



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2021 – 02:10 PM JST

PDB ID : 7E78
Title : the structure of cytosolic TaPGI with substrate
Authors : Gao, F.; Liu, C.M.
Deposited on : 2021-02-25
Resolution : 2.21 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 : 2.22
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) : 2.22

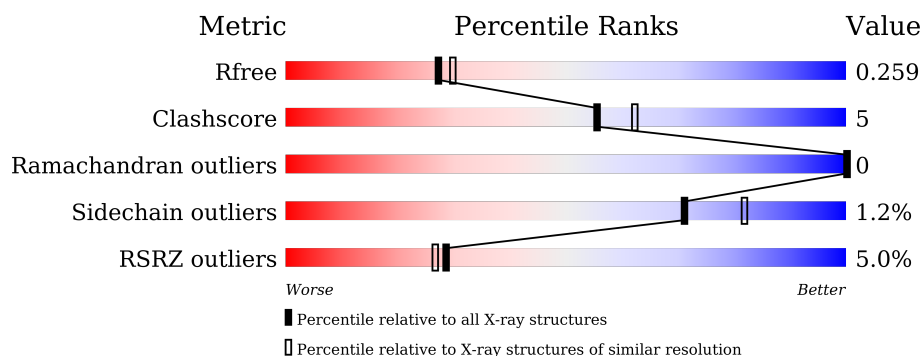
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	567	<div> <div>3%</div> <div>85% 13% ..</div> </div>
1	B	567	<div> <div>7%</div> <div>87% 12% .</div> </div>
1	C	567	<div> <div>4%</div> <div>86% 13% .</div> </div>
1	D	567	<div> <div>6%</div> <div>87% 11% .</div> </div>

2 Entry composition [i](#)

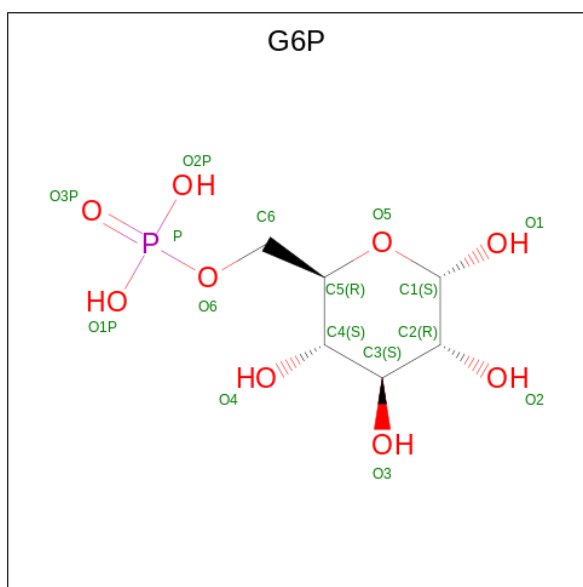
There are 3 unique types of molecules in this entry. The entry contains 17701 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4362	2791	745	815	11			
1	C	562	Total	C	N	O	S	0	0	0
			4360	2790	744	815	11			
1	B	562	Total	C	N	O	S	0	0	0
			4362	2791	745	815	11			
1	D	561	Total	C	N	O	S	0	0	0
			4353	2785	743	814	11			

- Molecule 2 is 6-O-phosphono-alpha-D-glucopyranose (three-letter code: G6P) (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		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		

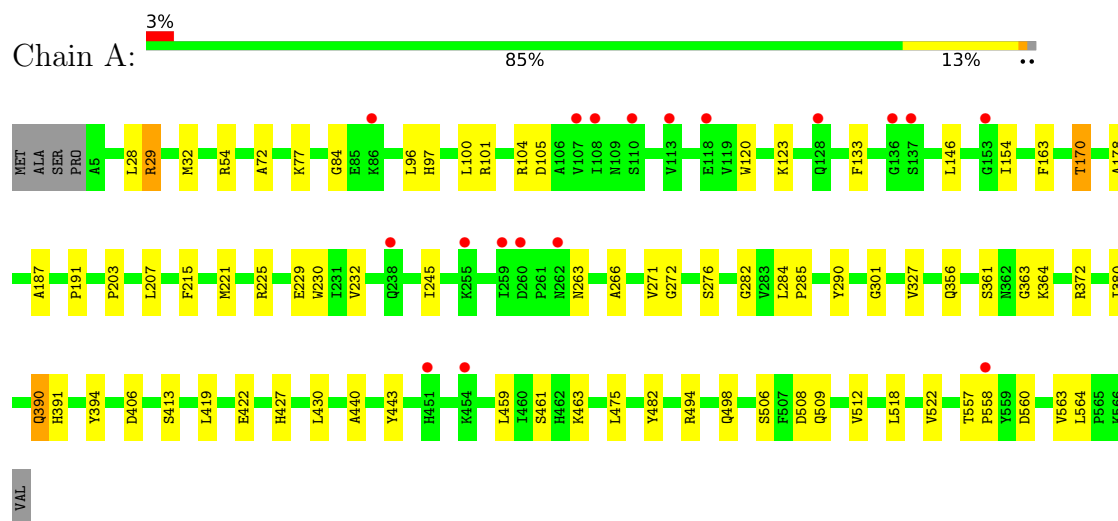
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total 58	O 58	0	0
3	C	56	Total 56	O 56	0	0
3	B	62	Total 62	O 62	0	0
3	D	56	Total 56	O 56	0	0

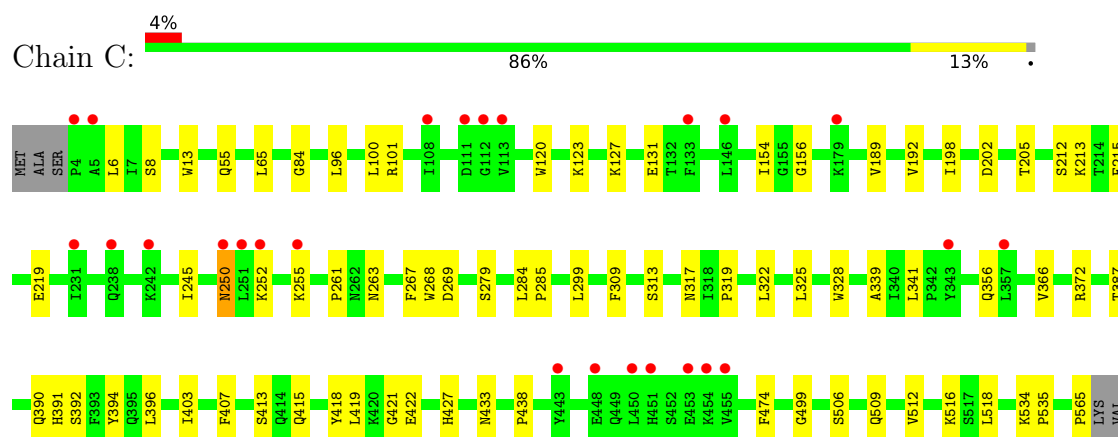
3 Residue-property plots

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.

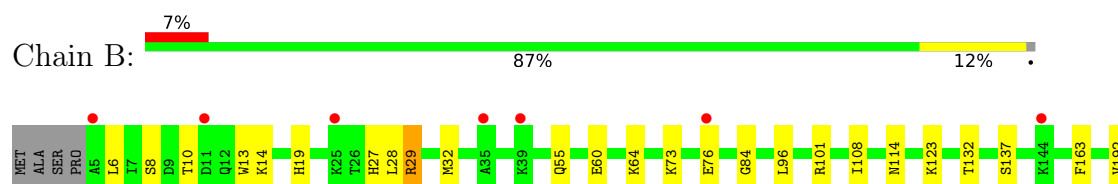
- Molecule 1: Glucose-6-phosphate isomerase

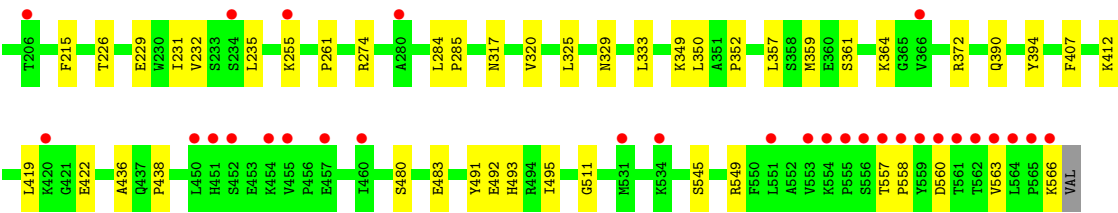


- Molecule 1: Glucose-6-phosphate isomerase

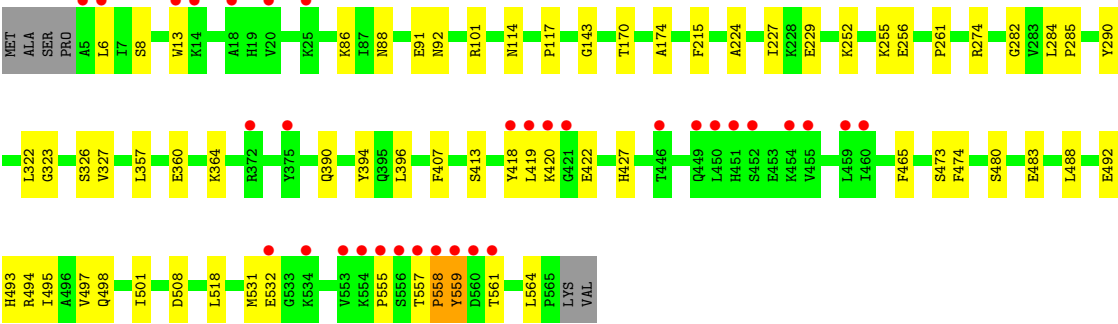
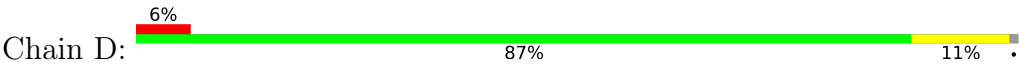


- Molecule 1: Glucose-6-phosphate isomerase





● Molecule 1: Glucose-6-phosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	243.62Å 74.45Å 125.58Å 90.00° 94.12° 90.00°	Depositor
Resolution (Å)	35.68 – 2.21 35.68 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.1 (35.68-2.21) 99.1 (35.68-2.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.233 , 0.258 0.234 , 0.259	Depositor DCC
R_{free} test set	1586 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17701	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: G6P

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	0.43	0/4464	0.59	0/6060
1	B	0.39	0/4464	0.57	0/6060
1	C	0.40	0/4463	0.57	0/6060
1	D	0.45	3/4455 (0.1%)	0.59	1/6049 (0.0%)
All	All	0.42	3/17846 (0.0%)	0.58	1/24229 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	559	TYR	C-N	7.85	1.52	1.34
1	D	143	GLY	C-N	-6.09	1.20	1.34
1	D	558	PRO	C-N	-5.72	1.20	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	558	PRO	O-C-N	-5.26	114.29	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	ALA	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	4362	0	4367	54	0
1	B	4362	0	4367	46	5
1	C	4360	0	4362	56	0
1	D	4353	0	4353	40	7
2	A	16	0	11	0	0
2	C	16	0	10	5	0
3	A	58	0	0	3	1
3	B	62	0	0	4	0
3	C	56	0	0	1	0
3	D	56	0	0	0	0
All	All	17701	0	17470	177	8

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 5.

All (177) 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:84:GLY:HA2	1:A:96:LEU:HD21	1.58	0.85
1:C:509:GLN:O	1:C:509:GLN:HG2	1.78	0.83
1:C:245:ILE:HG22	1:C:263:ASN:HB3	1.60	0.82
1:D:322:LEU:HD11	1:D:474:PHE:HZ	1.50	0.76
1:D:558:PRO:HB2	1:D:561:THR:HB	1.66	0.76
1:A:391:HIS:NE2	1:C:219:GLU:OE2	2.18	0.75
1:A:356:GLN:HG3	1:C:392:SER:HA	1.72	0.71
1:B:557:THR:HG22	1:B:558:PRO:O	1.91	0.71
1:A:406:ASP:OD2	1:A:494:ARG:NH1	2.17	0.70
1:C:212:SER:OG	2:C:601:G6P:O2P	2.08	0.70
1:B:132:THR:HG23	1:B:137:SER:HB2	1.75	0.67
1:D:255:LYS:HB2	1:D:261:PRO:HG3	1.76	0.66
1:A:97:HIS:HA	1:A:100:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:GLY:H	2:C:601:G6P:H1	1.59	0.66
1:A:170:THR:HG21	1:C:192:VAL:HG13	1.79	0.63
1:C:250:ASN:C	1:C:250:ASN:HD22	2.00	0.62
1:B:55:GLN:HG3	1:B:325:LEU:HD22	1.81	0.61
1:B:226:THR:HA	1:D:419:LEU:HD11	1.84	0.60
1:D:493:HIS:O	1:D:497:VAL:HG23	2.01	0.60
1:A:557:THR:HG21	1:A:563:VAL:CG1	2.32	0.59
1:C:534:LYS:HG2	1:C:535:PRO:HD2	1.85	0.59
1:C:245:ILE:HD12	1:C:284:LEU:HD21	1.86	0.58
1:B:84:GLY:HA2	1:B:96:LEU:HD21	1.86	0.57
1:D:357:LEU:HD21	1:D:492:GLU:HA	1.86	0.57
1:B:560:ASP:HA	1:D:418:TYR:HE2	1.68	0.57
1:B:27:HIS:ND1	1:B:29:ARG:HG2	2.19	0.57
1:A:100:LEU:HD21	1:A:271:VAL:HG22	1.87	0.56
1:B:192:VAL:HG13	1:D:170:THR:HG21	1.87	0.55
1:D:558:PRO:CB	1:D:561:THR:HB	2.35	0.55
1:A:146:LEU:HD13	1:A:207:LEU:HB2	1.87	0.55
1:A:154:ILE:HD12	1:C:391:HIS:CD2	2.42	0.54
1:C:356:GLN:HE22	2:C:601:G6P:H1	1.71	0.54
1:D:364:LYS:HE2	1:D:508:ASP:OD1	2.08	0.54
1:A:245:ILE:HG22	1:A:263:ASN:HB3	1.89	0.53
1:C:55:GLN:HG3	1:C:325:LEU:HD13	1.89	0.53
1:A:419:LEU:HB2	1:A:422:GLU:CG	2.39	0.53
1:D:229:GLU:HG3	1:D:564:LEU:HD11	1.91	0.53
1:B:284:LEU:HB3	1:B:285:PRO:HD3	1.91	0.53
1:C:390:GLN:OE1	1:C:433:ASN:HB3	2.09	0.52
1:C:8:SER:HA	1:C:13:TRP:CG	2.44	0.52
1:A:440:ALA:HB2	1:C:518:LEU:HD22	1.90	0.52
1:C:255:LYS:HE2	1:C:261:PRO:HB3	1.92	0.52
1:D:8:SER:HA	1:D:13:TRP:CG	2.45	0.52
1:B:560:ASP:O	1:B:560:ASP:OD1	2.27	0.52
1:A:557:THR:HG23	1:A:558:PRO:HD2	1.92	0.52
1:C:202:ASP:HB3	1:C:205:THR:OG1	2.10	0.52
1:A:327:VAL:HG23	1:A:498:GLN:HG2	1.92	0.51
1:C:198:ILE:HD11	1:C:565:PRO:HG2	1.93	0.51
1:B:255:LYS:HB2	1:B:261:PRO:HG3	1.92	0.51
1:A:364:LYS:HE3	1:A:508:ASP:OD1	2.11	0.51
1:B:73:LYS:HD2	1:B:76:GLU:OE2	2.11	0.50
1:C:387:THR:O	1:C:390:GLN:HB2	2.11	0.50
1:D:558:PRO:O	1:D:559:TYR:C	2.49	0.50
1:C:313:SER:O	1:C:317:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLY:O	1:A:276:SER:HB3	2.12	0.49
1:D:480:SER:OG	1:D:483:GLU:OE1	2.27	0.49
1:A:518:LEU:O	1:A:522:VAL:HG23	2.13	0.49
1:A:390:GLN:HA	1:A:394:TYR:CG	2.47	0.49
1:B:10:THR:O	1:B:14:LYS:HG3	2.13	0.49
1:A:557:THR:CG2	1:A:558:PRO:HD2	2.42	0.49
1:B:480:SER:OG	1:B:483:GLU:OE1	2.21	0.49
1:B:329:ASN:OD1	1:B:333:LEU:HD12	2.12	0.48
1:B:419:LEU:HB2	1:B:422:GLU:HG3	1.95	0.48
1:B:349:LYS:C	1:B:352:PRO:HD2	2.34	0.48
1:B:412:LYS:NZ	3:B:605:HOH:O	2.46	0.48
1:A:72:ALA:O	1:A:77:LYS:NZ	2.36	0.47
1:D:224:ALA:HA	1:D:227:ILE:HG22	1.97	0.47
1:C:123:LYS:HE2	1:C:299:LEU:HD13	1.95	0.47
1:C:267:PHE:HA	1:C:268:TRP:CE3	2.49	0.47
1:A:221:MET:O	1:A:225:ARG:HG3	2.15	0.47
1:C:284:LEU:HB3	1:C:285:PRO:HD3	1.96	0.47
1:B:357:LEU:HD21	1:B:492:GLU:HA	1.97	0.46
1:A:419:LEU:HB2	1:A:422:GLU:HG2	1.98	0.46
1:A:459:LEU:HD13	1:A:463:LYS:HE3	1.97	0.46
1:B:563:VAL:HG23	1:D:418:TYR:H	1.81	0.46
1:A:419:LEU:HB2	1:A:422:GLU:HG3	1.97	0.46
1:B:419:LEU:HB2	1:B:422:GLU:CG	2.45	0.46
1:D:274:ARG:HD3	1:D:360:GLU:OE1	2.16	0.46
1:A:557:THR:CG2	1:A:558:PRO:CD	2.94	0.46
1:D:323:GLY:O	1:D:327:VAL:HG23	2.16	0.46
3:A:748:HOH:O	1:C:421:GLY:HA2	2.16	0.46
1:B:491:TYR:O	1:B:495:ILE:HG12	2.15	0.46
1:A:104:ARG:N	3:A:701:HOH:O	2.20	0.45
1:A:203:PRO:HG3	1:A:230:TRP:CE2	2.52	0.45
1:A:509:GLN:O	1:A:512:VAL:HG12	2.15	0.45
1:C:127:LYS:NZ	1:C:131:GLU:OE2	2.46	0.45
1:C:213:LYS:HE3	1:C:269:ASP:HA	1.97	0.45
1:A:191:PRO:HB2	1:C:415:GLN:O	2.17	0.45
1:A:560:ASP:HA	1:C:418:TYR:HE2	1.80	0.45
1:C:509:GLN:O	1:C:509:GLN:CG	2.53	0.45
1:B:317:ASN:HB3	1:B:320:VAL:HB	1.98	0.45
1:A:29:ARG:NH1	1:A:443:TYR:O	2.50	0.45
1:B:8:SER:HA	1:B:13:TRP:CD2	2.52	0.45
1:B:545:SER:O	1:B:549:ARG:HG3	2.17	0.45
1:C:250:ASN:HD21	1:C:252:LYS:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:GLN:HG3	1:A:394:TYR:CE2	2.52	0.45
1:C:419:LEU:HB2	1:C:422:GLU:CG	2.47	0.45
1:B:123:LYS:HD2	3:B:636:HOH:O	2.16	0.45
1:C:213:LYS:H	2:C:601:G6P:P	2.40	0.44
1:C:65:LEU:HD11	1:C:328:TRP:HB2	1.99	0.44
1:C:499:GLY:HA3	1:C:506:SER:OG	2.17	0.44
1:D:88:ASN:ND2	1:D:91:GLU:HB2	2.32	0.44
1:A:361:SER:O	1:A:506:SER:HA	2.18	0.44
1:D:531:MET:SD	1:D:559:TYR:HB2	2.57	0.44
1:D:174:ALA:HB1	1:D:290:TYR:CD1	2.53	0.44
1:D:284:LEU:HB3	1:D:285:PRO:HD3	1.99	0.44
1:B:231:ILE:HG23	1:B:235:LEU:HD12	2.00	0.44
1:B:28:LEU:O	1:B:32:MET:HG2	2.18	0.44
1:D:86:LYS:HD3	1:D:92:ASN:OD1	2.18	0.44
1:D:413:SER:HB2	1:D:427:HIS:CG	2.53	0.43
1:C:212:SER:HG	2:C:601:G6P:P	2.38	0.43
1:C:84:GLY:HA2	1:C:96:LEU:HD21	2.00	0.43
1:B:361:SER:O	1:B:364:LYS:NZ	2.49	0.43
1:A:120:TRP:HA	1:A:123:LYS:HB2	2.00	0.43
1:C:512:VAL:HG22	1:C:516:LYS:HE3	2.01	0.43
1:B:84:GLY:HA2	3:B:633:HOH:O	2.18	0.43
1:B:493:HIS:ND1	3:B:603:HOH:O	2.37	0.43
1:C:309:PHE:CD1	1:C:319:PRO:HB2	2.54	0.43
1:D:390:GLN:HA	1:D:394:TYR:CG	2.53	0.43
1:C:250:ASN:C	1:C:250:ASN:ND2	2.70	0.43
1:B:436:ALA:HB1	1:D:518:LEU:HB3	2.00	0.43
1:B:560:ASP:HA	1:D:418:TYR:CE2	2.50	0.43
1:D:494:ARG:O	1:D:498:GLN:HG3	2.19	0.43
1:C:322:LEU:HD11	1:C:474:PHE:HZ	1.84	0.43
1:A:229:GLU:HA	1:A:232:VAL:HG22	2.00	0.42
1:A:391:HIS:CD2	1:C:154:ILE:HD12	2.54	0.42
1:D:555:PRO:C	1:D:557:THR:N	2.70	0.42
1:B:19:HIS:HB2	1:B:64:LYS:HE2	2.00	0.42
1:A:380:ILE:HG12	1:C:403:ILE:HD11	2.01	0.42
1:B:359:MET:HG2	1:D:396:LEU:HD13	2.01	0.42
1:D:407:PHE:O	1:D:473:SER:HA	2.19	0.42
1:A:301:GLY:HA3	1:A:482:TYR:O	2.20	0.42
1:C:100:LEU:HD13	1:C:279:SER:HB3	2.00	0.42
1:B:390:GLN:HA	1:B:394:TYR:CG	2.54	0.42
1:A:54:ARG:HB2	3:A:731:HOH:O	2.19	0.42
1:C:269:ASP:OD1	1:C:269:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLY:HA3	1:C:396:LEU:HB2	2.01	0.42
1:C:418:TYR:HA	3:C:726:HOH:O	2.19	0.42
1:B:511:GLY:HA2	1:D:465:PHE:CZ	2.55	0.42
1:D:497:VAL:O	1:D:501:ILE:HG12	2.20	0.42
1:A:284:LEU:HB3	1:A:285:PRO:HD3	2.01	0.41
1:B:60:GLU:O	1:B:64:LYS:HG3	2.20	0.41
1:B:407:PHE:CD2	1:B:438:PRO:HG3	2.56	0.41
1:B:566:LYS:HE3	1:B:566:LYS:HB3	1.86	0.41
1:A:413:SER:HB2	1:A:427:HIS:CG	2.55	0.41
1:A:430:LEU:HB2	1:C:189:VAL:HG13	2.03	0.41
1:C:390:GLN:HA	1:C:394:TYR:CG	2.55	0.41
1:B:274:ARG:NE	1:B:361:SER:OG	2.51	0.41
1:A:557:THR:HG23	1:A:558:PRO:CD	2.51	0.41
1:A:557:THR:HG21	1:A:563:VAL:HG11	2.01	0.41
1:C:413:SER:HB2	1:C:427:HIS:CG	2.55	0.41
1:A:282:GLY:O	1:A:285:PRO:HD2	2.20	0.41
1:A:154:ILE:HG22	1:A:187:ALA:O	2.21	0.41
1:A:178:ALA:HB2	1:A:290:TYR:CD1	2.56	0.41
1:A:475:LEU:HD12	1:A:475:LEU:HA	1.82	0.41
1:A:557:THR:HG21	1:A:563:VAL:HG13	2.02	0.41
1:B:372:ARG:NH1	1:B:372:ARG:HB2	2.36	0.41
1:D:114:ASN:O	1:D:117:PRO:HD2	2.21	0.41
1:C:120:TRP:CE3	1:C:123:LYS:HD2	2.55	0.41
1:C:322:LEU:HD11	1:C:474:PHE:CZ	2.55	0.41
1:C:407:PHE:CD2	1:C:438:PRO:HG3	2.56	0.41
1:D:282:GLY:O	1:D:285:PRO:HD2	2.21	0.41
1:C:339:ALA:HB1	1:C:341:LEU:HD21	2.02	0.41
1:B:163:PHE:CE1	1:B:350:LEU:HD13	2.56	0.41
1:A:133:PHE:CE1	1:A:207:LEU:HD22	2.56	0.40
1:A:564:LEU:HD23	1:A:564:LEU:HA	1.80	0.40
1:C:419:LEU:HB2	1:C:422:GLU:HG2	2.03	0.40
1:B:108:ILE:O	1:B:114:ASN:HA	2.21	0.40
1:D:252:LYS:O	1:D:256:GLU:HG3	2.21	0.40
1:D:326:SER:HB3	1:D:498:GLN:NE2	2.36	0.40
1:A:28:LEU:O	1:A:32:MET:HG2	2.21	0.40
1:C:366:VAL:HG12	1:C:372:ARG:HA	2.04	0.40
1:D:390:GLN:HA	1:D:394:TYR:CD2	2.56	0.40
1:B:8:SER:HA	1:B:13:TRP:CG	2.56	0.40
1:B:229:GLU:HA	1:B:232:VAL:HG22	2.02	0.40
1:D:88:ASN:ND2	1:D:91:GLU:OE1	2.41	0.40
1:D:419:LEU:HB2	1:D:422:GLU:HG3	2.03	0.40

All (8) 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:B:137:SER:OG	1:D:561:THR:CG2[4_445]	1.38	0.82
3:A:717:HOH:O	3:A:717:HOH:O[2_554]	1.48	0.72
1:B:560:ASP:OD2	1:D:532:GLU:OE2[1_545]	1.83	0.37
1:B:560:ASP:OD1	1:D:532:GLU:OE1[1_545]	1.92	0.28
1:D:420:LYS:NZ	1:D:531:MET:O[1_545]	1.98	0.22
1:D:420:LYS:CE	1:D:532:GLU:CG[1_545]	2.09	0.11
1:B:137:SER:OG	1:D:561:THR:CB[4_445]	2.12	0.08
1:B:560:ASP:CG	1:D:532:GLU:OE2[1_545]	2.16	0.04

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	560/567 (99%)	543 (97%)	17 (3%)	0	100	100
1	B	560/567 (99%)	547 (98%)	13 (2%)	0	100	100
1	C	560/567 (99%)	547 (98%)	13 (2%)	0	100	100
1	D	559/567 (99%)	546 (98%)	13 (2%)	0	100	100
All	All	2239/2268 (99%)	2183 (98%)	56 (2%)	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	477/481 (99%)	468 (98%)	9 (2%)	57	69
1	B	477/481 (99%)	473 (99%)	4 (1%)	81	89
1	C	477/481 (99%)	473 (99%)	4 (1%)	81	89
1	D	476/481 (99%)	471 (99%)	5 (1%)	73	84
All	All	1907/1924 (99%)	1885 (99%)	22 (1%)	71	82

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	101	ARG
1	A	105	ASP
1	A	163	PHE
1	A	170	THR
1	A	215	PHE
1	A	372	ARG
1	A	390	GLN
1	A	461	SER
1	C	6	LEU
1	C	101	ARG
1	C	215	PHE
1	C	250	ASN
1	B	6	LEU
1	B	29	ARG
1	B	101	ARG
1	B	215	PHE
1	D	6	LEU
1	D	101	ARG
1	D	215	PHE
1	D	488	LEU
1	D	495	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	250	ASN
1	C	437	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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	G6P	C	601	-	16,16,16	1.44	3 (18%)	24,24,24	1.48	4 (16%)
2	G6P	A	601	-	16,16,16	0.70	0	24,24,24	1.60	5 (20%)

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	G6P	C	601	-	-	2/6/26/26	0/1/1/1
2	G6P	A	601	-	-	4/6/26/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	G6P	O3-C3	2.81	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	G6P	O5-C1	2.20	1.48	1.42
2	C	601	G6P	O2-C2	2.10	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	G6P	C1-O5-C5	-4.68	104.84	113.66
2	C	601	G6P	C1-O5-C5	-3.98	106.16	113.66
2	C	601	G6P	C1-C2-C3	3.50	117.57	110.31
2	C	601	G6P	C4-C3-C2	2.56	115.29	110.82
2	A	601	G6P	C1-C2-C3	2.52	115.54	110.31
2	A	601	G6P	O5-C5-C6	2.27	111.25	106.67
2	A	601	G6P	O1P-P-O6	-2.20	100.89	106.73
2	C	601	G6P	O5-C1-C2	2.07	113.98	110.28
2	A	601	G6P	O2P-P-O1P	2.04	115.43	107.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	G6P	C4-C5-C6-O6
2	A	601	G6P	O5-C5-C6-O6
2	A	601	G6P	C6-O6-P-O3P
2	C	601	G6P	C4-C5-C6-O6
2	C	601	G6P	O5-C5-C6-O6
2	A	601	G6P	C6-O6-P-O1P

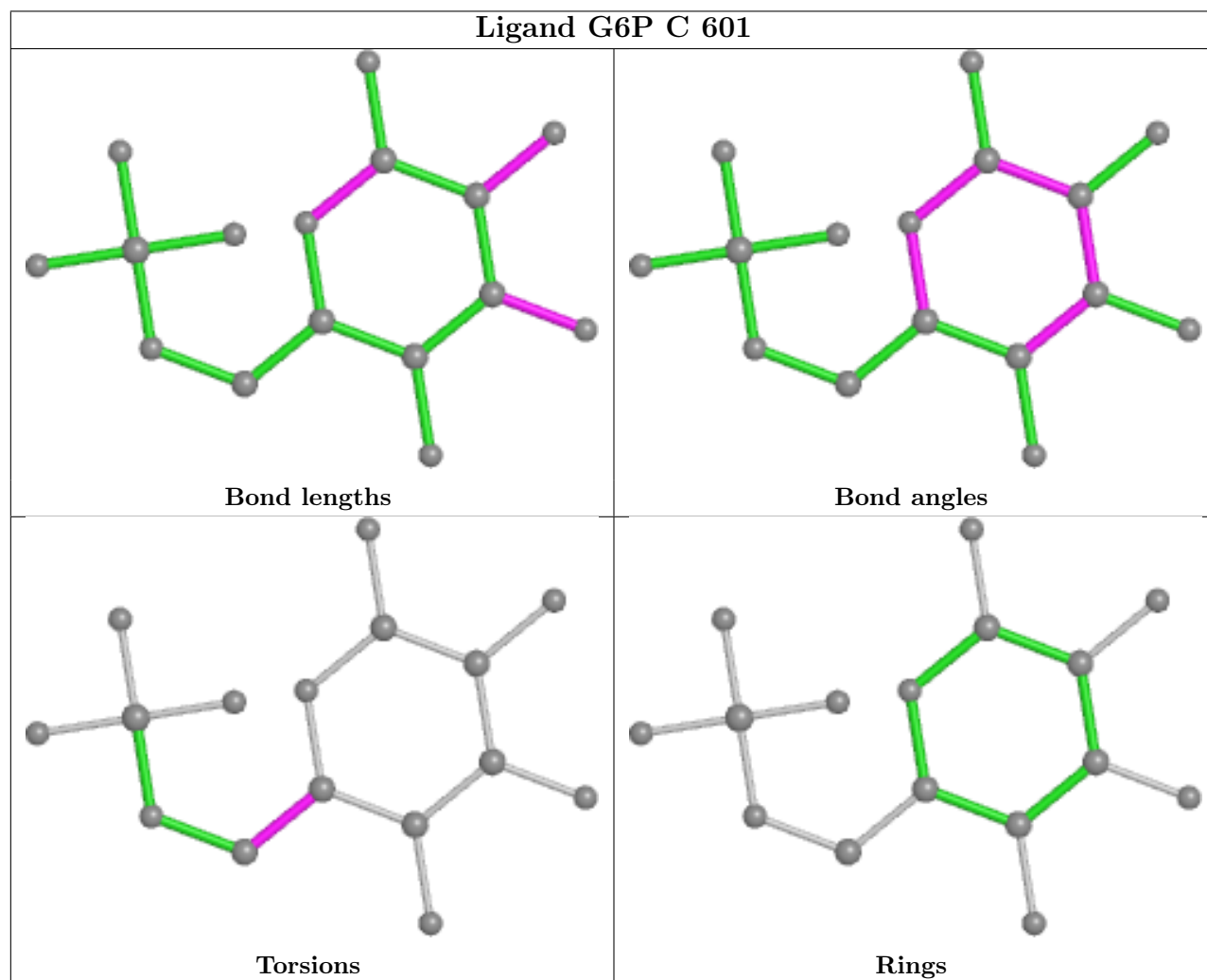
There are no ring outliers.

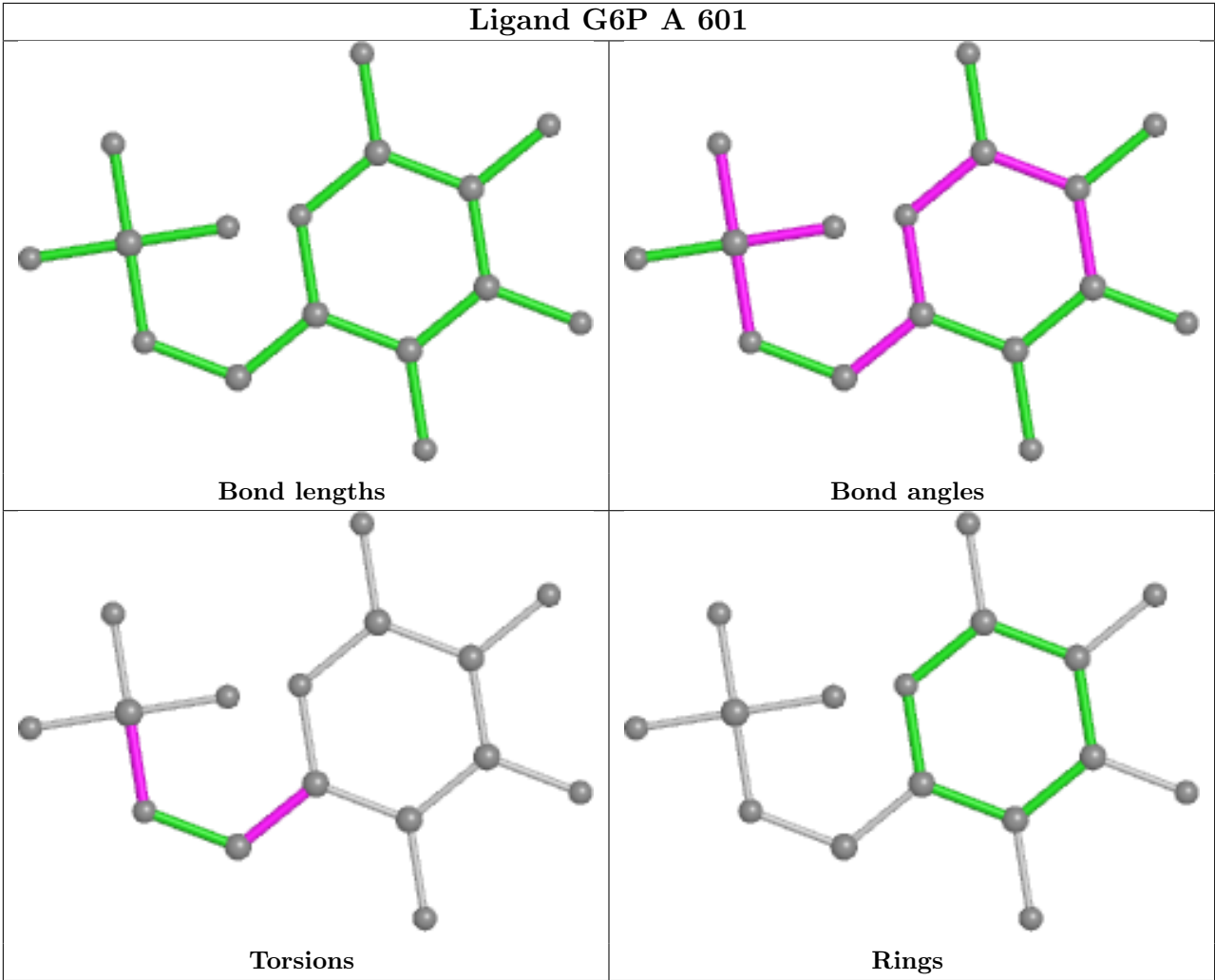
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	G6P	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	143:GLY	C	144:LYS	N	1.20

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	562/567 (99%)	0.23	18 (3%)	47	45	39, 51, 66, 78	0
1	B	562/567 (99%)	0.34	37 (6%)	18	17	42, 56, 71, 89	0
1	C	562/567 (99%)	0.33	25 (4%)	34	32	40, 53, 70, 80	0
1	D	561/567 (98%)	0.36	33 (5%)	22	21	39, 53, 73, 86	0
All	All	2247/2268 (99%)	0.31	113 (5%)	28	27	39, 53, 71, 89	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	421	GLY	9.6
1	B	557	THR	8.9
1	D	559	TYR	7.9
1	B	563	VAL	7.3
1	D	420	LYS	6.9
1	B	559	TYR	6.7
1	D	555	PRO	6.5
1	B	558	PRO	6.2
1	B	556	SER	6.0
1	B	560	ASP	5.6
1	D	556	SER	5.6
1	B	566	LYS	5.6
1	B	534	LYS	5.4
1	B	561	THR	5.1
1	D	418	TYR	5.0
1	D	451	HIS	4.9
1	D	558	PRO	4.7
1	C	455	VAL	4.7
1	D	557	THR	4.4
1	D	561	THR	4.4
1	D	455	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	113	VAL	4.0
1	D	560	ASP	3.8
1	B	555	PRO	3.7
1	D	460	ILE	3.7
1	C	112	GLY	3.7
1	B	562	THR	3.7
1	A	107	VAL	3.6
1	A	454	LYS	3.6
1	C	108	ILE	3.6
1	D	553	VAL	3.5
1	A	558	PRO	3.4
1	A	260	ASP	3.4
1	C	454	LYS	3.4
1	D	532	GLU	3.4
1	A	137	SER	3.3
1	A	451	HIS	3.3
1	C	5	ALA	3.2
1	D	450	LEU	3.2
1	D	13	TRP	3.2
1	D	554	LYS	3.1
1	B	460	ILE	3.1
1	C	255	LYS	3.0
1	D	6	LEU	3.0
1	B	554	LYS	3.0
1	C	443	TYR	3.0
1	B	454	LYS	2.9
1	B	234	SER	2.9
1	B	564	LEU	2.9
1	D	375	TYR	2.9
1	D	372	ARG	2.8
1	A	238	GLN	2.8
1	C	357	LEU	2.8
1	D	452	SER	2.8
1	B	25	LYS	2.8
1	A	255	LYS	2.7
1	A	262	ASN	2.7
1	D	5	ALA	2.7
1	B	144	LYS	2.7
1	C	231	ILE	2.7
1	B	565	PRO	2.7
1	C	146	LEU	2.7
1	B	450	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	448	GLU	2.7
1	B	39	LYS	2.7
1	D	454	LYS	2.7
1	A	113	VAL	2.7
1	C	252	LYS	2.7
1	A	136	GLY	2.6
1	C	450	LEU	2.6
1	B	5	ALA	2.6
1	D	25	LYS	2.6
1	A	259	ILE	2.6
1	A	128	GLN	2.6
1	B	531	MET	2.6
1	B	451	HIS	2.6
1	C	179	LYS	2.5
1	C	451	HIS	2.5
1	B	76	GLU	2.5
1	D	20	VAL	2.5
1	A	108	ILE	2.5
1	C	238	GLN	2.4
1	B	457	GLU	2.4
1	D	446	THR	2.4
1	D	419	LEU	2.4
1	D	459	LEU	2.4
1	B	553	VAL	2.3
1	C	133	PHE	2.3
1	B	35	ALA	2.3
1	D	14	LYS	2.2
1	C	111	ASP	2.2
1	B	11	ASP	2.2
1	C	453	GLU	2.2
1	B	280	ALA	2.2
1	D	18	ALA	2.2
1	B	551	LEU	2.2
1	B	455	VAL	2.2
1	A	86	LYS	2.2
1	A	110	SER	2.2
1	B	366	VAL	2.1
1	B	206	THR	2.1
1	C	251	LEU	2.1
1	D	534	LYS	2.1
1	A	153	GLY	2.1
1	B	452	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	250	ASN	2.1
1	B	255	LYS	2.1
1	C	4	PRO	2.1
1	D	449	GLN	2.1
1	B	420	LYS	2.1
1	C	343	TYR	2.0
1	C	242	LYS	2.0
1	A	118	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 monosaccharides in this entry.

6.4 Ligands [i](#)

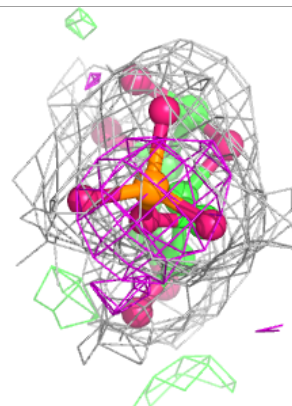
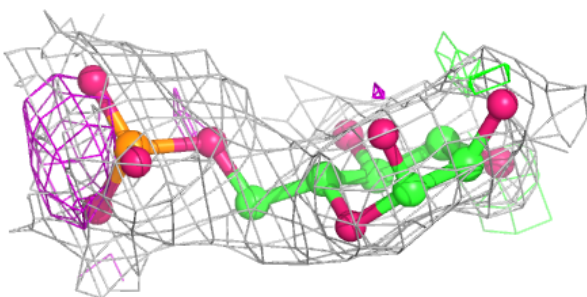
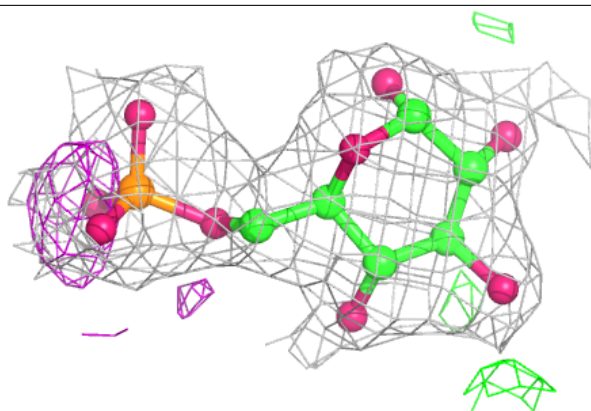
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	G6P	C	601	16/16	0.91	0.15	53,53,53,53	0
2	G6P	A	601	16/16	0.92	0.16	55,55,55,55	0

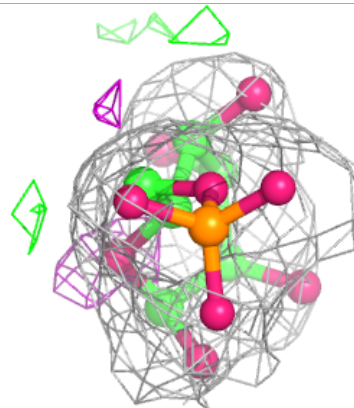
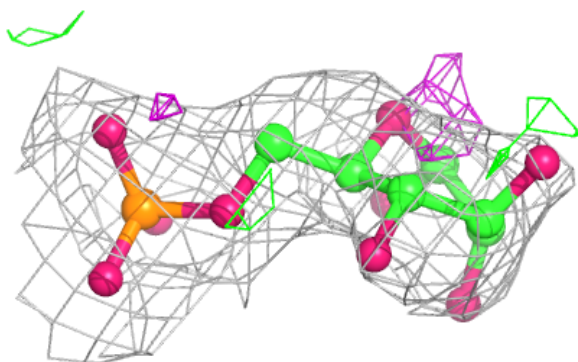
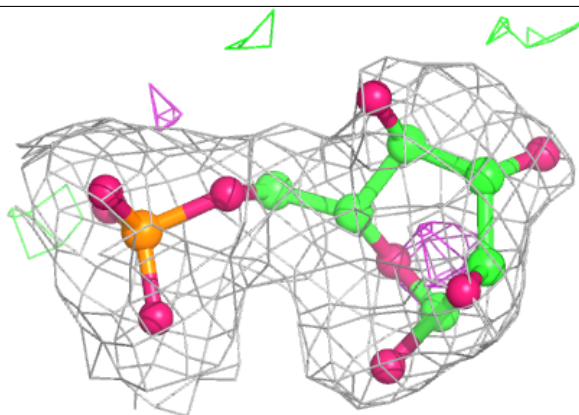
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G6P C 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 G6P 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 [i](#)

There are no such residues in this entry.