



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 04:05 am BST

PDB ID : 2O2C  
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](mailto: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.

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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 : 2.11  
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) : 2.11

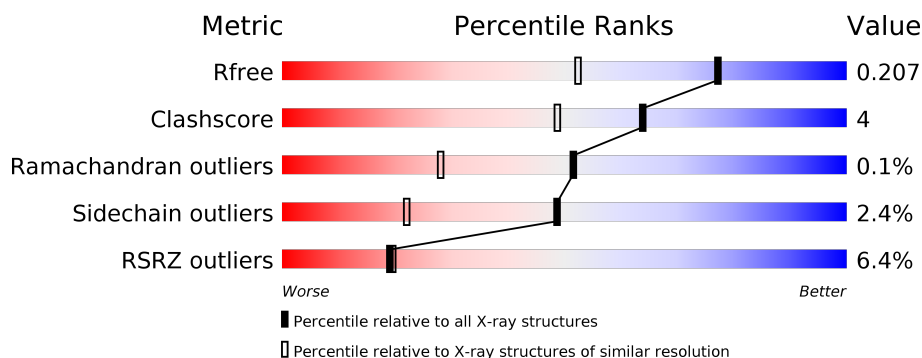
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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  $\geq 3$ , 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	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>8%</div> </div> </div>
1	B	613	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>
1	C	613	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>8%</div> </div> </div>

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.

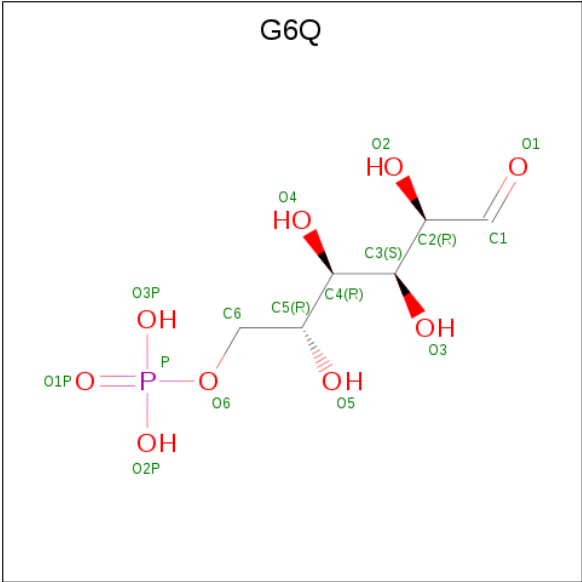
- Molecule 1 is a protein called Glucose-6-phosphate isomerase, glycosomal.

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:

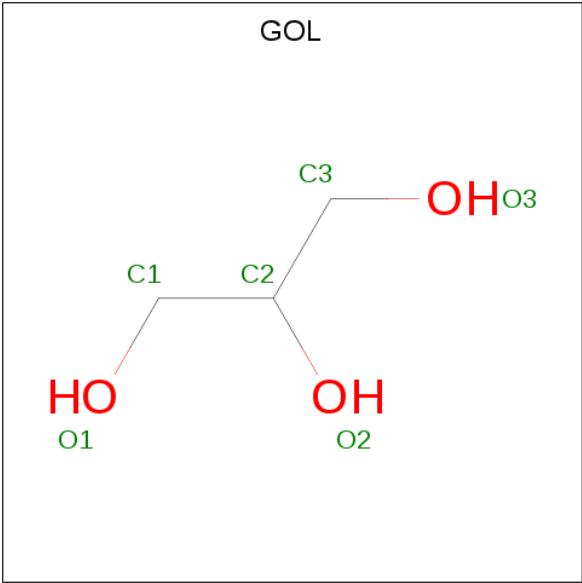
Chain	Residue	Modelled	Actual	Comment	Reference
A	77	THR	ALA	CONFLICT	UNP P13377
A	608	HIS	-	EXPRESSION TAG	UNP P13377
A	609	HIS	-	EXPRESSION TAG	UNP P13377
A	610	HIS	-	EXPRESSION TAG	UNP P13377
A	611	HIS	-	EXPRESSION TAG	UNP P13377
A	612	HIS	-	EXPRESSION TAG	UNP P13377
A	613	HIS	-	EXPRESSION TAG	UNP 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 (three-letter code: G6Q) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



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 (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

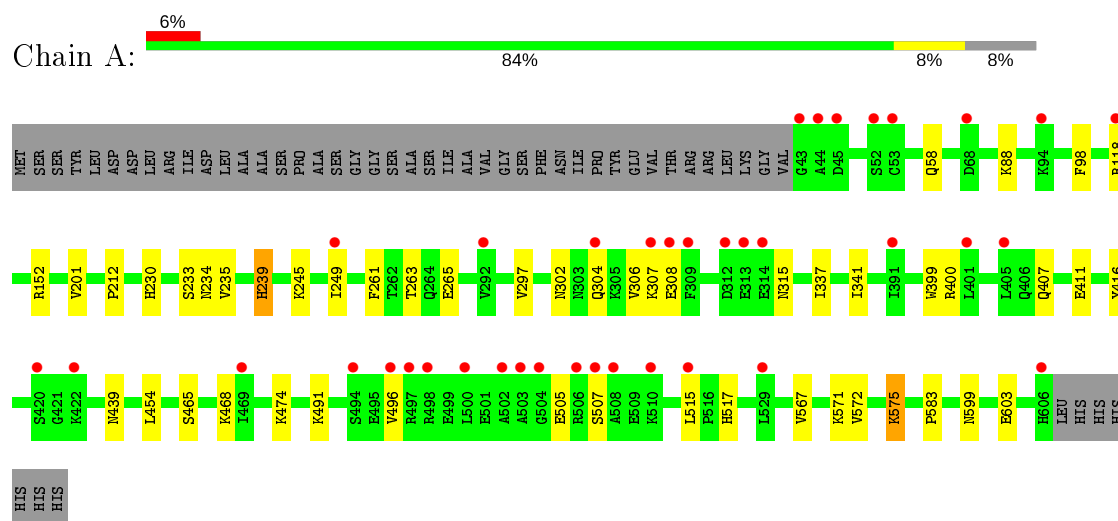
- Molecule 4 is water.

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

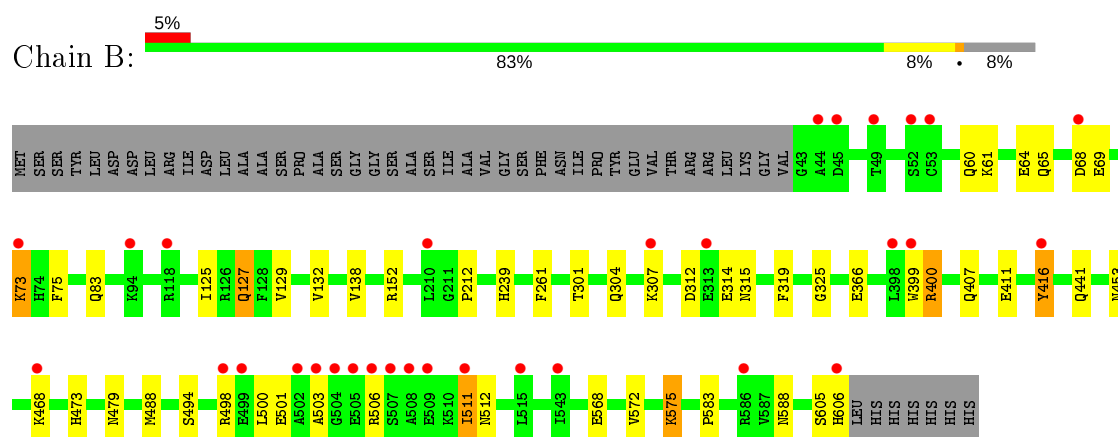
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

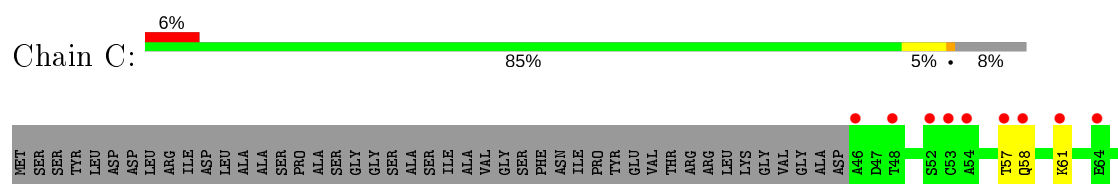
- Molecule 1: Glucose-6-phosphate isomerase, glycosomal

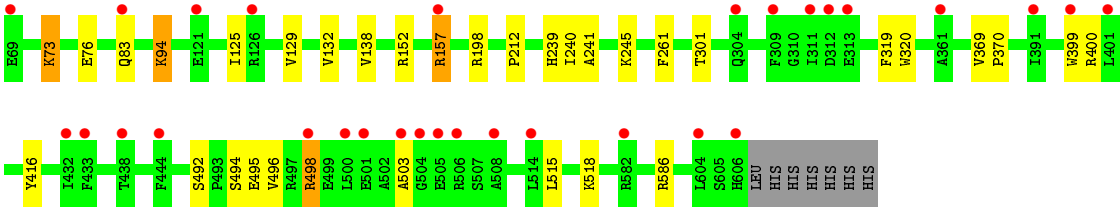


- Molecule 1: Glucose-6-phosphate isomerase, glycosomal



- Molecule 1: Glucose-6-phosphate isomerase, glycosomal







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.84Å 221.25Å 128.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.58 41.59 – 1.57	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.58) 99.4 (41.59-1.57)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 1.58Å)	Xtriage
Refinement program	CNS 1.0, REFMAC	Depositor
R, $R_{free}$	0.200 , 0.213 0.196 , 0.207	Depositor DCC
$R_{free}$ test set	12241 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.3	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, G6Q

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	0.60	0/4547	0.70	0/6155
1	B	0.63	0/4547	0.72	2/6155 (0.0%)
1	C	0.62	0/4530	0.71	0/6132
All	All	0.62	0/13624	0.71	2/18442 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	506	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	B	498	ARG	NE-CZ-NH2	7.35	123.98	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4449	0	4420	40	0
1	B	4449	0	4420	48	0
1	C	4432	0	4408	20	0
2	A	16	0	11	2	0
2	B	16	0	11	4	0
2	C	16	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	15	0
4	B	459	0	0	8	0
4	C	413	0	0	9	0
All	All	14725	0	13306	111	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 (111) 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: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:A:575:LYS:HB3	1:A:575:LYS:HZ2	1.47	0.78
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
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:A:575:LYS:HZ3	1:A:575:LYS:HB3	1.57	0.68
1:B:312:ASP:HB3	1:B:314:GLU:OE1	1.94	0.68
1:B:127:GLN:H	1:B:127:GLN:HE21	1.40	0.67
1:C:73:LYS:O	1:C:73:LYS:HD3	1.95	0.67
1:B:73:LYS:CB	1:B:73:LYS:NZ	2.58	0.67
1:A:263:THR:HB	4:A:7401:HOH:O	1.95	0.66
1:B:366:GLU:H	1:B:366:GLU:CD	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5002:G6Q:H3	4:B:7447:HOH:O	1.97	0.64
1:B:314:GLU:H	1:B:314:GLU:CD	2.01	0.63
1:B:73:LYS:CA	1:B:73:LYS:NZ	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:C:494:SER:O	1:C:498:ARG:HD3	2.04	0.58
1:A:575:LYS:CB	1:A:575:LYS:NZ	2.58	0.58
3:A:7001:GOL:HO1	3:A:7001:GOL:C1	2.08	0.57
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
1:B:473:HIS:HD2	4:C:7024:HOH:O	1.89	0.55
1:B:73:LYS:CA	1:B:73:LYS:HZ2	2.17	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
1:A:304:GLN:O	1:A:308:GLU:HG3	2.10	0.51
1:B:73:LYS:HZ3	1:B:73:LYS:HB2	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:HB2	1:B:73:LYS:NZ	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: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:HZ3	1:B:73:LYS:HA	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HZ3	1:B:73:LYS:CB	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: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:312:ASP:HB2	1:B:315:ASN:ND2	2.31	0.45
1:B:75:PHE:CE2	1:B:488:MET:SD	3.09	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:501:GLU:C	1:B:503:ALA:H	2.20	0.44
1:B:68:ASP:HB3	4:B:7421:HOH:O	2.15	0.44
1:A:245:LYS:NZ	4:A:7239:HOH:O	2.51	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:HZ3	1:B:73:LYS:CA	2.28	0.44
1:A:567:VAL:O	1:A:571:LYS:HG3	2.16	0.44
1:B:127:GLN:N	1:B:127:GLN:HE21	2.13	0.43
1:B:61:LYS:O	1:B:65:GLN:HG3	2.18	0.43
1:C:157:ARG:HB2	1:C:157:ARG:HE	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
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:C:518:LYS:NZ	4:C:7240:HOH:O	2.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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%)	47	25
All	All	1683/1839 (92%)	1639 (97%)	43 (3%)	1 (0%)	51	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	503	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	479/519 (92%)	470 (98%)	9 (2%)	57	31
1	B	479/519 (92%)	466 (97%)	13 (3%)	44	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	478/519 (92%)	465 (97%)	13 (3%)	44	18
All	All	1436/1557 (92%)	1401 (98%)	35 (2%)	49	22

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

Mol	Chain	Res	Type
1	A	152	ARG
1	A	212	PRO
1	A	239	HIS
1	A	249	ILE
1	A	261	PHE
1	A	416	TYR
1	A	474	LYS
1	A	515	LEU
1	A	575	LYS
1	B	73	LYS
1	B	127	GLN
1	B	152	ARG
1	B	212	PRO
1	B	239	HIS
1	B	261	PHE
1	B	400	ARG
1	B	416	TYR
1	B	468	LYS
1	B	511	ILE
1	B	512	ASN
1	B	575	LYS
1	B	588	ASN
1	C	73	LYS
1	C	83	GLN
1	C	94	LYS
1	C	152	ARG
1	C	157	ARG
1	C	212	PRO
1	C	239	HIS
1	C	240	ILE
1	C	261	PHE
1	C	416	TYR
1	C	498	ARG
1	C	515	LEU
1	C	586	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	HIS
1	A	315	ASN
1	A	467	ASN
1	A	473	HIS
1	A	517	HIS
1	B	127	GLN
1	B	156	ASN
1	B	171	ASN
1	B	304	GLN
1	B	315	ASN
1	B	367	GLN
1	B	441	GLN
1	B	473	HIS
1	B	588	ASN
1	B	606	HIS
1	C	83	GLN
1	C	473	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	A	7005	-	5,5,5	4.62	5 (100%)	5,5,5	5.79	3 (60%)
3	GOL	A	7001	-	5,5,5	4.86	5 (100%)	5,5,5	5.70	3 (60%)
2	G6Q	B	5002	-	14,15,15	0.74	0	20,21,21	1.21	2 (10%)
2	G6Q	C	5003	-	14,15,15	0.68	0	20,21,21	1.15	1 (5%)
3	GOL	B	7002	-	5,5,5	4.53	5 (100%)	5,5,5	5.61	3 (60%)
3	GOL	C	7003	-	5,5,5	4.55	5 (100%)	5,5,5	5.72	3 (60%)
3	GOL	B	7006	-	5,5,5	4.62	5 (100%)	5,5,5	5.81	3 (60%)
2	G6Q	A	5001	-	14,15,15	0.73	0	20,21,21	1.12	0
3	GOL	B	7004	-	5,5,5	4.54	4 (80%)	5,5,5	5.67	3 (60%)

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	A	7005	-	-	2/4/4/4	-
3	GOL	A	7001	-	-	2/4/4/4	-
2	G6Q	B	5002	-	-	1/18/20/20	-
2	G6Q	C	5003	-	-	0/18/20/20	-
3	GOL	B	7002	-	-	2/4/4/4	-
3	GOL	C	7003	-	-	2/4/4/4	-
3	GOL	B	7006	-	-	2/4/4/4	-
2	G6Q	A	5001	-	-	0/18/20/20	-
3	GOL	B	7004	-	-	2/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	7004	GOL	C3-C2	-7.83	1.19	1.51
3	A	7001	GOL	C3-C2	-7.61	1.20	1.51
3	B	7006	GOL	C3-C2	-7.57	1.20	1.51
3	C	7003	GOL	C3-C2	-7.51	1.20	1.51
3	A	7005	GOL	C3-C2	-7.48	1.20	1.51
3	B	7002	GOL	C3-C2	-7.43	1.21	1.51
3	A	7001	GOL	O1-C1	5.29	1.64	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	7005	GOL	O1-C1	4.57	1.61	1.42
3	C	7003	GOL	O1-C1	4.47	1.61	1.42
3	B	7006	GOL	O1-C1	4.47	1.61	1.42
3	B	7004	GOL	O1-C1	4.36	1.60	1.42
3	B	7002	GOL	O1-C1	4.21	1.60	1.42
3	A	7001	GOL	O3-C3	3.76	1.58	1.42
3	B	7002	GOL	O3-C3	3.62	1.57	1.42
3	B	7006	GOL	O3-C3	3.47	1.57	1.42
3	B	7004	GOL	O3-C3	3.44	1.56	1.42
3	A	7005	GOL	O3-C3	3.35	1.56	1.42
3	C	7003	GOL	O3-C3	3.33	1.56	1.42
3	B	7006	GOL	C1-C2	-3.28	1.38	1.51
3	A	7005	GOL	O2-C2	-3.22	1.33	1.43
3	B	7002	GOL	O2-C2	-3.18	1.33	1.43
3	A	7001	GOL	C1-C2	-2.98	1.39	1.51
3	A	7001	GOL	O2-C2	-2.98	1.34	1.43
3	C	7003	GOL	O2-C2	-2.91	1.34	1.43
3	B	7004	GOL	C1-C2	-2.88	1.39	1.51
3	A	7005	GOL	C1-C2	-2.88	1.39	1.51
3	C	7003	GOL	C1-C2	-2.73	1.40	1.51
3	B	7006	GOL	O2-C2	-2.59	1.35	1.43
3	B	7002	GOL	C1-C2	-2.52	1.41	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7005	GOL	O3-C3-C2	10.49	160.49	110.20
3	B	7006	GOL	O3-C3-C2	10.48	160.45	110.20
3	C	7003	GOL	O3-C3-C2	10.37	159.94	110.20
3	A	7001	GOL	O3-C3-C2	10.31	159.63	110.20
3	B	7004	GOL	O3-C3-C2	10.26	159.40	110.20
3	B	7002	GOL	O3-C3-C2	10.25	159.37	110.20
3	B	7006	GOL	O2-C2-C3	7.03	140.09	109.12
3	A	7005	GOL	O2-C2-C3	6.80	139.08	109.12
3	A	7001	GOL	O2-C2-C3	6.72	138.73	109.12
3	B	7004	GOL	O2-C2-C3	6.68	138.56	109.12
3	C	7003	GOL	O2-C2-C3	6.63	138.31	109.12
3	B	7002	GOL	O2-C2-C3	6.24	136.61	109.12
3	B	7002	GOL	O1-C1-C2	3.61	127.51	110.20
3	A	7005	GOL	O1-C1-C2	3.34	126.23	110.20
3	C	7003	GOL	O1-C1-C2	3.34	126.22	110.20
3	A	7001	GOL	O1-C1-C2	3.24	125.76	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	7006	GOL	O1-C1-C2	2.92	124.19	110.20
3	B	7004	GOL	O1-C1-C2	2.89	124.06	110.20
2	B	5002	G6Q	C4-C3-C2	2.62	118.11	113.54
2	C	5003	G6Q	C4-C3-C2	2.53	117.95	113.54
2	B	5002	G6Q	C5-C4-C3	-2.01	109.32	112.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	7005	GOL	O1-C1-C2-C3
3	A	7005	GOL	C1-C2-C3-O3
3	A	7001	GOL	O1-C1-C2-C3
3	A	7001	GOL	C1-C2-C3-O3
3	B	7002	GOL	O1-C1-C2-C3
3	B	7002	GOL	C1-C2-C3-O3
3	C	7003	GOL	O1-C1-C2-C3
3	B	7006	GOL	O1-C1-C2-C3
3	B	7006	GOL	C1-C2-C3-O3
3	B	7004	GOL	C1-C2-C3-O3
3	C	7003	GOL	C1-C2-C3-O3
3	B	7004	GOL	O1-C1-C2-O2
2	B	5002	G6Q	C2-C3-C4-O4

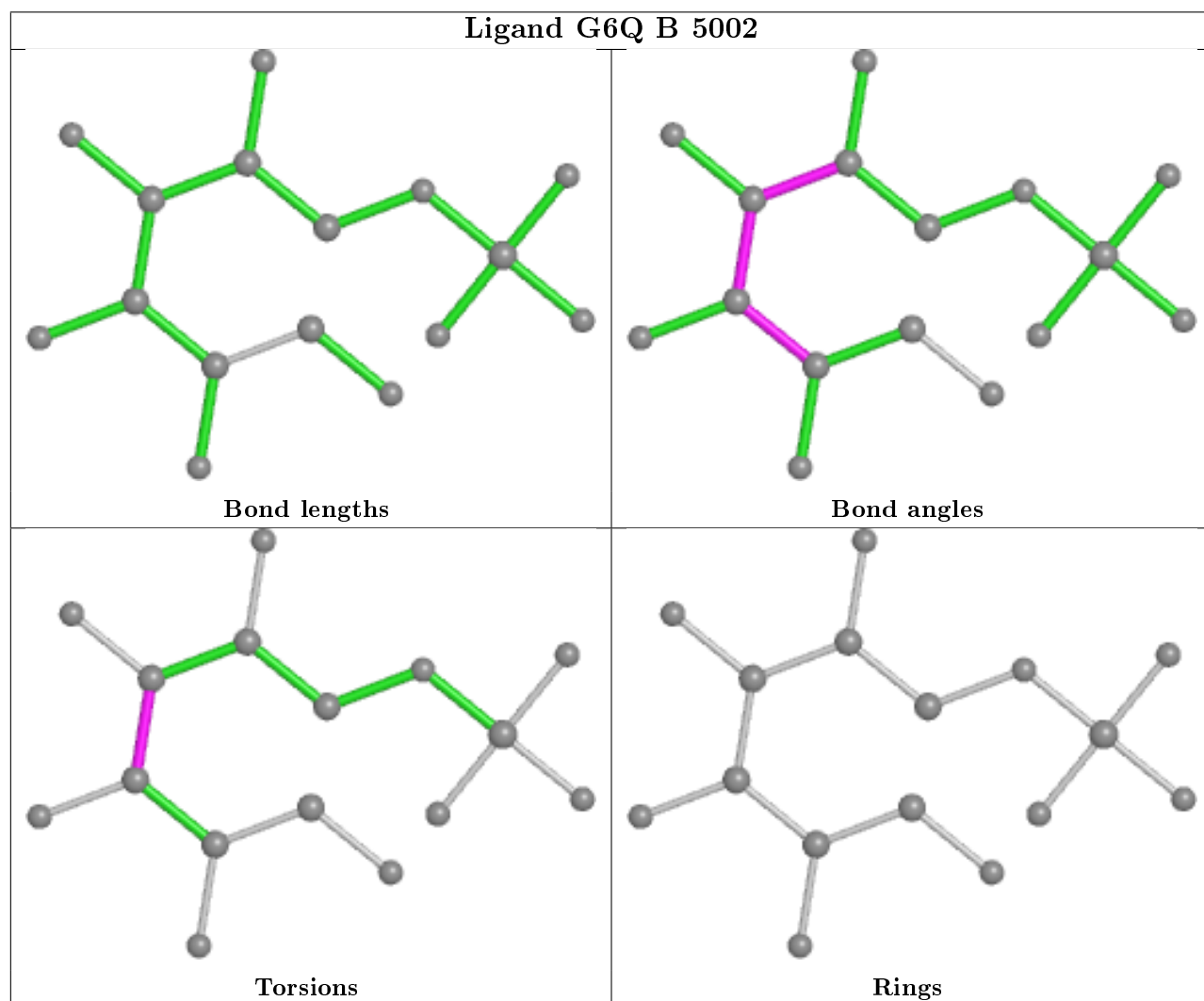
There are no ring outliers.

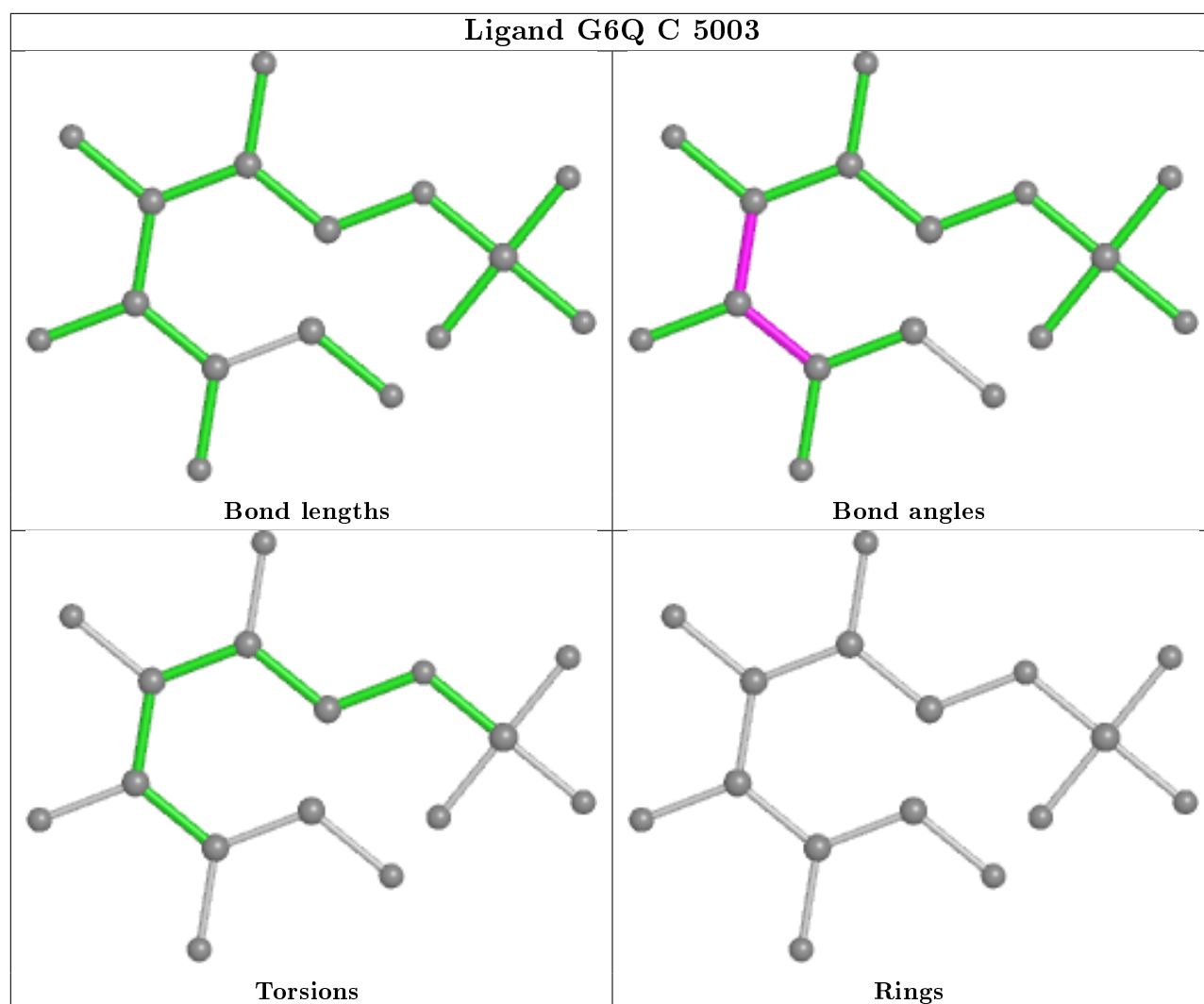
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	7001	GOL	2	0
2	B	5002	G6Q	4	0
2	A	5001	G6Q	2	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	564/613 (92%)	0.53	38 (6%) 17 18	9, 15, 32, 42	0
1	B	564/613 (92%)	0.41	31 (5%) 25 25	9, 14, 31, 44	0
1	C	561/613 (91%)	0.57	39 (6%) 16 16	9, 16, 31, 44	0
All	All	1689/1839 (91%)	0.51	108 (6%) 19 19	9, 15, 31, 44	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	503	ALA	9.2
1	A	606	HIS	8.8
1	C	504	GLY	7.2
1	B	606	HIS	6.9
1	B	504	GLY	6.8
1	B	44	ALA	6.6
1	A	44	ALA	6.4
1	B	502	ALA	6.0
1	C	312	ASP	4.9
1	A	502	ALA	4.7
1	A	504	GLY	4.7
1	C	505	GLU	4.7
1	B	503	ALA	4.5
1	A	43	GLY	4.4
1	C	606	HIS	4.2
1	A	500	LEU	4.0
1	A	307	LYS	3.8
1	C	508	ALA	3.7
1	C	506	ARG	3.6
1	C	582	ARG	3.6
1	A	52	SER	3.6
1	A	506	ARG	3.4
1	B	507	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	499	GLU	3.4
1	C	498	ARG	3.3
1	B	515	LEU	3.2
1	C	401	LEU	3.2
1	A	309	PHE	3.2
1	B	68	ASP	3.1
1	A	312	ASP	3.1
1	B	506	ARG	3.1
1	B	45	ASP	3.1
1	B	313	GLU	3.1
1	A	503	ALA	3.1
1	B	505	GLU	3.1
1	A	308	GLU	3.0
1	C	313	GLU	3.0
1	A	496	VAL	3.0
1	A	94	LYS	2.9
1	A	401	LEU	2.9
1	B	307	LYS	2.9
1	A	304	GLN	2.9
1	C	58	GLN	2.9
1	C	361	ALA	2.9
1	C	444	PHE	2.8
1	C	500	LEU	2.8
1	A	313	GLU	2.8
1	A	314	GLU	2.8
1	C	54	ALA	2.8
1	A	118	ARG	2.8
1	C	433	PHE	2.7
1	A	508	ALA	2.7
1	A	515	LEU	2.7
1	C	604	LEU	2.7
1	C	514	LEU	2.7
1	C	399	TRP	2.6
1	A	420	SER	2.6
1	A	497	ARG	2.6
1	B	586	ARG	2.6
1	B	416	TYR	2.6
1	A	405	LEU	2.6
1	C	157	ARG	2.5
1	A	469	ILE	2.5
1	C	121	GLU	2.5
1	A	422	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	46	ALA	2.4
1	A	249	ILE	2.4
1	C	57	THR	2.4
1	B	399	TRP	2.4
1	C	52	SER	2.4
1	B	94	LYS	2.4
1	C	64	GLU	2.4
1	A	510	LYS	2.3
1	C	69	GLU	2.3
1	A	45	ASP	2.3
1	A	391	ILE	2.3
1	B	511	ILE	2.3
1	C	432	ILE	2.3
1	A	529	LEU	2.3
1	C	309	PHE	2.3
1	A	53	CYS	2.3
1	B	398	LEU	2.3
1	B	53	CYS	2.2
1	C	61	LYS	2.2
1	B	73	LYS	2.2
1	A	292	VAL	2.2
1	C	391	ILE	2.2
1	C	83	GLN	2.2
1	B	118	ARG	2.2
1	C	48	THR	2.2
1	C	304	GLN	2.2
1	C	311	ILE	2.2
1	B	498	ARG	2.1
1	B	468	LYS	2.1
1	B	52	SER	2.1
1	B	508	ALA	2.1
1	B	543	ILE	2.1
1	A	494	SER	2.1
1	A	507	SER	2.1
1	C	53	CYS	2.1
1	B	210	LEU	2.1
1	A	68	ASP	2.1
1	B	49	THR	2.1
1	C	438	THR	2.1
1	A	498	ARG	2.0
1	C	126	ARG	2.0
1	B	509	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	501	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

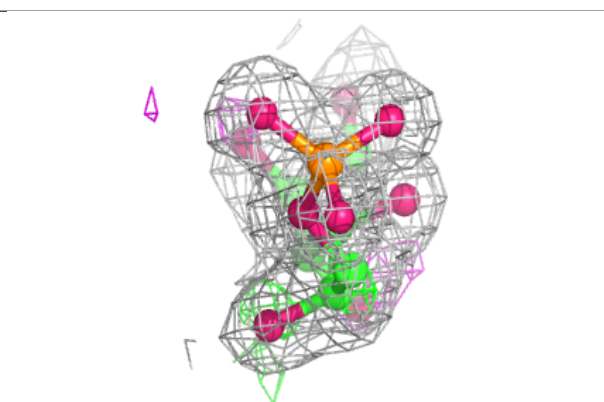
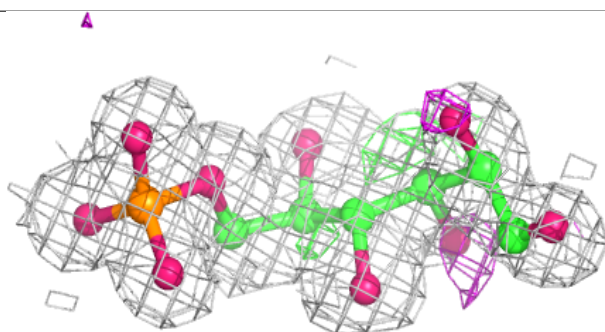
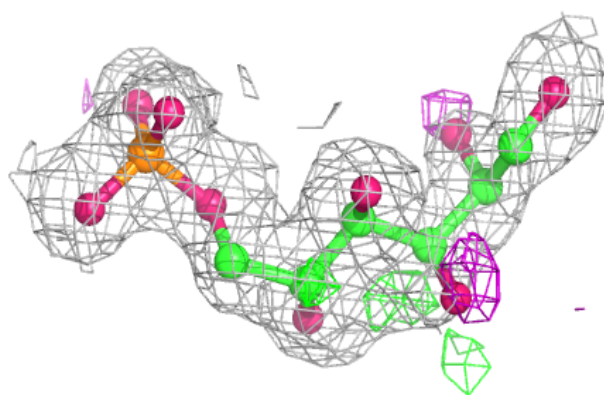
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	C	7003	6/6	0.70	0.15	26,29,30,32	0
3	GOL	A	7005	6/6	0.72	0.17	33,35,36,38	0
3	GOL	B	7004	6/6	0.72	0.24	36,37,37,38	0
3	GOL	B	7006	6/6	0.75	0.23	31,38,39,41	0
3	GOL	A	7001	6/6	0.77	0.18	24,27,28,31	0
3	GOL	B	7002	6/6	0.84	0.15	23,30,31,34	0
2	G6Q	C	5003	16/16	0.92	0.12	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	0.93	0.10	14,18,25,26	0

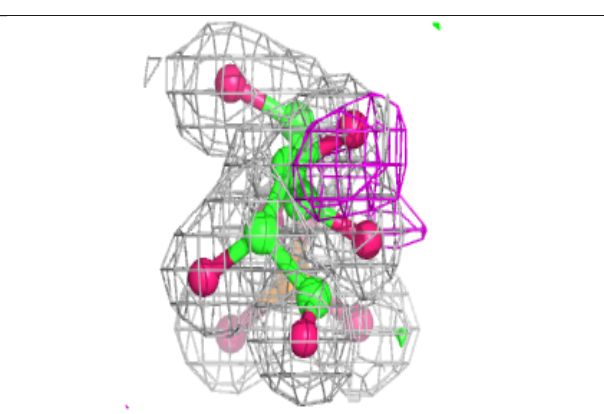
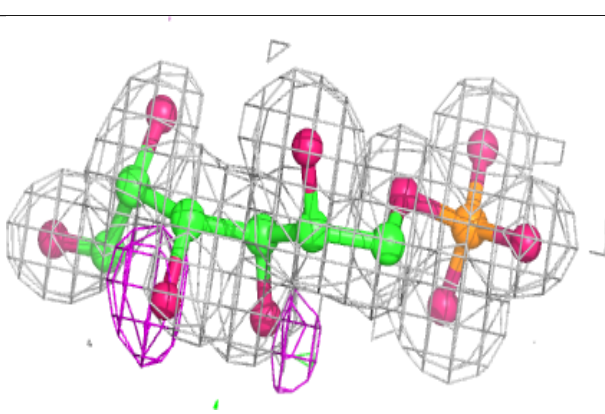
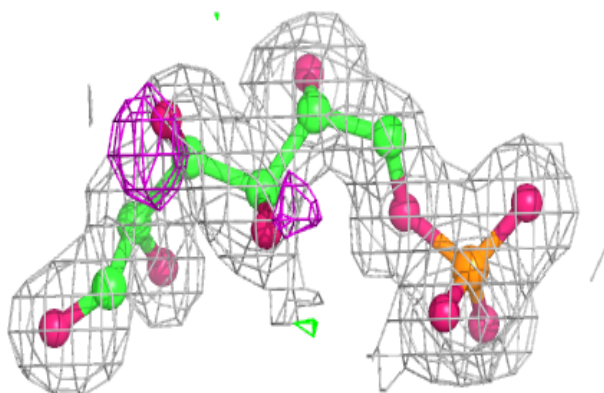
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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