



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2026 – 12:08 AM JST

PDB ID : 9VFZ / pdb_00009vfz
Title : Crystal structure of Phaeodactylibacter sp. phosphoglucomutase in complex with glucose-1-phosphate
Authors : Shen, Y.W.; Tu, T.
Deposited on : 2025-06-12
Resolution : 1.95 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 : 1.8.5 (274361), CSD as541be (2020)
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

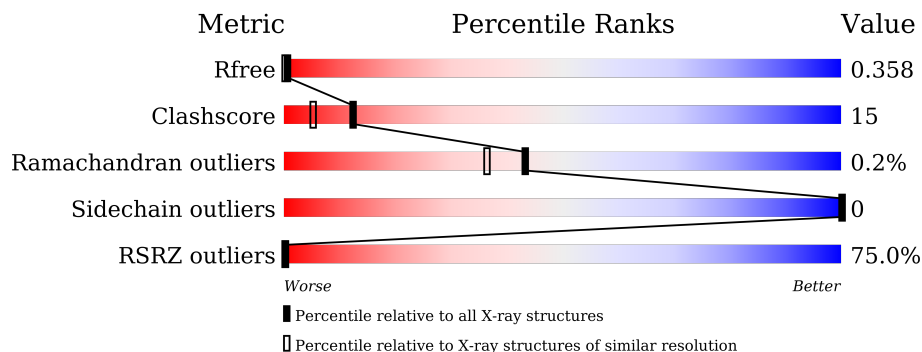
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	588	<div> <div>70%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8357 atoms, of which 4106 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 Phosphoglucomutase (Alpha-D-glucose-1,6-bisphosphate-dependent).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	545	Total	C	H	N	O	S	0	0	0
			8276	2627	4095	743	798	13			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP A0A959BHL9
A	-32	GLY	-	expression tag	UNP A0A959BHL9
A	-31	SER	-	expression tag	UNP A0A959BHL9
A	-30	SER	-	expression tag	UNP A0A959BHL9
A	-29	HIS	-	expression tag	UNP A0A959BHL9
A	-28	HIS	-	expression tag	UNP A0A959BHL9
A	-27	HIS	-	expression tag	UNP A0A959BHL9
A	-26	HIS	-	expression tag	UNP A0A959BHL9
A	-25	HIS	-	expression tag	UNP A0A959BHL9
A	-24	HIS	-	expression tag	UNP A0A959BHL9
A	-23	SER	-	expression tag	UNP A0A959BHL9
A	-22	SER	-	expression tag	UNP A0A959BHL9
A	-21	GLY	-	expression tag	UNP A0A959BHL9
A	-20	LEU	-	expression tag	UNP A0A959BHL9
A	-19	VAL	-	expression tag	UNP A0A959BHL9
A	-18	PRO	-	expression tag	UNP A0A959BHL9
A	-17	ARG	-	expression tag	UNP A0A959BHL9
A	-16	GLY	-	expression tag	UNP A0A959BHL9
A	-15	SER	-	expression tag	UNP A0A959BHL9
A	-14	HIS	-	expression tag	UNP A0A959BHL9
A	-13	MET	-	expression tag	UNP A0A959BHL9
A	-12	ALA	-	expression tag	UNP A0A959BHL9
A	-11	SER	-	expression tag	UNP A0A959BHL9
A	-10	MET	-	expression tag	UNP A0A959BHL9
A	-9	THR	-	expression tag	UNP A0A959BHL9
A	-8	GLY	-	expression tag	UNP A0A959BHL9

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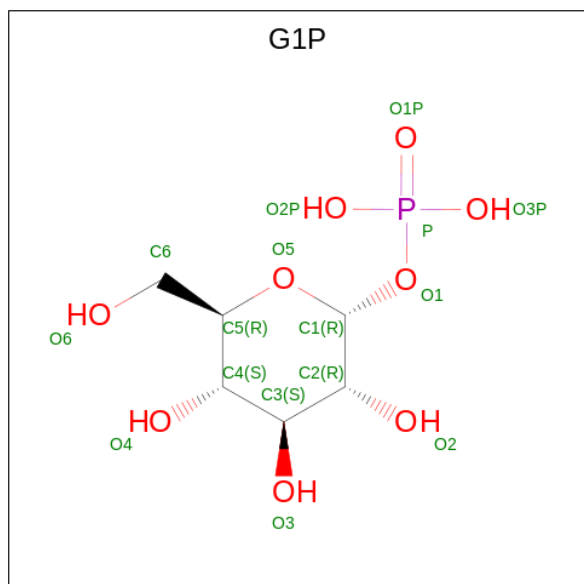
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP A0A959BHL9
A	-6	GLN	-	expression tag	UNP A0A959BHL9
A	-5	GLN	-	expression tag	UNP A0A959BHL9
A	-4	MET	-	expression tag	UNP A0A959BHL9
A	-3	GLY	-	expression tag	UNP A0A959BHL9
A	-2	ARG	-	expression tag	UNP A0A959BHL9
A	-1	GLY	-	expression tag	UNP A0A959BHL9
A	0	SER	-	expression tag	UNP A0A959BHL9
A	547	LEU	-	expression tag	UNP A0A959BHL9
A	548	GLU	-	expression tag	UNP A0A959BHL9
A	549	HIS	-	expression tag	UNP A0A959BHL9
A	550	HIS	-	expression tag	UNP A0A959BHL9
A	551	HIS	-	expression tag	UNP A0A959BHL9
A	552	HIS	-	expression tag	UNP A0A959BHL9
A	553	HIS	-	expression tag	UNP A0A959BHL9
A	554	HIS	-	expression tag	UNP A0A959BHL9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is 1-O-phosphono-alpha-D-glucopyranose (CCD ID: G1P) (formula: C₆H₁₃O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	0	0
			27	6	11	9	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.97Å 58.97Å 99.52Å 90.00° 118.22° 90.00°	Depositor
Resolution (Å)	49.16 – 1.95 49.16 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.16-1.95) 99.0 (49.16-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.272 , 0.359 0.271 , 0.358	Depositor DCC
R_{free} test set	2028 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.918	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8357	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: G1P, 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	0.65	1/4275 (0.0%)	0.84	3/5796 (0.1%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	MET	SD-CE	-11.48	1.50	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	MET	CG-SD-CE	7.51	117.41	100.90
1	A	283	SER	CA-C-N	-5.70	105.85	122.38
1	A	283	SER	C-N-CA	-5.70	105.85	122.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	MET	Peptide
1	A	474	GLN	Peptide

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	4181	4095	4094	128	6
2	A	1	0	0	0	0
3	A	16	11	11	0	0
4	A	53	0	0	5	0
All	All	4251	4106	4105	128	6

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 15.

All (128) 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:73:GLN:NE2	4:A:701:HOH:O	1.87	1.04
1:A:359:ARG:HA	1:A:362:ALA:HB3	1.52	0.88
1:A:424:THR:HG22	1:A:431:PRO:HD3	1.56	0.87
1:A:427:THR:HG23	1:A:429:LYS:H	1.38	0.87
1:A:70:LEU:HD23	1:A:177:LYS:HE3	1.65	0.79
1:A:478:GLU:HB2	1:A:501:THR:HG21	1.65	0.79
1:A:363:ARG:NH1	1:A:441:GLU:OE2	2.15	0.78
1:A:423:ILE:O	1:A:427:THR:HG22	1.88	0.73
1:A:474:GLN:HB2	1:A:479:LYS:HA	1.70	0.71
1:A:160:MET:HE2	1:A:170:VAL:HG21	1.72	0.71
1:A:474:GLN:CB	1:A:479:LYS:HA	2.20	0.70
1:A:494:ILE:HD11	1:A:496:GLY:O	1.96	0.66
1:A:359:ARG:HA	1:A:362:ALA:CB	2.25	0.65
1:A:420:ALA:O	1:A:424:THR:HG23	1.98	0.64
1:A:424:THR:HG22	1:A:430:ASP:HA	1.80	0.63
1:A:359:ARG:CA	1:A:362:ALA:HB3	2.26	0.62
1:A:478:GLU:HB2	1:A:501:THR:CG2	2.29	0.62
1:A:474:GLN:OE1	1:A:479:LYS:HB3	1.99	0.61
1:A:315:THR:HG21	1:A:432:GLY:H	1.65	0.61
1:A:219:VAL:HG21	1:A:407:TRP:CD2	2.38	0.59
1:A:348:GLY:O	1:A:390:GLY:HA2	2.03	0.58
1:A:257:THR:HG23	4:A:726:HOH:O	2.03	0.58
1:A:474:GLN:HA	1:A:480:ILE:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:VAL:HG13	1:A:409:THR:HB	1.86	0.58
1:A:148:HIS:CE1	1:A:149:ASN:OD1	2.57	0.57
1:A:342:LYS:HB2	1:A:345:THR:HG23	1.86	0.57
1:A:358:ASP:O	1:A:362:ALA:N	2.37	0.57
1:A:474:GLN:OE1	1:A:479:LYS:CA	2.52	0.57
1:A:288:MET:HE1	1:A:303:ALA:HB2	1.86	0.57
1:A:148:HIS:H	1:A:148:HIS:HD1	1.52	0.57
1:A:72:ARG:NH2	1:A:79:GLY:O	2.34	0.56
1:A:223:ASP:O	1:A:227:SER:HB3	2.05	0.56
1:A:44:THR:HG23	1:A:45:SER:H	1.71	0.56
1:A:359:ARG:O	1:A:362:ALA:HB3	2.05	0.55
1:A:454:ALA:HB2	1:A:517:TYR:HD2	1.72	0.55
1:A:458:GLN:OE1	1:A:545:ILE:HG21	2.07	0.55
1:A:436:ARG:O	1:A:439:THR:OG1	2.23	0.54
1:A:481:GLU:O	1:A:482:ALA:HB2	2.08	0.53
1:A:16:LEU:HD11	1:A:268:ARG:HG3	1.89	0.53
1:A:71:TYR:CZ	1:A:170:VAL:HG13	2.43	0.53
1:A:249:ALA:HB2	1:A:256:LEU:HB3	1.90	0.53
1:A:261:THR:HG22	4:A:704:HOH:O	2.10	0.52
1:A:288:MET:HE1	1:A:303:ALA:CB	2.40	0.52
1:A:494:ILE:HG13	1:A:496:GLY:N	2.25	0.52
1:A:424:THR:CG2	1:A:431:PRO:HD3	2.35	0.51
1:A:160:MET:CE	1:A:167:GLU:H	2.24	0.51
1:A:212:TYR:CE1	1:A:216:LEU:HD21	2.45	0.51
1:A:266:THR:OG1	1:A:268:ARG:HB2	2.10	0.51
1:A:464:LYS:O	1:A:464:LYS:HG2	2.11	0.51
1:A:384:ASP:OD1	1:A:384:ASP:C	2.54	0.50
1:A:474:GLN:OE1	1:A:479:LYS:CB	2.60	0.50
1:A:474:GLN:HB3	1:A:479:LYS:HA	1.92	0.50
1:A:497:LEU:HD23	1:A:498:LYS:N	2.27	0.50
1:A:515:ASP:OD1	1:A:515:ASP:N	2.45	0.49
1:A:329:VAL:HG22	1:A:434:ILE:HG22	1.92	0.49
1:A:483:ILE:HG23	1:A:497:LEU:HD21	1.94	0.49
1:A:359:ARG:C	1:A:362:ALA:HB3	2.37	0.49
1:A:432:GLY:O	1:A:436:ARG:HG2	2.12	0.49
1:A:300:VAL:HG11	1:A:431:PRO:HD2	1.94	0.49
1:A:271:SER:OG	1:A:286:TYR:O	2.27	0.49
1:A:495:GLY:O	1:A:510:PRO:HD2	2.12	0.48
1:A:147:SER:OG	1:A:148:HIS:N	2.37	0.48
1:A:427:THR:OG1	1:A:429:LYS:HE3	2.14	0.48
1:A:506:PHE:C	1:A:506:PHE:CD1	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLU:O	1:A:489:GLY:HA3	2.14	0.48
1:A:44:THR:HG23	1:A:45:SER:N	2.29	0.47
1:A:455:THR:HB	1:A:456:PRO:HD2	1.97	0.47
1:A:459:LYS:NZ	1:A:515:ASP:HA	2.29	0.47
1:A:222:MET:HE1	1:A:418:LEU:HD13	1.97	0.47
1:A:511:SER:OG	1:A:512:GLY:N	2.48	0.47
1:A:116:GLU:HG3	1:A:117:TYR:O	2.15	0.47
1:A:478:GLU:CB	1:A:501:THR:CG2	2.93	0.47
1:A:350:THR:HA	1:A:371:VAL:O	2.14	0.46
1:A:261:THR:HG22	1:A:261:THR:O	2.14	0.46
1:A:474:GLN:OE1	1:A:479:LYS:HA	2.15	0.46
1:A:19:ILE:HB	1:A:20:PRO:HD3	1.97	0.46
1:A:37:GLU:H	1:A:37:GLU:CD	2.23	0.46
1:A:107:VAL:HG22	4:A:701:HOH:O	2.15	0.46
1:A:4:HIS:CG	1:A:5:PRO:HD2	2.52	0.45
1:A:372:PRO:HG2	1:A:377:TRP:NE1	2.32	0.45
1:A:66:GLN:HE21	1:A:70:LEU:CD1	2.30	0.45
1:A:439:THR:HA	1:A:443:GLY:O	2.17	0.45
1:A:134:ARG:HD3	1:A:136:GLY:O	2.16	0.45
1:A:427:THR:HG21	1:A:434:ILE:HD11	1.99	0.45
1:A:462:LEU:O	1:A:465:LEU:HG	2.16	0.44
1:A:41:SER:O	1:A:47:HIS:HA	2.16	0.44
1:A:234:VAL:CG1	1:A:258:VAL:HG22	2.47	0.44
1:A:506:PHE:CG	1:A:537:ALA:HB2	2.52	0.44
1:A:30:GLN:HG2	1:A:59:GLN:NE2	2.31	0.43
1:A:50:SER:N	1:A:55:SER:OG	2.31	0.43
1:A:349:LYS:HG3	1:A:353:SER:HB2	1.99	0.43
1:A:86:ASP:C	1:A:86:ASP:OD1	2.61	0.43
1:A:393:GLU:OE2	1:A:394:SER:OG	2.35	0.43
1:A:59:GLN:HG2	1:A:186:LEU:HD11	2.01	0.43
1:A:349:LYS:HG2	1:A:350:THR:O	2.18	0.43
1:A:427:THR:HG23	1:A:429:LYS:N	2.20	0.43
1:A:71:TYR:CE1	1:A:170:VAL:HG13	2.54	0.43
1:A:179:ASN:O	1:A:183:GLU:HG3	2.19	0.43
1:A:182:LEU:HD12	1:A:186:LEU:HD21	2.00	0.43
1:A:359:ARG:C	1:A:362:ALA:H	2.27	0.42
1:A:473:SER:O	1:A:474:GLN:HB3	2.18	0.42
1:A:388:GLY:HA2	1:A:400:LEU:HG	2.01	0.42
1:A:333:TYR:CG	1:A:423:ILE:HG12	2.55	0.42
1:A:494:ILE:HD11	1:A:496:GLY:C	2.44	0.42
1:A:300:VAL:CG1	1:A:431:PRO:HD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:VAL:HB	1:A:372:PRO:HD2	2.02	0.42
1:A:2:ALA:HB1	1:A:274:TRP:HB2	2.00	0.42
1:A:219:VAL:HG21	1:A:407:TRP:CG	2.55	0.42
1:A:345:THR:HA	1:A:386:SER:O	2.19	0.42
1:A:64:THR:O	1:A:68:ILE:HG13	2.20	0.42
1:A:134:ARG:HG2	1:A:136:GLY:O	2.20	0.41
1:A:455:THR:O	1:A:457:ALA:N	2.52	0.41
1:A:474:GLN:HB2	1:A:478:GLU:O	2.19	0.41
1:A:342:LYS:HE2	4:A:702:HOH:O	2.20	0.41
1:A:160:MET:CE	1:A:170:VAL:HG21	2.46	0.41
1:A:455:THR:HB	1:A:456:PRO:CD	2.51	0.41
1:A:497:LEU:HD23	1:A:497:LEU:C	2.45	0.41
1:A:75:GLU:HA	1:A:75:GLU:OE2	2.21	0.41
1:A:430:ASP:OD1	1:A:432:GLY:N	2.54	0.41
1:A:85:ILE:HB	1:A:91:SER:HB3	2.02	0.41
1:A:221:ASP:HB3	1:A:422:GLU:CD	2.45	0.41
1:A:435:TYR:O	1:A:439:THR:HG23	2.21	0.41
1:A:7:ALA:O	1:A:9:LYS:NZ	2.54	0.41
1:A:42:PHE:HB3	1:A:175:GLU:HB2	2.03	0.41
1:A:119:PRO:HD3	1:A:244:TYR:CE1	2.56	0.40
1:A:500:VAL:HG12	1:A:501:THR:N	2.35	0.40
1:A:288:MET:HE3	1:A:288:MET:HB3	1.97	0.40
1:A:475:LEU:HD13	1:A:506:PHE:HE2	1.87	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ALA:O	1:A:479:LYS:NZ[2_656]	1.77	0.43
1:A:253:ARG:NH1	1:A:468:GLU:OE1[3_455]	1.96	0.24
1:A:361:ALA:O	1:A:479:LYS:HZ2[2_656]	1.40	0.20
1:A:21:ARG:HE	1:A:92:GLU:OE2[2_555]	1.47	0.13
1:A:361:ALA:O	1:A:479:LYS:HZ1[2_656]	1.52	0.08
1:A:253:ARG:O	1:A:468:GLU:OE2[3_455]	2.17	0.03

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	543/588 (92%)	502 (92%)	40 (7%)	1 (0%)	43	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	482	ALA

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	430/465 (92%)	430 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	184	ASN
1	A	538	GLN

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	$\# Z > 2$
3	G1P	A	602	-	15,16,16	1.30	1 (6%)	23,24,24	1.66	5 (21%)

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
3	G1P	A	602	-	-	1/7/27/27	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	G1P	O5-C1	2.98	1.49	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	G1P	O5-C5-C4	4.96	118.70	109.69
3	A	602	G1P	C3-C4-C5	2.72	115.08	110.24
3	A	602	G1P	C4-C3-C2	-2.63	106.22	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	G1P	C6-C5-C4	-2.46	107.23	113.00
3	A	602	G1P	C1-O5-C5	2.05	117.70	113.69

There are no chirality outliers.

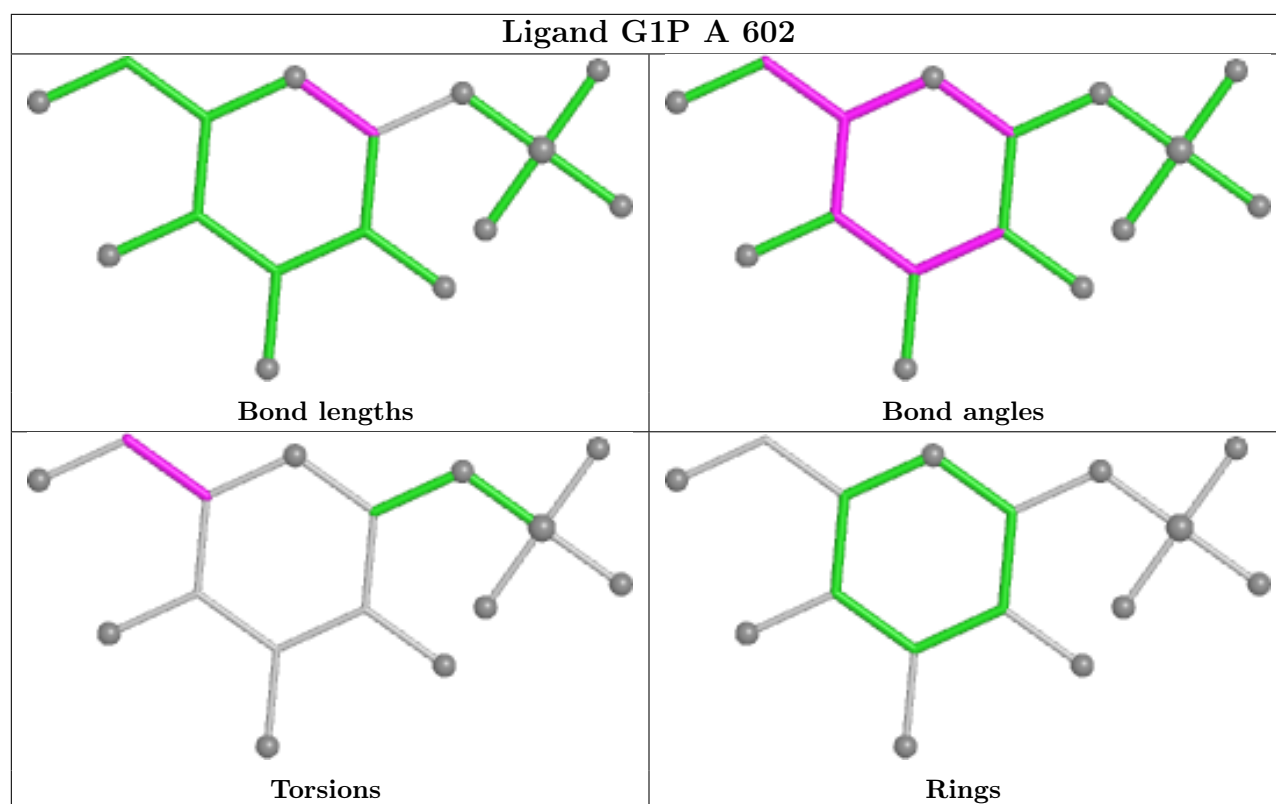
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	G1P	C4-C5-C6-O6

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 [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	545/588 (92%)	3.16	409 (75%) 0 0	30, 60, 144, 240	0

All (409) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	11.7
1	A	465	LEU	11.4
1	A	361	ALA	10.2
1	A	44	THR	10.1
1	A	508	ALA	9.6
1	A	362	ALA	9.5
1	A	291	LEU	8.5
1	A	462	LEU	8.3
1	A	517	TYR	7.9
1	A	224	ALA	7.8
1	A	545	ILE	7.5
1	A	270	MET	7.4
1	A	42	PHE	7.2
1	A	3	LEU	7.2
1	A	73	GLN	7.0
1	A	43	GLY	7.0
1	A	502	ALA	6.9
1	A	476	ALA	6.9
1	A	477	GLY	6.9
1	A	479	LYS	6.9
1	A	457	ALA	6.7
1	A	546	GLY	6.7
1	A	513	THR	6.6
1	A	258	VAL	6.5
1	A	542	ASP	6.5
1	A	483	ILE	6.5
1	A	274	TRP	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	485	THR	6.5
1	A	376	LYS	6.5
1	A	45	SER	6.4
1	A	454	ALA	6.4
1	A	223	ASP	6.4
1	A	544	VAL	6.3
1	A	456	PRO	6.2
1	A	300	VAL	6.2
1	A	40	VAL	6.2
1	A	475	LEU	6.1
1	A	527	GLU	6.1
1	A	74	LYS	6.1
1	A	494	ILE	6.1
1	A	472	SER	6.0
1	A	69	CYS	5.9
1	A	335	PHE	5.9
1	A	143	VAL	5.8
1	A	298	TYR	5.8
1	A	316	ARG	5.8
1	A	198	MET	5.7
1	A	480	ILE	5.7
1	A	284	SER	5.7
1	A	365	GLY	5.6
1	A	512	GLY	5.6
1	A	70	LEU	5.6
1	A	75	GLU	5.6
1	A	474	GLN	5.6
1	A	425	ALA	5.6
1	A	77	ILE	5.5
1	A	214	ASN	5.4
1	A	345	THR	5.4
1	A	463	LYS	5.4
1	A	17	VAL	5.3
1	A	46	GLY	5.3
1	A	107	VAL	5.2
1	A	516	ILE	5.1
1	A	466	SER	5.1
1	A	540	LEU	5.1
1	A	194	PHE	5.0
1	A	379	VAL	5.0
1	A	68	ILE	5.0
1	A	142	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	157	LYS	5.0
1	A	288	MET	5.0
1	A	507	ALA	4.9
1	A	468	GLU	4.9
1	A	341	TRP	4.9
1	A	377	TRP	4.9
1	A	260	ASP	4.8
1	A	71	TYR	4.8
1	A	191	ARG	4.8
1	A	439	THR	4.8
1	A	269	PHE	4.8
1	A	389	PHE	4.8
1	A	184	ASN	4.7
1	A	230	LEU	4.7
1	A	418	LEU	4.7
1	A	148	HIS	4.7
1	A	237	LEU	4.6
1	A	497	LEU	4.6
1	A	524	PHE	4.6
1	A	9	LYS	4.6
1	A	268	ARG	4.6
1	A	448	GLY	4.6
1	A	169	ASN	4.5
1	A	375	PHE	4.5
1	A	255	ASN	4.5
1	A	173	TRP	4.5
1	A	286	TYR	4.5
1	A	123	VAL	4.5
1	A	179	ASN	4.5
1	A	348	GLY	4.5
1	A	504	GLY	4.5
1	A	10	THR	4.5
1	A	343	PRO	4.4
1	A	397	ALA	4.4
1	A	78	ASN	4.4
1	A	354	SER	4.4
1	A	294	LEU	4.3
1	A	450	ILE	4.3
1	A	510	PRO	4.3
1	A	304	CYS	4.3
1	A	518	LYS	4.3
1	A	515	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	219	VAL	4.2
1	A	464	LYS	4.2
1	A	407	TRP	4.2
1	A	514	GLU	4.2
1	A	482	ALA	4.2
1	A	283	SER	4.2
1	A	222	MET	4.2
1	A	455	THR	4.2
1	A	35	VAL	4.1
1	A	182	LEU	4.1
1	A	295	LYS	4.1
1	A	249	ALA	4.1
1	A	252	TYR	4.1
1	A	189	VAL	4.1
1	A	126	ALA	4.1
1	A	257	THR	4.1
1	A	470	VAL	4.0
1	A	471	THR	4.0
1	A	536	GLU	4.0
1	A	488	PRO	4.0
1	A	253	ARG	4.0
1	A	293	ARG	4.0
1	A	297	ASP	4.0
1	A	506	PHE	4.0
1	A	528	GLU	4.0
1	A	225	ILE	3.9
1	A	242	VAL	3.9
1	A	369	VAL	3.9
1	A	256	LEU	3.9
1	A	452	ALA	3.9
1	A	133	GLY	3.9
1	A	13	PRO	3.9
1	A	529	HIS	3.8
1	A	500	VAL	3.8
1	A	289	GLN	3.8
1	A	201	SER	3.8
1	A	20	PRO	3.8
1	A	526	GLY	3.8
1	A	532	GLN	3.8
1	A	244	TYR	3.8
1	A	357	ILE	3.8
1	A	263	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	281	ASP	3.7
1	A	6	GLN	3.7
1	A	76	GLY	3.7
1	A	495	GLY	3.7
1	A	246	GLY	3.7
1	A	374	GLY	3.7
1	A	209	LEU	3.7
1	A	29	GLY	3.7
1	A	196	ARG	3.7
1	A	228	SER	3.7
1	A	492	ALA	3.6
1	A	314	VAL	3.6
1	A	261	THR	3.6
1	A	137	GLY	3.6
1	A	188	GLU	3.5
1	A	505	TRP	3.5
1	A	312	GLY	3.5
1	A	259	VAL	3.5
1	A	218	GLN	3.5
1	A	355	GLN	3.5
1	A	503	ASN	3.5
1	A	229	GLY	3.5
1	A	419	LEU	3.5
1	A	265	PRO	3.4
1	A	26	TYR	3.4
1	A	19	ILE	3.4
1	A	21	ARG	3.4
1	A	404	GLY	3.4
1	A	496	GLY	3.4
1	A	543	ARG	3.4
1	A	51	SER	3.4
1	A	186	LEU	3.4
1	A	417	ALA	3.4
1	A	267	PHE	3.4
1	A	467	ARG	3.4
1	A	7	ALA	3.3
1	A	166	ALA	3.3
1	A	16	LEU	3.3
1	A	426	ARG	3.3
1	A	490	ASN	3.3
1	A	330	ALA	3.3
1	A	282	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	205	ARG	3.3
1	A	440	ARG	3.3
1	A	511	SER	3.3
1	A	278	ILE	3.3
1	A	101	VAL	3.3
1	A	499	ALA	3.3
1	A	469	GLN	3.3
1	A	5	PRO	3.3
1	A	366	ARG	3.3
1	A	541	VAL	3.2
1	A	48	ARG	3.2
1	A	128	LEU	3.2
1	A	383	PHE	3.2
1	A	14	ASP	3.2
1	A	61	ILE	3.2
1	A	63	ALA	3.2
1	A	93	PRO	3.2
1	A	99	LEU	3.2
1	A	27	PHE	3.2
1	A	310	ARG	3.2
1	A	307	ASP	3.2
1	A	135	ALA	3.2
1	A	453	PRO	3.2
1	A	340	LYS	3.2
1	A	351	LEU	3.2
1	A	30	GLN	3.2
1	A	248	ILE	3.1
1	A	461	LYS	3.1
1	A	272	LEU	3.1
1	A	364	LEU	3.1
1	A	363	ARG	3.1
1	A	302	PHE	3.1
1	A	537	ALA	3.1
1	A	509	ARG	3.1
1	A	90	LEU	3.1
1	A	82	PHE	3.1
1	A	12	THR	3.1
1	A	487	ALA	3.1
1	A	81	VAL	3.1
1	A	429	LYS	3.1
1	A	187	ARG	3.1
1	A	226	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	315	THR	3.1
1	A	287	ALA	3.1
1	A	519	ILE	3.0
1	A	498	LYS	3.0
1	A	245	TRP	3.0
1	A	290	ARG	3.0
1	A	442	PHE	3.0
1	A	109	THR	3.0
1	A	37	GLU	3.0
1	A	262	GLU	3.0
1	A	168	SER	3.0
1	A	33	PRO	3.0
1	A	119	PRO	3.0
1	A	433	GLU	3.0
1	A	234	VAL	3.0
1	A	72	ARG	3.0
1	A	197	ALA	3.0
1	A	352	VAL	2.9
1	A	451	ASP	2.9
1	A	531	ARG	2.9
1	A	530	LEU	2.9
1	A	132	ARG	2.9
1	A	150	PRO	2.9
1	A	523	SER	2.9
1	A	385	GLY	2.9
1	A	285	PRO	2.9
1	A	438	PHE	2.9
1	A	124	SER	2.9
1	A	347	ILE	2.9
1	A	49	GLY	2.9
1	A	161	THR	2.8
1	A	80	PRO	2.8
1	A	251	HIS	2.8
1	A	98	ALA	2.8
1	A	484	LEU	2.8
1	A	241	GLY	2.8
1	A	271	SER	2.8
1	A	62	LEU	2.8
1	A	4	HIS	2.8
1	A	144	ILE	2.8
1	A	436	ARG	2.8
1	A	199	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	31	PRO	2.8
1	A	165	PRO	2.8
1	A	221	ASP	2.8
1	A	380	ASP	2.8
1	A	334	LEU	2.8
1	A	533	LEU	2.8
1	A	212	TYR	2.7
1	A	129	ALA	2.7
1	A	181	LEU	2.7
1	A	23	ILE	2.7
1	A	115	ASP	2.7
1	A	449	ARG	2.7
1	A	458	GLN	2.7
1	A	478	GLU	2.7
1	A	491	GLY	2.7
1	A	104	ALA	2.6
1	A	215	GLY	2.6
1	A	318	ALA	2.6
1	A	489	GLY	2.6
1	A	435	TYR	2.6
1	A	441	GLU	2.6
1	A	190	LYS	2.6
1	A	79	GLY	2.6
1	A	176	ALA	2.6
1	A	460	ASP	2.6
1	A	87	SER	2.6
1	A	102	LEU	2.6
1	A	138	LEU	2.6
1	A	54	ARG	2.6
1	A	232	MET	2.6
1	A	413	GLY	2.6
1	A	180	GLU	2.6
1	A	403	GLU	2.6
1	A	200	ALA	2.6
1	A	447	TYR	2.6
1	A	445	PRO	2.6
1	A	399	PHE	2.6
1	A	327	LEU	2.6
1	A	183	GLU	2.6
1	A	192	ILE	2.6
1	A	437	GLU	2.6
1	A	319	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	428	GLY	2.6
1	A	11	ALA	2.6
1	A	473	SER	2.6
1	A	520	TYR	2.5
1	A	406	ALA	2.5
1	A	254	LEU	2.5
1	A	353	SER	2.5
1	A	359	ARG	2.5
1	A	240	ALA	2.5
1	A	195	GLN	2.5
1	A	486	GLU	2.5
1	A	217	GLY	2.5
1	A	368	LEU	2.5
1	A	416	ALA	2.5
1	A	170	VAL	2.5
1	A	390	GLY	2.4
1	A	117	TYR	2.4
1	A	22	LEU	2.4
1	A	111	ILE	2.4
1	A	481	GLU	2.4
1	A	539	GLU	2.4
1	A	112	ALA	2.4
1	A	151	PRO	2.4
1	A	332	ASP	2.4
1	A	213	VAL	2.4
1	A	216	LEU	2.3
1	A	378	PHE	2.3
1	A	91	SER	2.3
1	A	371	VAL	2.3
1	A	136	GLY	2.3
1	A	386	SER	2.3
1	A	231	GLU	2.3
1	A	356	MET	2.3
1	A	130	TYR	2.3
1	A	411	LYS	2.3
1	A	459	LYS	2.3
1	A	94	ALA	2.3
1	A	146	PRO	2.3
1	A	8	GLY	2.3
1	A	174	ILE	2.3
1	A	233	GLY	2.3
1	A	414	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	415	ILE	2.3
1	A	41	SER	2.3
1	A	92	GLU	2.3
1	A	534	GLN	2.3
1	A	373	VAL	2.3
1	A	145	THR	2.3
1	A	206	TYR	2.2
1	A	344	GLU	2.2
1	A	127	ILE	2.2
1	A	367	LYS	2.2
1	A	382	LEU	2.2
1	A	162	ASN	2.2
1	A	444	GLU	2.2
1	A	427	THR	2.2
1	A	55	SER	2.2
1	A	114	GLY	2.2
1	A	358	ASP	2.2
1	A	525	LYS	2.2
1	A	329	VAL	2.2
1	A	32	ASP	2.2
1	A	207	ASP	2.2
1	A	141	GLY	2.2
1	A	163	GLY	2.2
1	A	47	HIS	2.1
1	A	208	TYR	2.1
1	A	424	THR	2.1
1	A	36	ARG	2.1
1	A	52	LEU	2.1
1	A	431	PRO	2.1
1	A	53	ASN	2.1
1	A	333	TYR	2.1
1	A	147	SER	2.1
1	A	317	SER	2.1
1	A	155	GLY	2.1
1	A	118	THR	2.1
1	A	306	THR	2.1
1	A	172	ALA	2.1
1	A	280	MET	2.0
1	A	501	THR	2.0
1	A	372	PRO	2.0
1	A	96	ALA	2.0
1	A	301	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	395	ALA	2.0
1	A	292	ILE	2.0
1	A	24	THR	2.0
1	A	402	ARG	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](#)

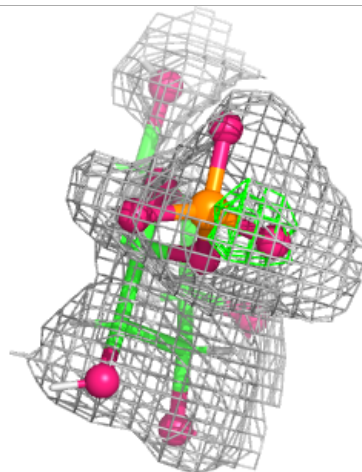
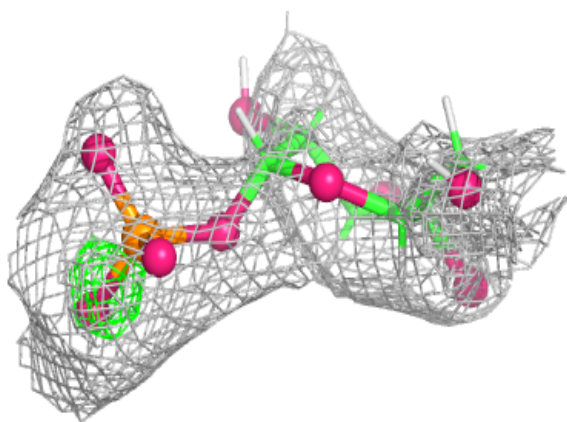
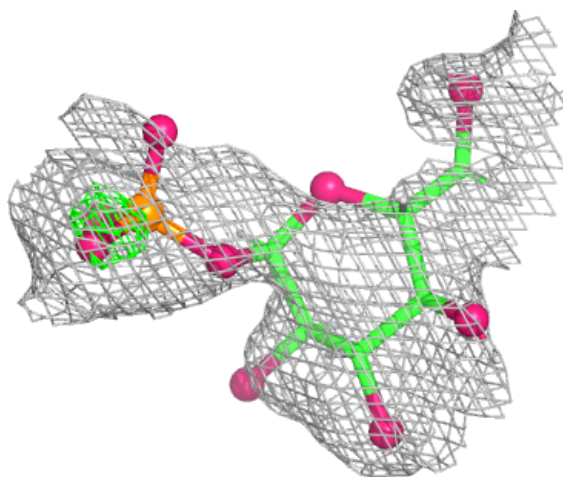
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	G1P	A	602	16/16	0.62	0.26	58,124,165,192	0
2	MG	A	601	1/1	0.96	0.08	32,32,32,32	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.

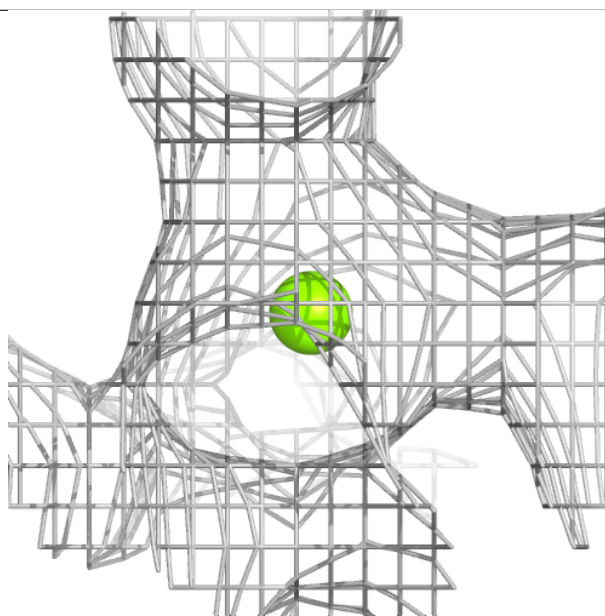
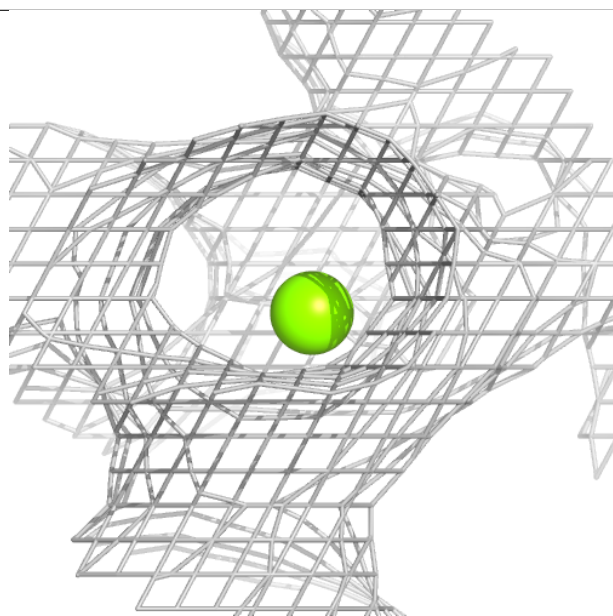
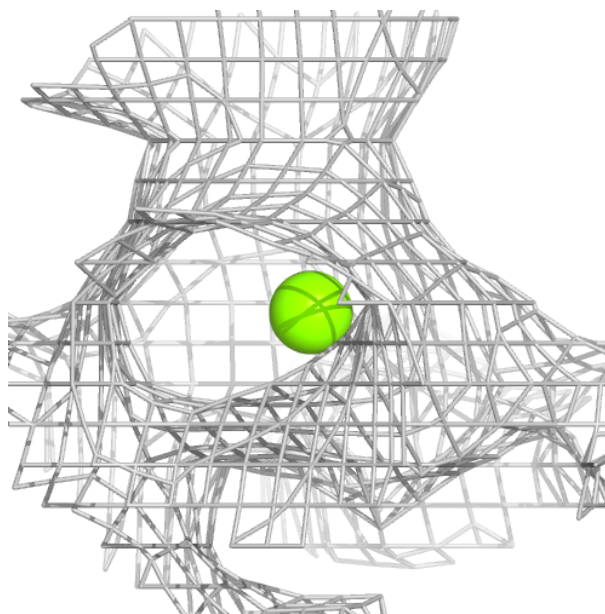
Electron density around G1P A 602:

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



Electron density around MG 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.