



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:45 AM BST

PDB ID : 2VF5
Title : Glucosamine-6-phosphate synthase in complex with glucosamine-6- phosphate
Authors : Mouilleron, S.; Golinelli-Pimpaneau, B.
Deposited on : 2007-10-30
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

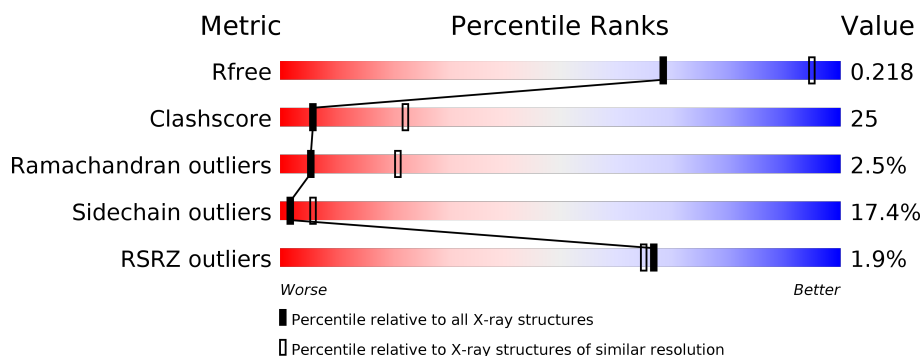
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	X	608	<div> <div> <div></div> <div>31%</div> <div>23%</div> <div>5%</div> <div>40%</div> </div> </div>

2 Entry composition [i](#)

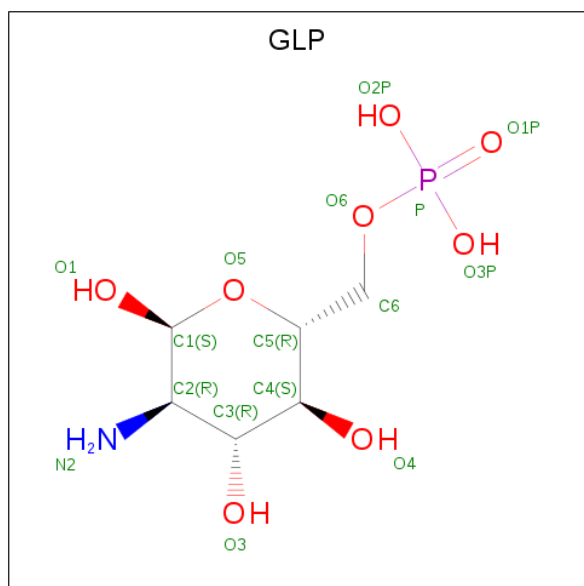
There are 3 unique types of molecules in this entry. The entry contains 2853 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINO-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	366	Total	C	N	O	S	0	2	0
			2825	1786	483	544	12			

- Molecule 2 is 2-amino-2-deoxy-6-O-phosphono-alpha-D-glucopyranose (three-letter code: GLP) (formula: C₆H₁₄NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	X	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	X	12	Total 12 O 12	0	0

- Molecule 1: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	144.76Å 144.76Å 171.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.90 14.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.00-2.90) 99.8 (14.95-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.242 0.180 , 0.218	Depositor DCC
R_{free} test set	767 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.012 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.002 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2853	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: GLP

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	X	0.95	3/2881 (0.1%)	1.08	10/3899 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	587	VAL	CB-CG1	-7.13	1.37	1.52
1	X	312	TYR	CE1-CZ	6.66	1.47	1.38
1	X	607	VAL	CB-CG2	5.34	1.64	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	518	VAL	CB-CA-C	-6.92	98.26	111.40
1	X	288	LEU	CA-CB-CG	6.71	130.72	115.30
1	X	463	ASP	CB-CG-OD2	6.59	124.23	118.30
1	X	511	ASP	CB-CG-OD2	6.36	124.03	118.30
1	X	286	ASP	CB-CG-OD2	6.15	123.83	118.30
1	X	513	ASP	CB-CG-OD2	5.50	123.25	118.30
1	X	402	THR	OG1-CB-CG2	-5.46	97.44	110.00
1	X	453	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	X	323	ASP	CB-CG-OD2	5.20	122.98	118.30
1	X	311	ARG	NE-CZ-NH2	-5.16	117.72	120.30

There are no chirality outliers.

There are no planarity outliers.

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	X	2825	0	2853	144	0
2	X	16	0	11	0	0
3	X	12	0	0	0	0
All	All	2853	0	2864	144	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 25.

All (144) 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:X:577:THR:HG22	1:X:581:GLN:HE21	1.08	1.07
1:X:351:GLU:OE2	1:X:379:SER:HB2	1.60	1.00
1:X:443:ARG:HD2	1:X:567:VAL:HG12	1.43	1.00
1:X:466:HIS:HB3	1:X:514:MET:HG3	1.48	0.95
1:X:577:THR:HG22	1:X:581:GLN:NE2	1.88	0.88
1:X:443:ARG:CD	1:X:567:VAL:HG12	2.03	0.88
1:X:310:SER:CB	1:X:412:LEU:HD22	2.09	0.81
1:X:327:ALA:HB2	1:X:355:THR:HG22	1.62	0.81
1:X:412:LEU:O	1:X:416:VAL:HG23	1.86	0.75
1:X:278:LEU:HD12	1:X:418:LYS:HB2	1.69	0.74
1:X:377:PRO:HA	1:X:390:MET:CE	2.19	0.73
1:X:299:ALA:HA	1:X:355:THR:CG2	2.18	0.73
1:X:430:GLU:O	1:X:434:VAL:HG23	1.89	0.73
1:X:572:ALA:HB3	1:X:573:PRO:HD3	1.69	0.72
1:X:450:GLN:HB3	1:X:453:ARG:HH21	1.57	0.70
1:X:277:ASP:OD1	1:X:279:SER:OG	2.11	0.69
1:X:299:ALA:HA	1:X:355:THR:HG21	1.72	0.69
1:X:295:ILE:CG2	1:X:344:ILE:HD12	2.23	0.69
1:X:532:ASN:O	1:X:535:GLU:HB2	1.93	0.68
1:X:578:VAL:N	1:X:579:PRO:HD2	2.08	0.68
1:X:353:ALA:HB2	1:X:606:THR:O	1.92	0.68
1:X:466:HIS:CB	1:X:514:MET:HG3	2.24	0.66
1:X:577:THR:O	1:X:581:GLN:HG3	1.95	0.66
1:X:455:GLU:HG3	1:X:586:HIS:ND1	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:257:TYR:CD2	1:X:448:LEU:HD22	2.31	0.65
1:X:433:ILE:HG22	1:X:437:LEU:HD12	1.79	0.65
1:X:461:PHE:CE2	1:X:517:ILE:HD11	2.33	0.64
1:X:311:ARG:HG3	1:X:322:CYS:HB3	1.80	0.63
1:X:377:PRO:CA	1:X:390:MET:HE1	2.28	0.63
1:X:567:VAL:HG21	1:X:575:PHE:CD2	2.34	0.63
1:X:344:ILE:HA	1:X:371:LEU:O	1.98	0.62
1:X:377:PRO:HA	1:X:390:MET:HE1	1.80	0.62
1:X:263:ILE:HG21	1:X:440:LEU:HD23	1.80	0.62
1:X:380:SER:O	1:X:384:GLU:HG3	1.98	0.61
1:X:572:ALA:HB3	1:X:573:PRO:CD	2.29	0.61
1:X:259:GLN:N	1:X:260:PRO:HD2	2.15	0.61
1:X:310:SER:HB2	1:X:412:LEU:HD22	1.82	0.61
1:X:374:CYS:O	1:X:390:MET:HA	2.01	0.61
1:X:418:LYS:HG3	1:X:422:LEU:HD12	1.84	0.60
1:X:443:ARG:HD2	1:X:567:VAL:CG1	2.26	0.60
1:X:532:ASN:HA	1:X:535:GLU:OE2	2.02	0.60
1:X:252:MET:O	1:X:256:ILE:HG13	2.04	0.58
1:X:476:TYR:HB3	1:X:477:PRO:HD3	1.85	0.58
1:X:379:SER:O	1:X:380:SER:C	2.41	0.57
1:X:278:LEU:O	1:X:281:LEU:HB2	2.05	0.57
1:X:297:ILE:HB	1:X:324:VAL:HG12	1.85	0.56
1:X:302:THR:O	1:X:305:ASN:HB2	2.05	0.56
1:X:309:VAL:HG22	1:X:477:PRO:HB2	1.87	0.56
1:X:313:TRP:CE3	1:X:413:LEU:HD13	2.41	0.56
1:X:341:SER:HB3	1:X:367:TYR:CE2	2.40	0.56
1:X:481:GLU:OE2	1:X:485:LYS:NZ	2.38	0.56
1:X:278:LEU:CD1	1:X:418:LYS:HB2	2.36	0.55
1:X:414:MET:O	1:X:417:ALA:N	2.38	0.55
1:X:261:ASN:O	1:X:264:LYS:N	2.39	0.55
1:X:327:ALA:HB2	1:X:355:THR:CG2	2.36	0.55
1:X:362:SER:HB2	1:X:367:TYR:CD1	2.41	0.54
1:X:347:SER:O	1:X:374:CYS:HA	2.07	0.54
1:X:278:LEU:HD12	1:X:418:LYS:CB	2.37	0.54
1:X:287:GLU:O	1:X:291:LYS:HG3	2.07	0.54
1:X:400:ALA:HB1	1:X:485:LYS:HE3	1.90	0.54
1:X:399:VAL:HB	1:X:598:PRO:HD2	1.90	0.54
1:X:401[A]:SER:HB2	1:X:404:ALA:HB3	1.88	0.53
1:X:413:LEU:HG	1:X:433:ILE:HG23	1.90	0.53
1:X:355:THR:O	1:X:358:GLY:N	2.41	0.53
1:X:415:LEU:HG	1:X:419:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:379:SER:H	1:X:382:VAL:HB	1.74	0.53
1:X:250:HIS:HD2	1:X:585:TYR:OH	1.91	0.52
1:X:401[B]:SER:HB3	1:X:404:ALA:HB3	1.91	0.52
1:X:299:ALA:HA	1:X:355:THR:HG22	1.89	0.52
1:X:472:ARG:HG2	1:X:473:GLY:N	2.24	0.52
1:X:295:ILE:HG21	1:X:344:ILE:HD12	1.93	0.51
1:X:310:SER:OG	1:X:412:LEU:HD22	2.10	0.51
1:X:256:ILE:HG12	1:X:402:THR:HG21	1.91	0.51
1:X:287:GLU:HA	1:X:290:SER:OG	2.10	0.51
1:X:453:ARG:HH22	1:X:564:MET:HE2	1.74	0.51
1:X:448:LEU:O	1:X:451:ASP:HB2	2.11	0.50
1:X:345:THR:OG1	1:X:381:LEU:HD22	2.11	0.50
1:X:446:GLN:O	1:X:449:SER:OG	2.29	0.50
1:X:447:MET:HG2	1:X:578:VAL:HB	1.92	0.50
1:X:421:ARG:C	1:X:423:LYS:H	2.15	0.50
1:X:374:CYS:SG	1:X:375:ASN:N	2.84	0.49
1:X:486:LEU:HD12	1:X:490:SER:OG	2.12	0.49
1:X:445:GLU:HA	1:X:448:LEU:HD12	1.94	0.49
1:X:257:TYR:CE2	1:X:448:LEU:HD22	2.47	0.49
1:X:421:ARG:HB3	1:X:421:ARG:NH1	2.27	0.49
1:X:421:ARG:HB3	1:X:421:ARG:CZ	2.43	0.48
1:X:245:LYS:HB2	1:X:245:LYS:HE2	1.48	0.48
1:X:443:ARG:NH1	1:X:446:GLN:HE22	2.12	0.48
1:X:285:ALA:O	1:X:288:LEU:HB3	2.14	0.48
1:X:276:VAL:HG21	1:X:417:ALA:CB	2.43	0.47
1:X:391:THR:HG22	1:X:411:VAL:HG23	1.96	0.47
1:X:351:GLU:OE2	1:X:379:SER:CB	2.49	0.47
1:X:520:ALA:N	1:X:521:PRO:CD	2.78	0.47
1:X:400:ALA:HB1	1:X:485:LYS:CE	2.43	0.47
1:X:276:VAL:HG21	1:X:417:ALA:HB3	1.97	0.47
1:X:379:SER:O	1:X:382:VAL:N	2.41	0.47
1:X:377:PRO:N	1:X:390:MET:HE1	2.30	0.47
1:X:578:VAL:N	1:X:579:PRO:CD	2.77	0.47
1:X:377:PRO:CA	1:X:390:MET:CE	2.90	0.46
1:X:449:SER:C	1:X:451:ASP:H	2.18	0.46
1:X:297:ILE:HA	1:X:344:ILE:O	2.15	0.46
1:X:311:ARG:HD2	1:X:322:CYS:O	2.15	0.46
1:X:261:ASN:O	1:X:262:ALA:C	2.53	0.46
1:X:411:VAL:O	1:X:412:LEU:C	2.50	0.46
1:X:452:LYS:HB3	1:X:452:LYS:HE2	1.88	0.46
1:X:506:PRO:O	1:X:509:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:562:ILE:HD12	1:X:562:ILE:N	2.32	0.45
1:X:455:GLU:HG3	1:X:586:HIS:CE1	2.51	0.45
1:X:305:ASN:O	1:X:308:MET:HB2	2.17	0.44
1:X:391:THR:HG22	1:X:411:VAL:CG2	2.48	0.44
1:X:434:VAL:O	1:X:437:LEU:N	2.50	0.44
1:X:341:SER:O	1:X:368:LEU:HB2	2.17	0.44
1:X:298:LEU:HD11	1:X:330:PHE:CD2	2.53	0.44
1:X:510:ILE:N	1:X:510:ILE:HD13	2.32	0.44
1:X:312:TYR:CE1	1:X:473:GLY:HA2	2.53	0.44
1:X:372:ALA:HB2	1:X:385:SER:OG	2.18	0.44
1:X:501:GLU:O	1:X:502:LEU:C	2.56	0.44
1:X:390:MET:HE3	1:X:390:MET:HB3	1.86	0.43
1:X:304:TYR:CE1	1:X:326:ILE:HG12	2.54	0.43
1:X:413:LEU:HD12	1:X:413:LEU:HA	1.65	0.43
1:X:263:ILE:HG21	1:X:440:LEU:CD2	2.48	0.43
1:X:443:ARG:HD3	1:X:567:VAL:HG12	1.95	0.43
1:X:260:PRO:HD3	1:X:444:ILE:CG2	2.49	0.43
1:X:507:LEU:HA	1:X:507:LEU:HD12	1.50	0.43
1:X:350:GLY:HA2	1:X:381:LEU:HD12	2.00	0.43
1:X:480:LEU:HD23	1:X:496:ALA:HB3	2.01	0.42
1:X:362:SER:O	1:X:363:LYS:C	2.58	0.42
1:X:473:GLY:O	1:X:475:GLN:N	2.52	0.42
1:X:379:SER:O	1:X:381:LEU:N	2.53	0.42
1:X:440:LEU:HD12	1:X:571:ILE:HB	2.02	0.42
1:X:284:ASN:HB3	1:X:285:ALA:H	1.70	0.42
1:X:266:THR:OG1	1:X:391:THR:O	2.32	0.42
1:X:356:LEU:HD11	1:X:380:SER:HB3	2.02	0.41
1:X:543:LEU:HA	1:X:543:LEU:HD23	1.88	0.41
1:X:448:LEU:O	1:X:451:ASP:CB	2.69	0.41
1:X:440:LEU:HD12	1:X:571:ILE:HD12	2.02	0.41
1:X:327:ALA:HB1	1:X:354:ASP:O	2.20	0.41
1:X:305:ASN:O	1:X:309:VAL:HG23	2.21	0.40
1:X:512:ALA:HA	1:X:540:GLY:O	2.21	0.40
1:X:476:TYR:CB	1:X:477:PRO:HD3	2.50	0.40
1:X:475:GLN:HG3	1:X:520:ALA:HB3	2.03	0.40
1:X:390:MET:HG2	1:X:390:MET:H	1.73	0.40
1:X:518:VAL:HG23	1:X:545:VAL:HG22	2.04	0.40
1:X:406:THR:HG22	1:X:574:ILE:HG23	2.03	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	X	366/608 (60%)	308 (84%)	49 (13%)	9 (2%)	5	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	284	ASN
1	X	380	SER
1	X	337	VAL
1	X	390	MET
1	X	422	LEU
1	X	448	LEU
1	X	607	VAL
1	X	280	GLU
1	X	314	PHE

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	X	307/500 (61%)	254 (83%)	53 (17%)	2	6

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	244	ASP
1	X	245	LYS

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Mol	Chain	Res	Type
1	X	264	LYS
1	X	266	THR
1	X	271	ILE
1	X	280	GLU
1	X	287	GLU
1	X	288	LEU
1	X	293	GLU
1	X	297	ILE
1	X	298	LEU
1	X	311	ARG
1	X	324	VAL
1	X	326	ILE
1	X	334	LYS
1	X	335	SER
1	X	337	VAL
1	X	341	SER
1	X	348	GLN
1	X	354	ASP
1	X	364	GLU
1	X	368	LEU
1	X	374	CYS
1	X	376	VAL
1	X	379	SER
1	X	380	SER
1	X	391	THR
1	X	402	THR
1	X	406	THR
1	X	419	LEU
1	X	421	ARG
1	X	426	ASP
1	X	438	GLN
1	X	440	LEU
1	X	444	ILE
1	X	450	GLN
1	X	452	LYS
1	X	453	ARG
1	X	497	TYR
1	X	510	ILE
1	X	518	VAL
1	X	524	GLU
1	X	526	LEU
1	X	533	ILE

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Mol	Chain	Res	Type
1	X	535	GLU
1	X	537	ARG
1	X	543	LEU
1	X	549	GLN
1	X	554	VAL
1	X	570	VAL
1	X	573	PRO
1	X	591	LYS
1	X	603	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	250	HIS
1	X	259	GLN
1	X	348	GLN
1	X	446	GLN
1	X	581	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	GLP	X	609	-	16,16,16	1.51	3 (18%)	23,24,24	3.22	11 (47%)

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	GLP	X	609	-	-	1/6/26/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	609	GLP	C1-C2	-2.87	1.49	1.52
2	X	609	GLP	P-O1P	2.79	1.59	1.50
2	X	609	GLP	C2-N2	-2.72	1.43	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	609	GLP	C1-O5-C5	8.67	130.02	113.66
2	X	609	GLP	O3-C3-C4	5.24	122.47	110.35
2	X	609	GLP	C1-C2-C3	5.17	117.40	110.60
2	X	609	GLP	C4-C3-C2	5.13	119.88	111.07
2	X	609	GLP	O5-C1-C2	4.82	115.13	109.51
2	X	609	GLP	O5-C5-C4	4.09	117.12	109.69
2	X	609	GLP	O4-C4-C3	3.10	117.51	110.35
2	X	609	GLP	C3-C2-N2	2.80	116.80	111.05
2	X	609	GLP	C3-C4-C5	2.39	114.51	110.24
2	X	609	GLP	O2P-P-O6	-2.20	100.87	106.73
2	X	609	GLP	O3P-P-O2P	2.15	115.84	107.64

There are no chirality outliers.

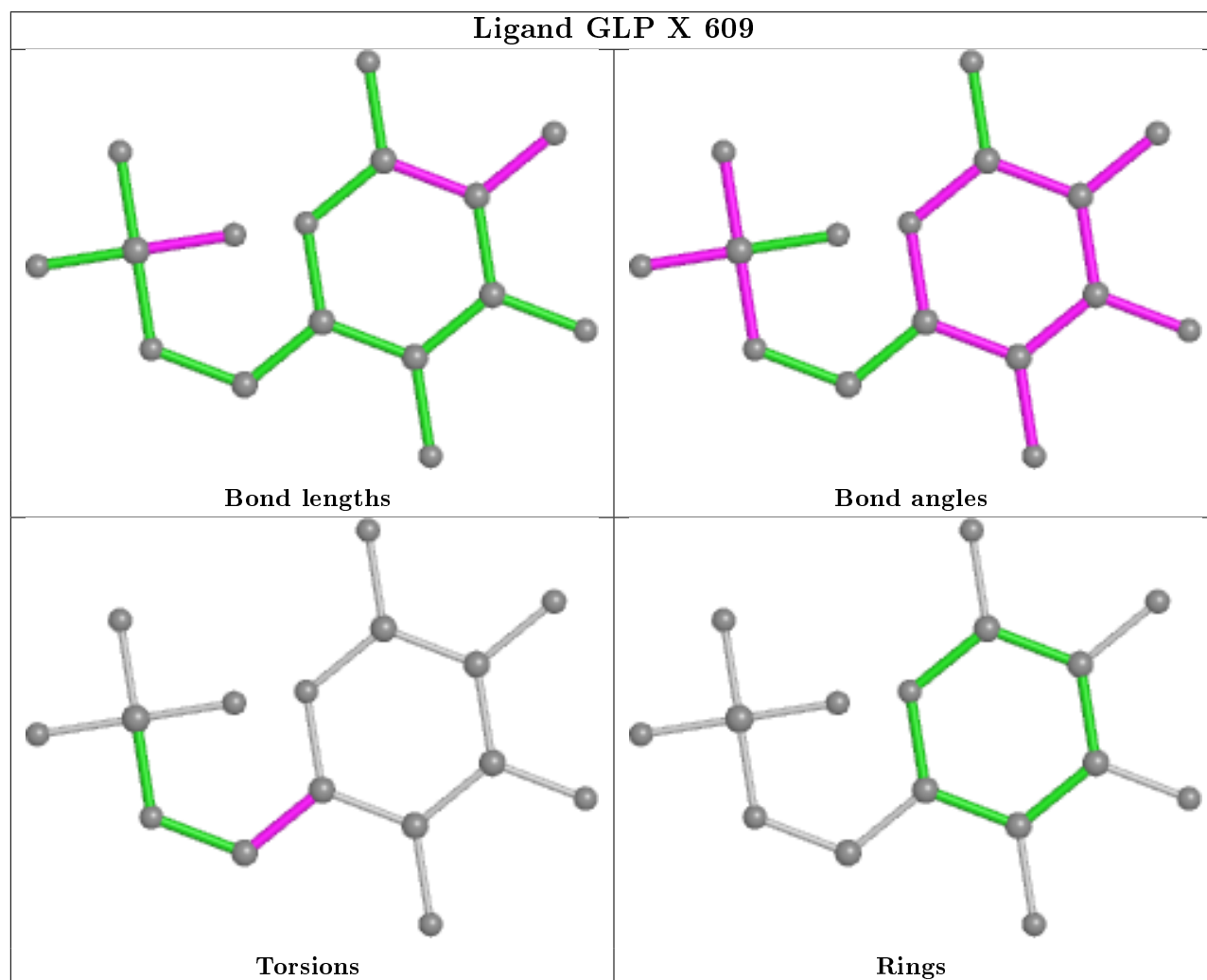
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	609	GLP	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 ⓘ

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	X	366/608 (60%)	-0.55	7 (1%) 66 65	18, 27, 33, 44	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	282	GLY	4.0
1	X	269	GLY	3.5
1	X	243	GLY	3.5
1	X	283	PRO	2.7
1	X	608	GLU	2.7
1	X	244	ASP	2.2
1	X	425	LEU	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 ⓘ

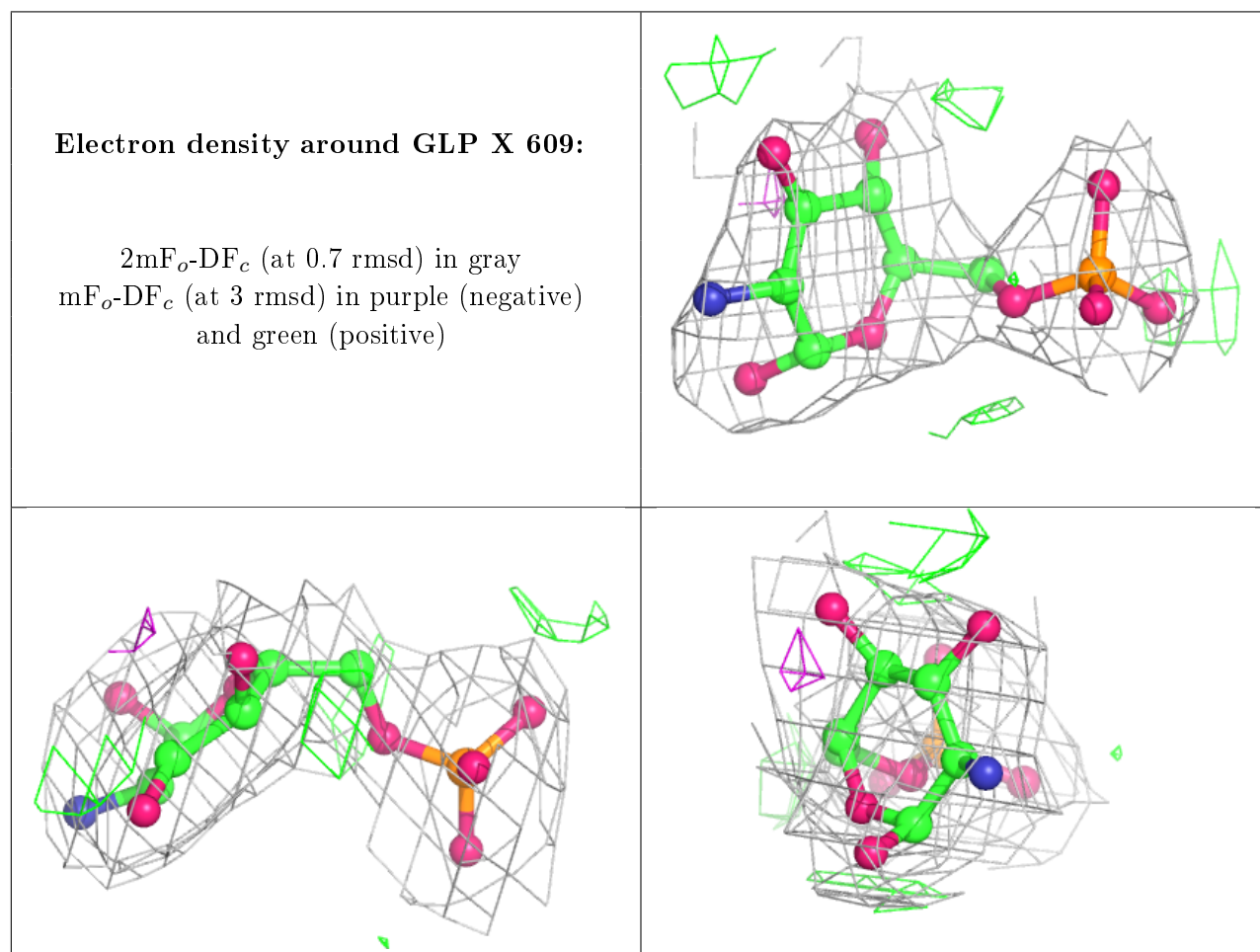
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	GLP	X	609	16/16	0.98	0.08	17,26,28,30	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.