



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 02:15 AM UTC

PDB ID : 2O2C / pdb_00002o2c
Title : Crystal structure of phosphoglucose isomerase from *T. brucei* containing glucose-6-phosphate in the active site
Authors : Arsenieva, D.; Mazock, G.H.; Appavu, B.L.; Jeffery, C.J.
Deposited on : 2006-11-29
Resolution : 1.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

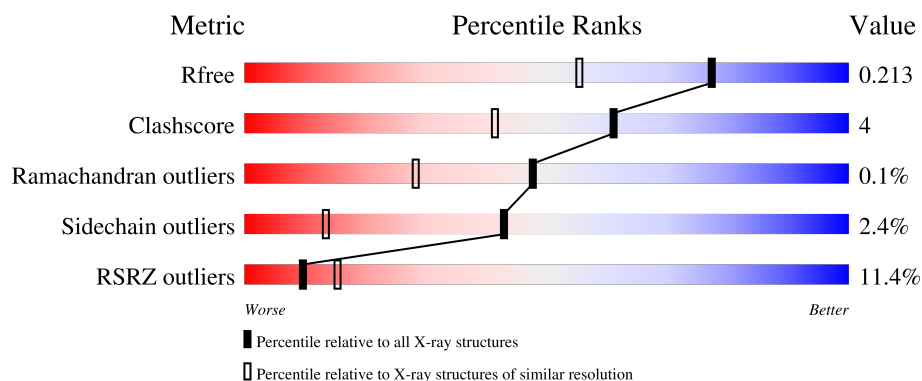
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	613	10% 81% 10% 8%
1	B	613	8% 80% 10% 8%
1	C	613	13% 83% 7% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	7001	-	X	-	-
3	GOL	A	7005	-	X	-	-
3	GOL	B	7002	-	X	-	-
3	GOL	B	7004	-	X	-	-
3	GOL	B	7006	-	X	-	-
3	GOL	C	7003	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14725 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.

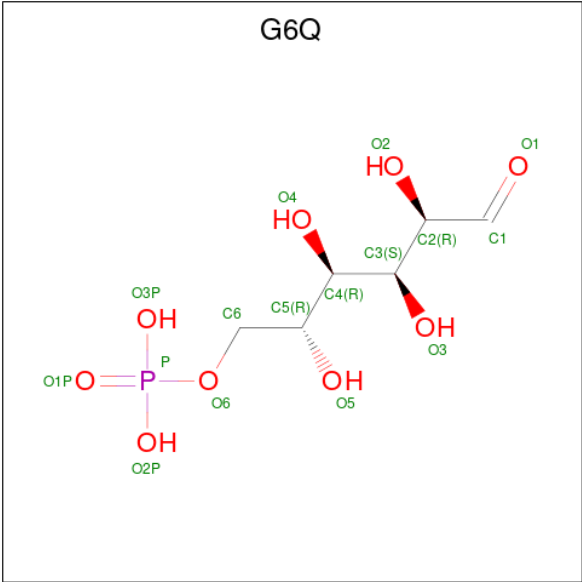
- Molecule 1 is a protein called Glucose-6-phosphate isomerase, glycosomal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4449	2827	781	826	15			
1	B	564	Total	C	N	O	S	0	0	0
			4449	2827	781	826	15			
1	C	561	Total	C	N	O	S	0	0	0
			4432	2818	778	821	15			

There are 21 discrepancies between the modelled and reference sequences:

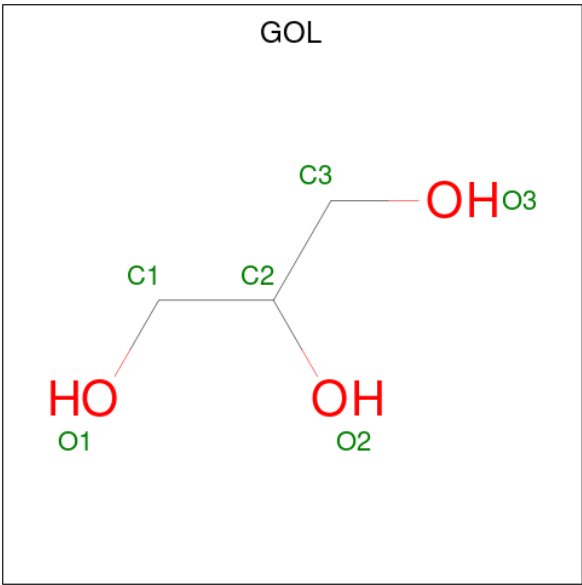
Chain	Residue	Modelled	Actual	Comment	Reference
A	77	THR	ALA	conflict	UNP P13377
A	608	HIS	-	expression tag	UNP P13377
A	609	HIS	-	expression tag	UNP P13377
A	610	HIS	-	expression tag	UNP P13377
A	611	HIS	-	expression tag	UNP P13377
A	612	HIS	-	expression tag	UNP P13377
A	613	HIS	-	expression tag	UNP P13377
B	77	THR	ALA	conflict	UNP P13377
B	608	HIS	-	expression tag	UNP P13377
B	609	HIS	-	expression tag	UNP P13377
B	610	HIS	-	expression tag	UNP P13377
B	611	HIS	-	expression tag	UNP P13377
B	612	HIS	-	expression tag	UNP P13377
B	613	HIS	-	expression tag	UNP P13377
C	77	THR	ALA	conflict	UNP P13377
C	608	HIS	-	expression tag	UNP P13377
C	609	HIS	-	expression tag	UNP P13377
C	610	HIS	-	expression tag	UNP P13377
C	611	HIS	-	expression tag	UNP P13377
C	612	HIS	-	expression tag	UNP P13377
C	613	HIS	-	expression tag	UNP P13377

- Molecule 2 is GLUCOSE-6-PHOSPHATE (CCD ID: G6Q) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	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 GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

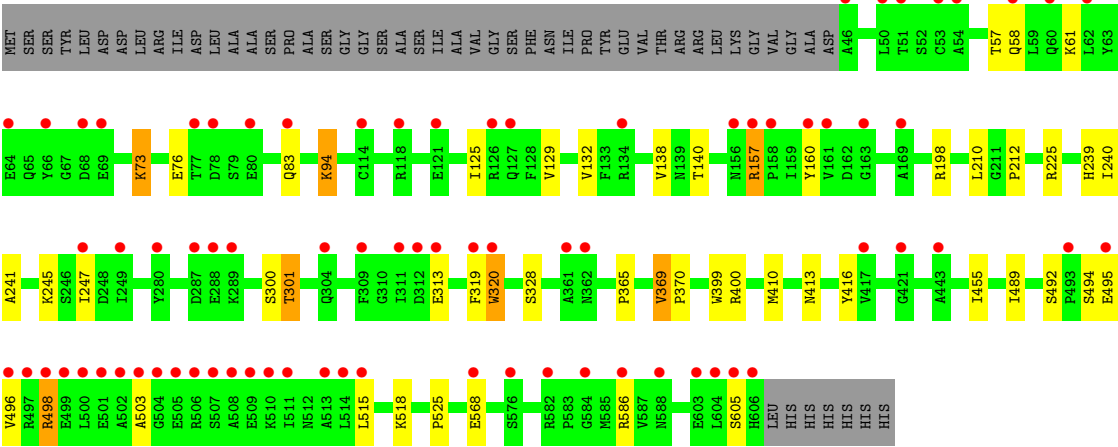
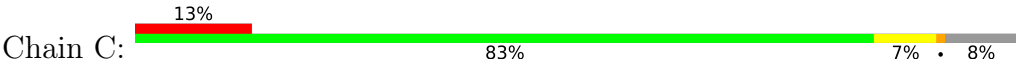
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	439	Total 439	O 439	0	0
4	B	459	Total 459	O 459	0	0
4	C	413	Total 413	O 413	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	125.84Å 221.25Å 128.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.58 40.00 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.58) 99.8 (40.00-1.58)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 1.58Å)	Xtriage
Refinement program	CNS 1.0, REFMAC	Depositor
R, R_{free}	0.200 , 0.213 0.203 , 0.213	Depositor DCC
R_{free} test set	12241 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.014 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14725	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: G6Q, GOL

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	1/4547 (0.0%)	1.05	16/6155 (0.3%)
1	B	0.67	2/4547 (0.0%)	1.06	21/6155 (0.3%)
1	C	0.66	1/4530 (0.0%)	1.06	16/6132 (0.3%)
All	All	0.66	4/13624 (0.0%)	1.06	53/18442 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	VAL	CA-CB	8.70	1.59	1.54
1	B	369	VAL	CA-CB	7.21	1.58	1.54
1	C	320	TRP	NE1-CE2	-5.49	1.31	1.37
1	B	320	TRP	NE1-CE2	-5.45	1.31	1.37

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	GLU	N-CA-C	6.88	118.78	111.28
1	C	568	GLU	N-CA-C	6.88	118.44	111.07
1	B	568	GLU	N-CA-C	6.84	118.81	111.36
1	B	247	ILE	O-C-N	6.65	128.30	122.12
1	A	455	ILE	N-CA-C	6.55	114.64	108.15
1	C	413	ASN	N-CA-C	6.51	120.93	112.92
1	C	455	ILE	N-CA-C	6.45	114.54	108.15
1	B	455	ILE	N-CA-C	6.34	114.42	108.15
1	B	160	TYR	N-CA-C	6.27	120.04	109.76
1	A	413	ASN	N-CA-C	6.26	120.62	112.92
1	C	525	PRO	N-CA-C	6.23	120.76	111.41
1	B	413	ASN	N-CA-C	6.13	120.46	112.92
1	B	210	LEU	N-CA-C	6.12	117.95	111.28
1	B	489	ILE	N-CA-C	6.07	117.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	THR	N-CA-C	5.98	118.58	111.71
1	C	605	SER	N-CA-C	5.97	117.45	111.07
1	B	225	ARG	N-CA-C	5.94	119.63	112.38
1	A	160	TYR	N-CA-C	5.94	119.50	109.76
1	B	525	PRO	N-CA-C	5.94	120.60	111.57
1	C	410	MET	N-CA-C	5.92	117.73	111.28
1	A	301	THR	N-CA-C	-5.91	106.41	113.97
1	C	225	ARG	N-CA-C	5.85	119.52	112.38
1	A	225	ARG	N-CA-C	5.85	119.52	112.38
1	C	328	SER	N-CA-C	5.66	120.30	113.17
1	B	562	TYR	N-CA-C	5.57	120.77	113.30
1	A	210	LEU	N-CA-C	5.52	118.01	111.33
1	B	301	THR	N-CA-C	-5.46	106.98	113.97
1	C	247	ILE	O-C-N	5.45	127.76	122.69
1	C	140	THR	N-CA-C	5.45	117.98	111.71
1	A	328	SER	N-CA-C	5.43	120.01	113.17
1	A	300	SER	N-CA-C	5.39	115.66	108.38
1	B	506	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	C	301	THR	N-CA-C	-5.32	107.16	113.97
1	A	362	ASN	N-CA-C	5.32	120.42	113.88
1	B	498	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	B	382	ASN	N-CA-C	5.27	119.43	112.89
1	A	49	THR	N-CA-C	5.23	116.98	111.28
1	A	140	THR	N-CA-C	5.23	117.72	111.71
1	C	369	VAL	O-C-N	-5.21	115.17	121.10
1	C	210	LEU	N-CA-C	5.19	117.61	111.33
1	A	525	PRO	N-CA-C	5.19	119.19	111.41
1	B	300	SER	N-CA-C	5.18	115.38	108.38
1	C	160	TYR	N-CA-C	5.13	118.18	109.76
1	A	410	MET	N-CA-C	5.13	116.95	111.36
1	A	592	SER	N-CA-C	5.13	117.61	111.71
1	C	300	SER	N-CA-C	5.12	115.29	108.38
1	B	410	MET	N-CA-C	5.11	116.93	111.36
1	B	473	HIS	N-CA-C	5.11	116.85	111.28
1	B	482	ALA	N-CA-C	5.10	116.92	111.36
1	B	328	SER	N-CA-C	5.08	119.57	113.17
1	C	489	ILE	N-CA-C	5.04	118.19	111.44
1	A	320	TRP	N-CA-C	5.04	117.51	109.81
1	B	592	SER	N-CA-C	5.01	117.48	111.71

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	A	4449	0	4420	41	0
1	B	4449	0	4420	49	0
1	C	4432	0	4408	20	0
2	A	16	0	11	3	0
2	B	16	0	11	4	0
2	C	16	0	11	0	0
3	A	12	0	8	2	0
3	B	18	0	13	0	0
3	C	6	0	4	0	0
4	A	439	0	0	14	0
4	B	459	0	0	8	0
4	C	413	0	0	9	0
All	All	14725	0	13306	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (113) 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)
3:A:7001:GOL:O1	3:A:7001:GOL:C1	1.64	1.41
1:B:583:PRO:HG3	1:B:606:HIS:CD2	1.78	1.17
1:A:468:LYS:HD3	4:A:7098:HOH:O	1.60	0.99
1:B:69:GLU:OE2	1:B:73:LYS:HG2	1.61	0.98
1:A:575:LYS:HB3	1:A:575:LYS:NZ	1.82	0.95
1:A:411:GLU:OE1	2:A:5001:G6Q:H2	1.68	0.93
1:A:307:LYS:HE3	4:A:7390:HOH:O	1.71	0.91
1:C:492:SER:OG	1:C:495:GLU:HG3	1.71	0.90
1:A:468:LYS:HE3	4:A:7133:HOH:O	1.72	0.89
1:A:575:LYS:HB3	1:A:575:LYS:HZ2	1.37	0.88
1:B:73:LYS:HA	1:B:73:LYS:NZ	1.94	0.82
1:A:599:ASN:O	1:A:603:GLU:HG3	1.81	0.80
1:B:73:LYS:HA	1:B:73:LYS:HZ2	1.47	0.78
1:A:572:VAL:HG23	4:A:7412:HOH:O	1.84	0.77
1:B:441:GLN:HE22	1:B:479:ASN:HB3	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:LEU:HB3	1:B:511:ILE:HD13	1.70	0.71
1:B:575:LYS:HE3	4:B:7244:HOH:O	1.89	0.71
1:B:366:GLU:H	1:B:366:GLU:CD	1.99	0.70
1:B:312:ASP:HB3	1:B:314:GLU:OE1	1.94	0.68
1:B:127:GLN:HE21	1:B:127:GLN:H	1.40	0.67
1:B:314:GLU:H	1:B:314:GLU:CD	2.01	0.67
1:C:73:LYS:O	1:C:73:LYS:HD3	1.95	0.67
1:B:73:LYS:NZ	1:B:73:LYS:CB	2.58	0.67
1:A:263:THR:HB	4:A:7401:HOH:O	1.95	0.66
1:B:399:TRP:CZ3	1:B:400:ARG:HD3	2.32	0.65
1:A:465:SER:HB3	1:A:468:LYS:HD2	1.79	0.64
1:C:301:THR:HG22	1:C:319:PHE:O	1.98	0.64
2:B:5002:G6Q:H3	4:B:7447:HOH:O	1.97	0.64
1:B:73:LYS:NZ	1:B:73:LYS:CA	2.62	0.62
1:B:605:SER:OG	1:B:606:HIS:CD2	2.53	0.62
1:B:83:GLN:HG3	4:B:7218:HOH:O	2.01	0.60
1:C:73:LYS:HE2	1:C:76:GLU:OE1	2.02	0.60
1:B:416:TYR:CD1	4:C:7409:HOH:O	2.51	0.59
4:B:7331:HOH:O	1:C:245:LYS:HE3	2.01	0.59
1:C:496:VAL:HG13	4:C:7311:HOH:O	2.03	0.59
1:A:233:SER:H	1:A:239:HIS:CD2	2.21	0.58
1:A:88:LYS:HE2	1:A:98:PHE:CD2	2.39	0.58
1:A:575:LYS:HB3	1:A:575:LYS:HZ3	1.67	0.58
1:C:494:SER:O	1:C:498:ARG:HD3	2.04	0.58
1:A:575:LYS:NZ	1:A:575:LYS:CB	2.58	0.58
1:B:605:SER:OG	1:B:606:HIS:HD2	1.86	0.57
1:A:454:LEU:CD1	4:A:7250:HOH:O	2.52	0.57
3:A:7001:GOL:C1	3:A:7001:GOL:HO1	2.08	0.56
1:B:73:LYS:HZ2	1:B:73:LYS:CA	2.17	0.55
1:B:473:HIS:HD2	4:C:7024:HOH:O	1.89	0.55
1:A:58:GLN:HG2	1:A:118:ARG:HH22	1.71	0.55
1:A:88:LYS:HE2	1:A:98:PHE:CG	2.42	0.54
1:B:304:GLN:HE22	1:B:307:LYS:NZ	2.05	0.54
1:A:505:GLU:OE2	1:A:507:SER:HB3	2.07	0.54
1:A:234:ASN:H	1:A:239:HIS:HD2	1.57	0.52
1:B:416:TYR:CE1	4:C:7409:HOH:O	2.61	0.52
1:B:568:GLU:O	1:B:572:VAL:HG23	2.09	0.52
1:C:94:LYS:HD3	4:C:7254:HOH:O	2.09	0.52
1:A:454:LEU:HD12	4:A:7250:HOH:O	2.09	0.52
1:A:297:VAL:HG12	1:A:315:ASN:HB3	1.91	0.52
1:B:60:GLN:O	1:B:64:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLN:O	1:A:308:GLU:HG3	2.10	0.51
1:B:73:LYS:HB2	1:B:73:LYS:HZ3	1.74	0.51
1:B:325:GLY:HA3	2:B:5002:G6Q:H1	1.92	0.51
1:B:416:TYR:CE1	4:C:7328:HOH:O	2.55	0.50
1:B:73:LYS:NZ	1:B:73:LYS:HB2	2.24	0.50
1:A:583:PRO:HG3	4:A:7210:HOH:O	2.11	0.50
1:B:301:THR:HG22	1:B:319:PHE:O	2.12	0.49
1:A:233:SER:H	1:A:239:HIS:HD2	1.58	0.49
1:B:501:GLU:C	1:B:503:ALA:H	2.20	0.49
1:C:399:TRP:CZ3	1:C:400:ARG:HD3	2.47	0.49
1:B:68:ASP:CB	4:B:7421:HOH:O	2.60	0.48
1:C:198:ARG:HD3	4:C:7218:HOH:O	2.13	0.48
1:B:73:LYS:HA	1:B:73:LYS:HZ3	1.76	0.48
1:A:468:LYS:HE3	1:A:468:LYS:HA	1.96	0.48
1:A:454:LEU:HA	4:A:7250:HOH:O	2.13	0.48
1:B:500:LEU:CB	1:B:511:ILE:HD13	2.39	0.48
1:B:73:LYS:CB	1:B:73:LYS:HZ3	2.26	0.47
1:B:312:ASP:HB2	1:B:315:ASN:HD22	1.80	0.47
1:C:57:THR:O	1:C:61:LYS:HG3	2.15	0.47
1:A:399:TRP:CZ3	1:A:400:ARG:HD3	2.50	0.47
1:C:369:VAL:HB	1:C:370:PRO:HD3	1.97	0.46
1:A:575:LYS:HZ2	1:A:575:LYS:CB	2.19	0.46
1:A:307:LYS:HG2	4:A:7422:HOH:O	2.16	0.46
1:A:302:ASN:O	1:A:306:VAL:HG23	2.16	0.46
1:A:439:ASN:HB2	4:A:7207:HOH:O	2.16	0.46
1:A:235:VAL:HB	1:A:265:GLU:HG3	1.96	0.46
1:B:132:VAL:HG22	1:B:138:VAL:HG21	1.96	0.46
1:B:75:PHE:CE2	1:B:488:MET:SD	3.09	0.45
1:B:312:ASP:HB2	1:B:315:ASN:ND2	2.31	0.45
1:A:491:LYS:HE3	1:A:496:VAL:HG22	1.98	0.45
1:A:454:LEU:HD13	4:A:7250:HOH:O	2.15	0.44
1:B:68:ASP:HB3	4:B:7421:HOH:O	2.15	0.44
1:B:494:SER:HB2	4:B:7378:HOH:O	2.18	0.44
1:C:58:GLN:HG3	4:C:7202:HOH:O	2.17	0.44
1:B:73:LYS:CA	1:B:73:LYS:HZ3	2.28	0.44
1:A:567:VAL:O	1:A:571:LYS:HG3	2.16	0.44
1:B:127:GLN:HE21	1:B:127:GLN:N	2.13	0.43
1:B:61:LYS:O	1:B:65:GLN:HG3	2.18	0.43
1:C:157:ARG:HE	1:C:157:ARG:HB2	1.73	0.43
1:B:407:GLN:NE2	2:B:5002:G6Q:O3	2.51	0.43
1:C:125:ILE:O	1:C:129:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLU:CD	2:A:5001:G6Q:H2	2.41	0.42
1:B:411:GLU:OE1	2:B:5002:G6Q:H2	2.19	0.42
1:A:407:GLN:NE2	2:A:5001:G6Q:O3	2.52	0.42
1:B:400:ARG:HD2	1:B:400:ARG:HA	1.66	0.41
1:A:517:HIS:HE1	4:A:7138:HOH:O	2.02	0.41
1:C:320:TRP:CD2	1:C:320:TRP:N	2.89	0.41
1:C:399:TRP:CH2	1:C:400:ARG:HD3	2.56	0.41
1:A:201:VAL:HG22	1:A:230:HIS:HB2	2.02	0.41
1:B:125:ILE:O	1:B:129:VAL:HG23	2.21	0.41
1:C:518:LYS:NZ	4:C:7240:HOH:O	2.52	0.41
1:C:132:VAL:HG22	1:C:138:VAL:HG21	2.01	0.41
1:A:337:ILE:O	1:A:341:ILE:HG12	2.21	0.41
1:B:453:ASN:ND2	4:B:7418:HOH:O	2.53	0.41
1:C:241:ALA:O	1:C:245:LYS:HG3	2.20	0.41
1:A:315:ASN:ND2	4:A:7416:HOH:O	2.52	0.40
1:B:69:GLU:CD	1:B:73:LYS:HG2	2.41	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	562/613 (92%)	547 (97%)	15 (3%)	0	100	100
1	B	562/613 (92%)	547 (97%)	15 (3%)	0	100	100
1	C	559/613 (91%)	545 (98%)	13 (2%)	1 (0%)	43	26
All	All	1683/1839 (92%)	1639 (97%)	43 (3%)	1 (0%)	48	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	503	ALA

5.3.2 Protein sidechains ⓘ

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	479/519 (92%)	470 (98%)	9 (2%)	50	21
1	B	479/519 (92%)	466 (97%)	13 (3%)	39	10
1	C	478/519 (92%)	465 (97%)	13 (3%)	39	10
All	All	1436/1557 (92%)	1401 (98%)	35 (2%)	43	13

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	PRO
1	A	239	HIS
1	A	249	ILE
1	A	289	LYS
1	A	416	TYR
1	A	474	LYS
1	A	515	LEU
1	A	536	PRO
1	A	575	LYS
1	B	73	LYS
1	B	127	GLN
1	B	212	PRO
1	B	239	HIS
1	B	366	GLU
1	B	400	ARG
1	B	416	TYR
1	B	468	LYS
1	B	499	GLU
1	B	511	ILE
1	B	512	ASN
1	B	536	PRO
1	B	588	ASN
1	C	73	LYS
1	C	83	GLN
1	C	94	LYS
1	C	157	ARG

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Mol	Chain	Res	Type
1	C	212	PRO
1	C	239	HIS
1	C	240	ILE
1	C	313	GLU
1	C	365	PRO
1	C	416	TYR
1	C	498	ARG
1	C	515	LEU
1	C	586	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	239	HIS
1	A	315	ASN
1	A	362	ASN
1	A	406	GLN
1	A	467	ASN
1	A	517	HIS
1	A	580	GLN
1	A	589	ASN
1	B	127	GLN
1	B	156	ASN
1	B	171	ASN
1	B	304	GLN
1	B	315	ASN
1	B	441	GLN
1	B	453	ASN
1	B	473	HIS
1	B	512	ASN
1	B	580	GLN
1	B	588	ASN
1	B	606	HIS
1	C	83	GLN
1	C	156	ASN
1	C	171	ASN
1	C	367	GLN
1	C	473	HIS
1	C	580	GLN
1	C	588	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
3	GOL	C	7003	-	5,5,5	4.79	5 (100%)	5,5,5	6.07	3 (60%)
3	GOL	B	7002	-	5,5,5	4.77	5 (100%)	5,5,5	5.95	3 (60%)
3	GOL	A	7001	-	5,5,5	5.10	5 (100%)	5,5,5	6.05	3 (60%)
2	G6Q	B	5002	-	14,15,15	0.76	0	19,21,21	1.25	2 (10%)
3	GOL	B	7006	-	5,5,5	4.88	5 (100%)	5,5,5	6.16	3 (60%)
3	GOL	B	7004	-	5,5,5	4.81	4 (80%)	5,5,5	6.02	3 (60%)
3	GOL	A	7005	-	5,5,5	4.87	5 (100%)	5,5,5	6.15	3 (60%)
2	G6Q	A	5001	-	14,15,15	0.75	0	19,21,21	1.16	0
2	G6Q	C	5003	-	14,15,15	0.70	0	19,21,21	1.20	1 (5%)

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	GOL	C	7003	-	-	2/4/4/4	-
3	GOL	B	7002	-	-	2/4/4/4	-
3	GOL	A	7001	-	-	2/4/4/4	-
2	G6Q	B	5002	-	-	2/19/20/20	-
3	GOL	B	7006	-	-	2/4/4/4	-
3	GOL	B	7004	-	-	2/4/4/4	-
3	GOL	A	7005	-	-	2/4/4/4	-
2	G6Q	A	5001	-	-	1/19/20/20	-
2	G6Q	C	5003	-	-	1/19/20/20	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	7004	GOL	C3-C2	-8.46	1.19	1.51
3	A	7001	GOL	C3-C2	-8.23	1.20	1.51
3	B	7006	GOL	C3-C2	-8.18	1.20	1.51
3	C	7003	GOL	C3-C2	-8.12	1.20	1.51
3	A	7005	GOL	C3-C2	-8.09	1.20	1.51
3	B	7002	GOL	C3-C2	-8.03	1.21	1.51
3	A	7001	GOL	O1-C1	5.32	1.64	1.42
3	A	7005	GOL	O1-C1	4.59	1.61	1.42
3	C	7003	GOL	O1-C1	4.49	1.61	1.42
3	B	7006	GOL	O1-C1	4.49	1.61	1.42
3	B	7004	GOL	O1-C1	4.38	1.60	1.42
3	B	7002	GOL	O1-C1	4.23	1.60	1.42
3	A	7001	GOL	O3-C3	3.78	1.58	1.42
3	B	7002	GOL	O3-C3	3.64	1.57	1.42
3	B	7006	GOL	C1-C2	-3.55	1.38	1.51
3	B	7006	GOL	O3-C3	3.48	1.57	1.42
3	B	7004	GOL	O3-C3	3.46	1.56	1.42
3	A	7005	GOL	O3-C3	3.36	1.56	1.42
3	C	7003	GOL	O3-C3	3.34	1.56	1.42
3	A	7005	GOL	O2-C2	-3.30	1.33	1.43
3	B	7002	GOL	O2-C2	-3.25	1.33	1.43
3	A	7001	GOL	C1-C2	-3.23	1.39	1.51
3	B	7004	GOL	C1-C2	-3.13	1.39	1.51
3	A	7005	GOL	C1-C2	-3.12	1.39	1.51
3	A	7001	GOL	O2-C2	-3.05	1.34	1.43
3	C	7003	GOL	O2-C2	-2.98	1.34	1.43
3	C	7003	GOL	C1-C2	-2.96	1.40	1.51
3	B	7002	GOL	C1-C2	-2.74	1.41	1.51
3	B	7006	GOL	O2-C2	-2.66	1.35	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7005	GOL	O3-C3-C2	11.13	160.49	110.38
3	B	7006	GOL	O3-C3-C2	11.12	160.45	110.38
3	C	7003	GOL	O3-C3-C2	11.01	159.94	110.38
3	A	7001	GOL	O3-C3-C2	10.94	159.63	110.38
3	B	7004	GOL	O3-C3-C2	10.89	159.40	110.38
3	B	7002	GOL	O3-C3-C2	10.88	159.37	110.38
3	B	7006	GOL	O2-C2-C3	7.47	140.09	109.18
3	A	7005	GOL	O2-C2-C3	7.22	139.08	109.18
3	A	7001	GOL	O2-C2-C3	7.14	138.73	109.18
3	B	7004	GOL	O2-C2-C3	7.10	138.56	109.18
3	C	7003	GOL	O2-C2-C3	7.04	138.31	109.18
3	B	7002	GOL	O2-C2-C3	6.63	136.61	109.18
3	B	7002	GOL	O1-C1-C2	3.81	127.51	110.38
3	A	7005	GOL	O1-C1-C2	3.52	126.23	110.38
3	C	7003	GOL	O1-C1-C2	3.52	126.22	110.38
3	A	7001	GOL	O1-C1-C2	3.42	125.76	110.38
3	B	7006	GOL	O1-C1-C2	3.07	124.19	110.38
3	B	7004	GOL	O1-C1-C2	3.04	124.06	110.38
2	B	5002	G6Q	C4-C3-C2	2.64	118.11	113.49
2	C	5003	G6Q	C4-C3-C2	2.54	117.95	113.49
2	B	5002	G6Q	C5-C4-C3	-2.05	109.32	112.48

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5001	G6Q	O1-C1-C2-C3
2	B	5002	G6Q	O1-C1-C2-C3
2	C	5003	G6Q	O1-C1-C2-C3
3	A	7001	GOL	O1-C1-C2-C3
3	A	7001	GOL	C1-C2-C3-O3
3	A	7005	GOL	O1-C1-C2-C3
3	A	7005	GOL	C1-C2-C3-O3
3	B	7002	GOL	O1-C1-C2-C3
3	B	7002	GOL	C1-C2-C3-O3
3	B	7004	GOL	C1-C2-C3-O3
3	B	7006	GOL	O1-C1-C2-C3
3	B	7006	GOL	C1-C2-C3-O3
3	C	7003	GOL	O1-C1-C2-C3
3	C	7003	GOL	C1-C2-C3-O3
3	B	7004	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	5002	G6Q	C2-C3-C4-O4

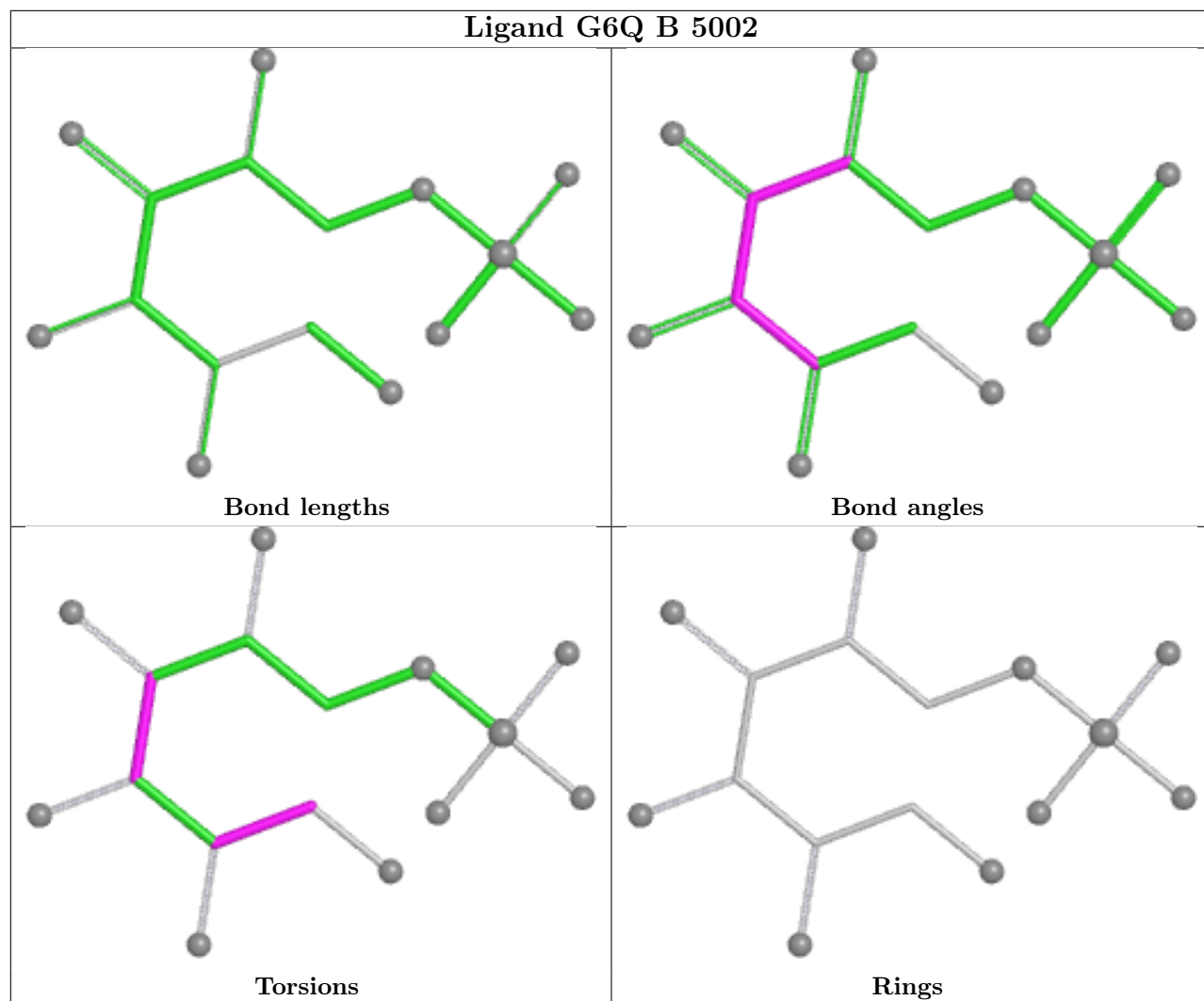
There are no ring outliers.

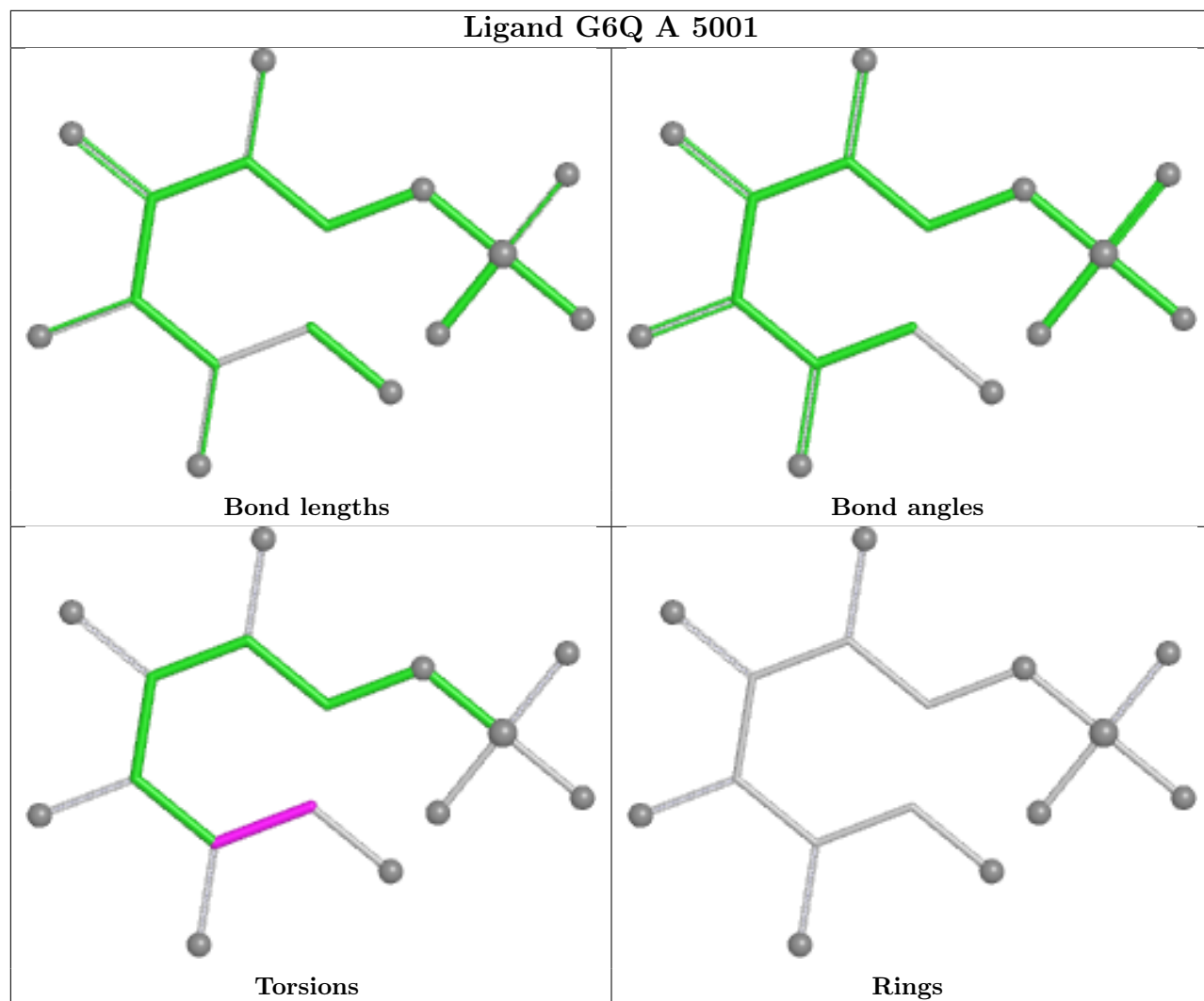
3 monomers are involved in 9 short contacts:

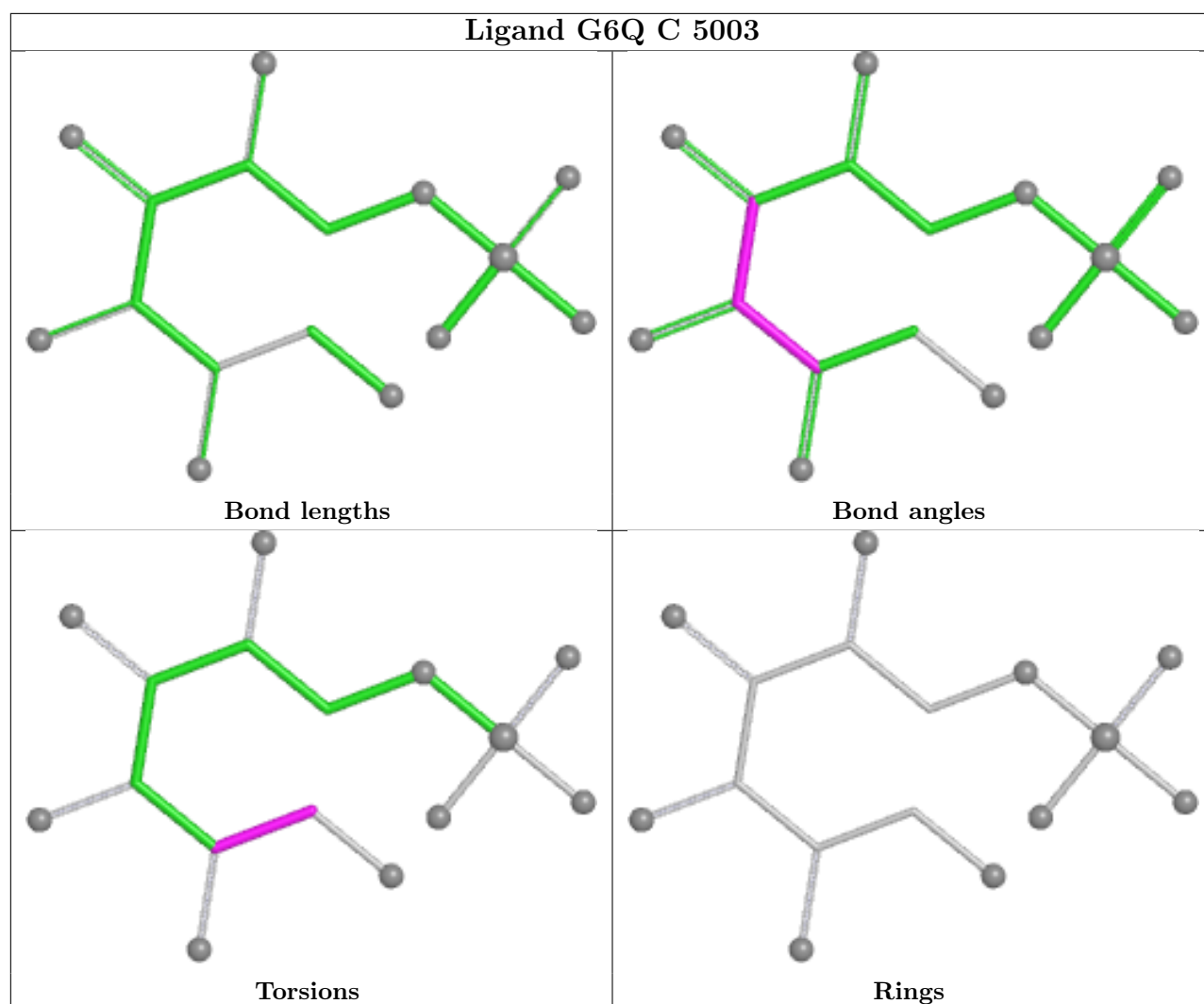
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	7001	GOL	2	0
2	B	5002	G6Q	4	0
2	A	5001	G6Q	3	0

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.

Ligand G6Q B 5002







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	564/613 (92%)	0.77	63 (11%) 10 16	9, 15, 32, 42	0
1	B	564/613 (92%)	0.60	51 (9%) 15 23	9, 14, 31, 44	0
1	C	561/613 (91%)	0.86	78 (13%) 6 11	9, 16, 31, 44	0
All	All	1689/1839 (91%)	0.74	192 (11%) 10 15	9, 15, 31, 44	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	503	ALA	9.7
1	B	502	ALA	5.6
1	A	43	GLY	5.6
1	B	504	GLY	5.5
1	A	606	HIS	5.4
1	A	503	ALA	5.4
1	B	503	ALA	5.3
1	B	44	ALA	5.0
1	B	606	HIS	4.7
1	C	312	ASP	4.6
1	C	514	LEU	4.5
1	C	508	ALA	4.5
1	C	504	GLY	4.5
1	A	44	ALA	4.5
1	B	43	GLY	4.4
1	B	604	LEU	4.4
1	C	502	ALA	4.3
1	C	500	LEU	4.3
1	B	507	SER	4.3
1	A	500	LEU	4.2
1	B	500	LEU	4.2
1	B	515	LEU	4.2
1	A	306	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	502	ALA	4.1
1	C	46	ALA	4.1
1	C	606	HIS	3.9
1	C	507	SER	3.9
1	C	361	ALA	3.9
1	C	498	ARG	3.9
1	A	469	ILE	3.9
1	A	496	VAL	3.8
1	C	505	GLU	3.8
1	B	468	LYS	3.8
1	B	508	ALA	3.7
1	B	53	CYS	3.6
1	B	499	GLU	3.6
1	A	52	SER	3.6
1	A	504	GLY	3.5
1	A	286	ILE	3.5
1	A	46	ALA	3.5
1	A	292	VAL	3.5
1	A	310	GLY	3.4
1	B	505	GLU	3.4
1	A	420	SER	3.4
1	B	506	ARG	3.4
1	A	309	PHE	3.4
1	B	494	SER	3.3
1	B	511	ILE	3.3
1	B	73	LYS	3.2
1	B	52	SER	3.2
1	A	45	ASP	3.2
1	C	157	ARG	3.2
1	C	604	LEU	3.2
1	B	68	ASP	3.2
1	C	506	ARG	3.1
1	C	126	ARG	3.1
1	A	94	LYS	3.1
1	B	45	ASP	3.1
1	C	313	GLU	3.1
1	B	493	PRO	3.1
1	A	307	LYS	3.0
1	C	280	TYR	3.0
1	B	313	GLU	3.0
1	A	507	SER	3.0
1	A	249	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	312	ASP	3.0
1	C	69	GLU	3.0
1	B	510	LYS	3.0
1	C	64	GLU	2.9
1	A	515	LEU	2.9
1	C	68	ASP	2.9
1	A	308	GLU	2.9
1	A	497	ARG	2.9
1	A	422	LYS	2.9
1	A	80	GLU	2.9
1	B	51	THR	2.9
1	C	362	ASN	2.9
1	A	285	GLY	2.9
1	C	309	PHE	2.8
1	A	511	ILE	2.8
1	C	58	GLN	2.8
1	A	118	ARG	2.8
1	B	498	ARG	2.8
1	A	493	PRO	2.8
1	C	158	PRO	2.8
1	B	69	GLU	2.8
1	C	121	GLU	2.8
1	C	421	GLY	2.8
1	C	160	TYR	2.8
1	C	51	THR	2.8
1	C	247	ILE	2.8
1	B	416	TYR	2.8
1	B	605	SER	2.7
1	A	311	ILE	2.7
1	C	582	ARG	2.7
1	A	54	ALA	2.7
1	B	307	LYS	2.7
1	C	568	GLU	2.7
1	A	53	CYS	2.7
1	B	46	ALA	2.6
1	C	515	LEU	2.6
1	A	68	ASP	2.6
1	C	83	GLN	2.6
1	A	137	ARG	2.6
1	A	498	ARG	2.6
1	B	509	GLU	2.6
1	B	311	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	576	SER	2.6
1	B	496	VAL	2.6
1	C	163	GLY	2.6
1	C	54	ALA	2.5
1	A	247	ILE	2.5
1	C	53	CYS	2.5
1	A	302	ASN	2.5
1	A	313	GLU	2.5
1	A	529	LEU	2.5
1	B	513	ALA	2.4
1	C	114	CYS	2.4
1	A	495	GLU	2.4
1	C	586	ARG	2.4
1	A	287	ASP	2.4
1	C	588	ASN	2.4
1	B	454	LEU	2.4
1	A	314	GLU	2.4
1	B	469	ILE	2.4
1	A	99	LEU	2.4
1	A	506	ARG	2.4
1	B	586	ARG	2.4
1	C	510	LYS	2.4
1	B	163	GLY	2.4
1	C	319	PHE	2.4
1	A	114	CYS	2.3
1	A	605	SER	2.3
1	C	511	ILE	2.3
1	C	443	ALA	2.3
1	C	499	GLU	2.3
1	C	584	GLY	2.3
1	C	497	ARG	2.3
1	A	120	ALA	2.3
1	C	513	ALA	2.3
1	C	493	PRO	2.3
1	C	156	ASN	2.3
1	B	82	GLY	2.3
1	C	320	TRP	2.3
1	A	468	LYS	2.3
1	A	514	LEU	2.3
1	C	62	LEU	2.3
1	A	603	GLU	2.3
1	C	249	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	321	ASP	2.2
1	C	118	ARG	2.2
1	A	421	GLY	2.2
1	C	311	ILE	2.2
1	A	513	ALA	2.2
1	C	127	GLN	2.2
1	C	169	ALA	2.2
1	B	114	CYS	2.2
1	C	495	GLU	2.2
1	B	75	PHE	2.2
1	A	419	ARG	2.2
1	C	50	LEU	2.2
1	B	501	GLU	2.2
1	C	288	GLU	2.2
1	C	501	GLU	2.2
1	C	509	GLU	2.2
1	C	66	TYR	2.2
1	C	289	LYS	2.2
1	C	77	THR	2.2
1	A	501	GLU	2.2
1	C	496	VAL	2.2
1	A	491	LYS	2.2
1	B	309	PHE	2.1
1	C	161	VAL	2.1
1	B	310	GLY	2.1
1	A	508	ALA	2.1
1	B	361	ALA	2.1
1	C	60	GLN	2.1
1	C	304	GLN	2.1
1	C	80	GLU	2.1
1	C	417	VAL	2.1
1	C	78	ASP	2.1
1	C	287	ASP	2.1
1	B	54	ALA	2.1
1	B	363	ALA	2.1
1	A	586	ARG	2.1
1	A	510	LYS	2.0
1	B	57	THR	2.0
1	B	121	GLU	2.0
1	C	603	GLU	2.0
1	A	305	LYS	2.0
1	C	134	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	605	SER	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](#)

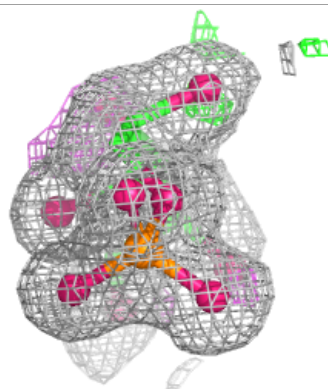
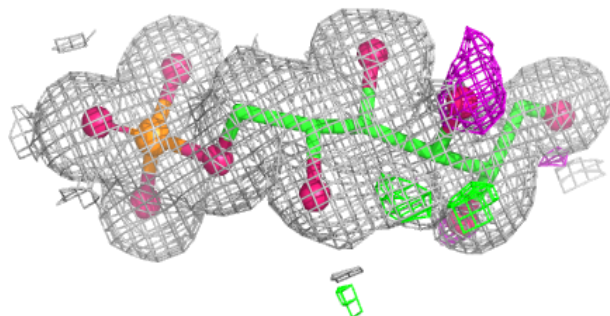
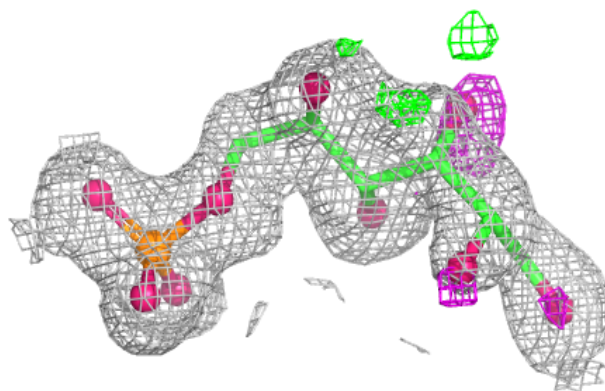
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	GOL	B	7004	6/6	0.59	0.28	36,37,37,38	0
3	GOL	A	7005	6/6	0.65	0.21	33,35,36,38	0
3	GOL	B	7006	6/6	0.70	0.18	31,38,39,41	0
3	GOL	C	7003	6/6	0.77	0.16	26,29,30,32	0
3	GOL	A	7001	6/6	0.78	0.17	24,27,28,31	0
3	GOL	B	7002	6/6	0.80	0.16	23,30,31,34	0
2	G6Q	C	5003	16/16	0.92	0.11	17,23,29,29	0
2	G6Q	A	5001	16/16	0.93	0.11	16,21,27,28	0
2	G6Q	B	5002	16/16	0.94	0.10	14,18,25,26	0

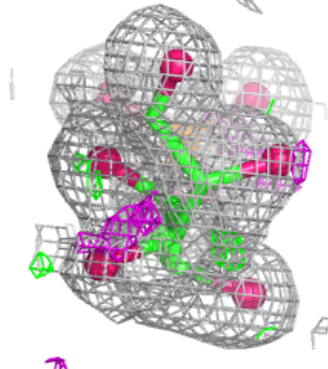
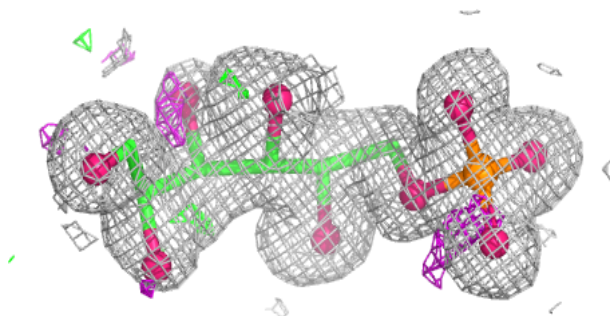
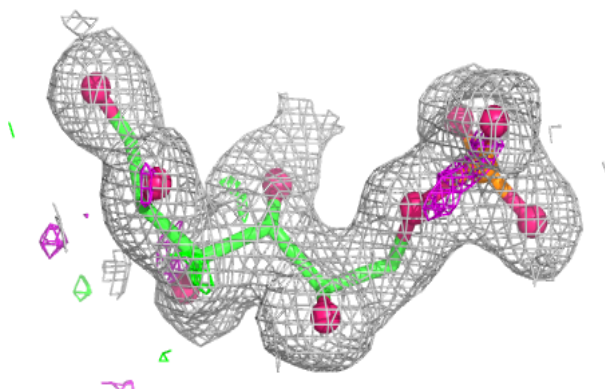
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G6Q C 5003:

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

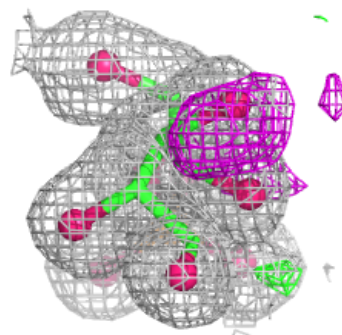
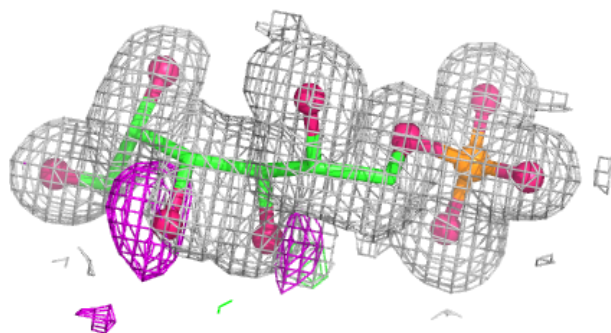
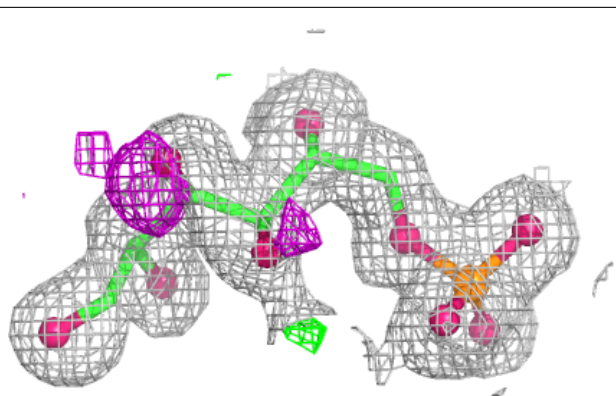
**Electron density around G6Q A 5001:**

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



Electron density around G6Q B 5002:

$2mF_o-DF_c$ (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.