atoms
2	A	801	XGP	C4-C5-C6-O6
2	A	801	XGP	O5-C5-C6-O6
2	A	801	XGP	C1-O1-P-OP3
2	A	801	XGP	C1-O1-P-OP2

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	775/777 (99%)	1.18	116 (14%) 5 6	21, 32, 47, 74	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	687	THR	5.6
1	A	683	ILE	5.4
1	A	533	SER	4.1
1	A	123	PRO	3.7
1	A	11	ASN	3.5
1	A	682	ASP	3.4
1	A	680	TYR	3.4
1	A	681	TYR	3.4
1	A	260	VAL	3.4
1	A	213	ASP	3.3
1	A	672	LEU	3.3
1	A	407	THR	3.2
1	A	678	SER	3.2
1	A	231	GLY	3.2
1	A	408	VAL	3.2
1	A	463	ALA	3.2
1	A	684	GLN	3.1
1	A	578	GLY	3.1
1	A	739	GLY	3.1
1	A	242	GLN	3.1
1	A	46	GLU	3.1
1	A	284	GLU	3.1
1	A	686	GLY	3.1
1	A	78	LEU	3.0
1	A	478	GLY	3.0
1	A	488	GLY	3.0
1	A	744	PHE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	567	ALA	3.0
1	A	750	ALA	3.0
1	A	429	TYR	3.0
1	A	530	ASP	3.0
1	A	241	VAL	2.9
1	A	294	ASP	2.9
1	A	404	HIS	2.8
1	A	217	PHE	2.8
1	A	56	GLY	2.8
1	A	717	LEU	2.7
1	A	283	GLN	2.7
1	A	359	THR	2.7
1	A	380	LEU	2.7
1	A	189	ALA	2.7
1	A	297	ASP	2.6
1	A	475	GLY	2.6
1	A	606	LEU	2.6
1	A	229	SER	2.6
1	A	685	GLY	2.6
1	A	134	ALA	2.5
1	A	579	ASP	2.5
1	A	563	PHE	2.5
1	A	122	VAL	2.5
1	A	307	ASN	2.5
1	A	534	ASP	2.5
1	A	202	ILE	2.5
1	A	559	TYR	2.5
1	A	303	MET	2.5
1	A	298	PRO	2.5
1	A	203	ASP	2.4
1	A	309	PHE	2.4
1	A	124	GLN	2.4
1	A	315	ALA	2.4
1	A	698	GLY	2.4
1	A	531	PHE	2.4
1	A	416	ASN	2.4
1	A	664	ASN	2.4
1	A	679	ASP	2.4
1	A	349	VAL	2.3
1	A	532	GLY	2.3
1	A	581	HIS	2.3
1	A	91	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	708	PHE	2.3
1	A	711	VAL	2.3
1	A	741	MET	2.3
1	A	126	GLN	2.3
1	A	143	LEU	2.3
1	A	90	ASP	2.3
1	A	535	TRP	2.3
1	A	308	ILE	2.3
1	A	582	ARG	2.2
1	A	482	TYR	2.2
1	A	626	TYR	2.2
1	A	545	GLY	2.2
1	A	526	ALA	2.2
1	A	256	SER	2.2
1	A	93	VAL	2.2
1	A	300	MET	2.2
1	A	410	ASN	2.2
1	A	670	ASP	2.2
1	A	37	GLY	2.2
1	A	351	TYR	2.1
1	A	47	HIS	2.1
1	A	125	GLY	2.1
1	A	95	ILE	2.1
1	A	624	LEU	2.1
1	A	406	ASN	2.1
1	A	84	PHE	2.1
1	A	413	GLU	2.1
1	A	192	ILE	2.1
1	A	405	LEU	2.1
1	A	494	ILE	2.1
1	A	627	ASP	2.1
1	A	412	TRP	2.1
1	A	177	ALA	2.1
1	A	9	MET	2.1
1	A	104	GLU	2.1
1	A	580	ILE	2.1
1	A	584	ASP	2.1
1	A	65	VAL	2.1
1	A	525	VAL	2.1
1	A	674	THR	2.0
1	A	769	SER	2.0
1	A	155	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	102	HIS	2.0
1	A	164	ASP	2.0
1	A	663	ASN	2.0
1	A	181	ARG	2.0
1	A	16	GLU	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](#)

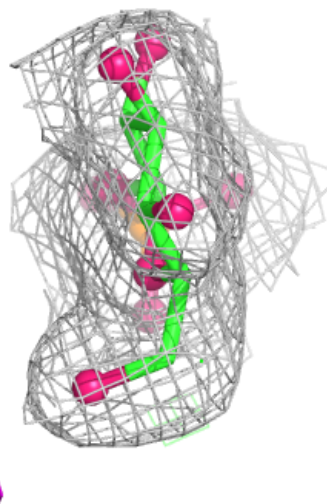
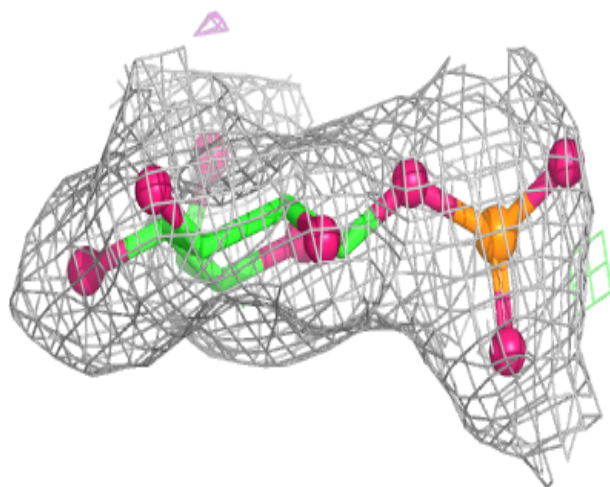
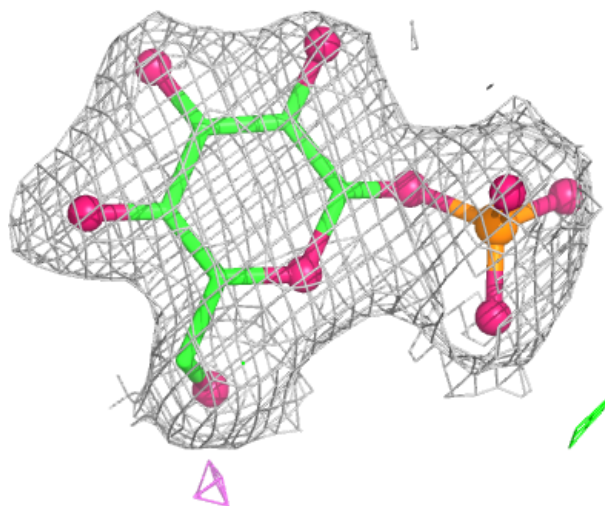
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	XGP	A	801	16/16	0.92	0.11	22,31,41,48	0
3	MG	A	802	1/1	0.94	0.13	26,26,26,26	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 XGP A 801:

$2mF_o-DF_c$ (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.