



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:05 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

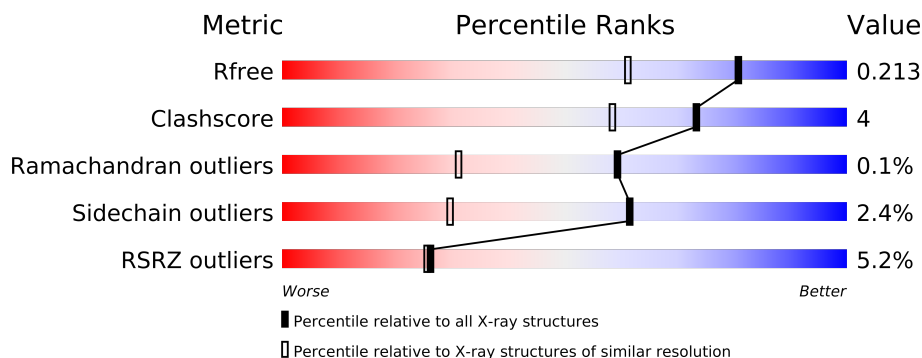
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2778 (1.60-1.56)
Clashscore	79885	3207 (1.60-1.56)
Ramachandran outliers	78287	3107 (1.60-1.56)
Sidechain outliers	78261	3104 (1.60-1.56)
RSRZ outliers	66119	2778 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	613	
1	B	613	
1	C	613	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14725 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

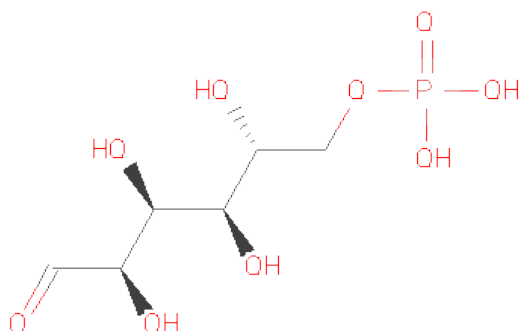
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4449	2827	781	826	15			
1	B	564	Total	C	N	O	S	0	0	0
			4449	2827	781	826	15			
1	C	561	Total	C	N	O	S	0	0	0
			4432	2818	778	821	15			

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

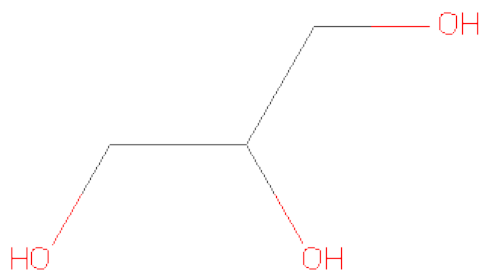
- Molecule 2 is SUGAR (GLUCOSE-6-PHOSPHATE) (three-letter code: G6Q) (formula:

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 (three-letter code: GOL) (formula: C₃H₈O₃).



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

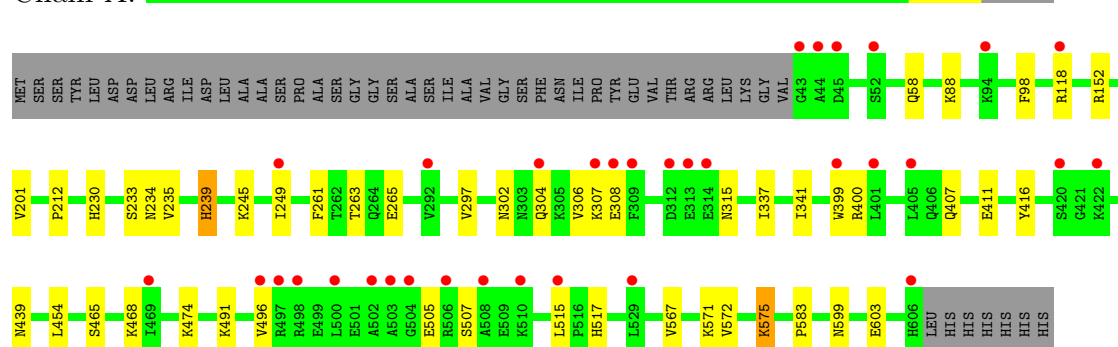
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	439	Total 439	O 439	0	0
4	B	459	Total 459	O 459	0	0
4	C	413	Total 413	O 413	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

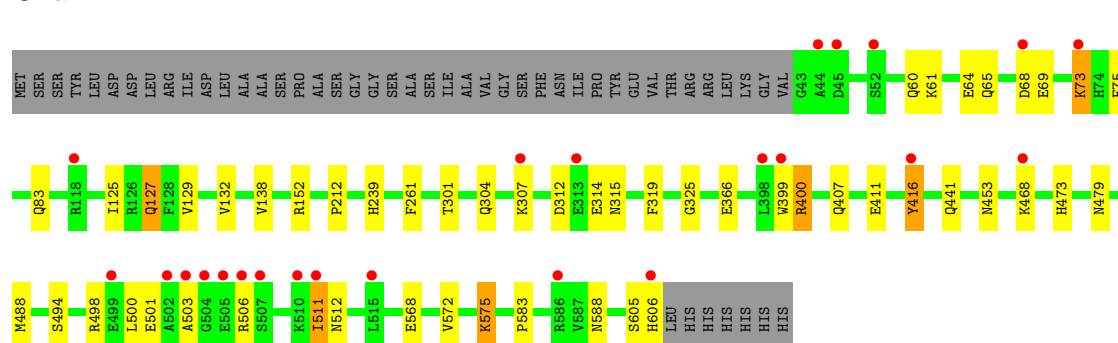
- Molecule 1: Glucose-6-phosphate isomerase, glycosomal

Chain A:



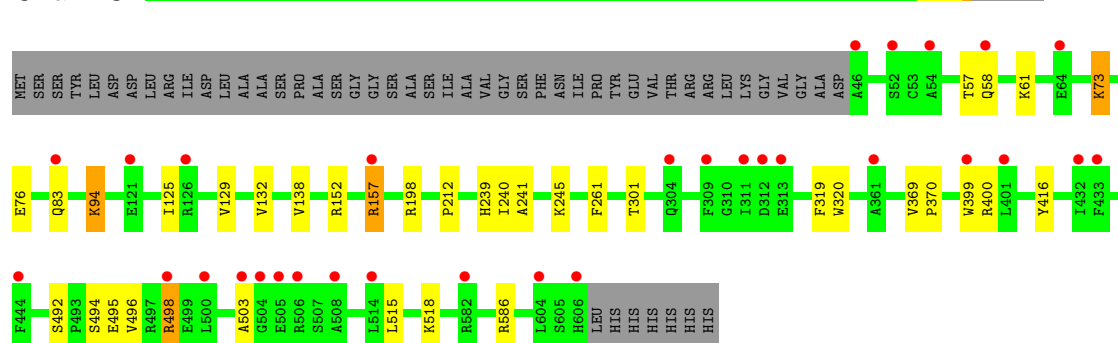
- Molecule 1: Glucose-6-phosphate isomerase, glycosomal

Chain B:



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

Chain C:



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 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
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 1.58Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.200 , 0.213 0.203 , 0.213	Depositor DCC
R_{free} test set	12151 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.6	EDS
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
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 243951 reflections	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	15	0
4	B	459	0	0	8	0
4	C	413	0	0	9	0
All	All	14725	0	13306	111	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (111) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:B:73:LYS:HA	1:B:73:LYS:HZ2	1.47	0.78
1:A:575:LYS:HB3	1:A:575: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:5002:G6Q:H3	4:B:7447:HOH:O	1.97	0.64
1:B:314:GLU:CD	1:B:314:GLU:H	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:73:LYS:CA	1:B:73:LYS:HZ2	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:C:94:LYS:HD3	4:C:7254:HOH:O	2.09	0.52
1:B:568:GLU:O	1:B:572:VAL:HG23	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
1:A:468:LYS:HE3	1:A:468:LYS:HA	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:125:ILE:O	1:B:129:VAL:HG23	2.21	0.41
1:A:201:VAL:HG22	1:A:230:HIS:HB2	2.02	0.41
1:C:132:VAL:HG22	1:C:138:VAL:HG21	2.01	0.41
1:C:241:ALA:O	1:C:245:LYS:HG3	2.20	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:A:315:ASN:ND2	4:A:7416:HOH:O	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	56	28
All	All	1683/1839 (92%)	1639 (97%)	43 (3%)	1 (0%)	59	31

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%)	69	41
1	B	479/519 (92%)	466 (97%)	13 (3%)	57	25
1	C	478/519 (92%)	465 (97%)	13 (3%)	57	25
All	All	1436/1557 (92%)	1401 (98%)	35 (2%)	61	30

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

Mol	Chain	Res	Type
1	A	152	ARG
1	A	212	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 carbohydrates 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	$\# Z > 2$
2	G6Q	A	5001	-	15,15,15	0.67	0	21,21,21	1.37	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	7001	-	5,5,5	4.86	5 (100%)	5,5,5	5.67	3 (60%)
3	GOL	A	7005	-	5,5,5	4.63	5 (100%)	5,5,5	5.76	3 (60%)
2	G6Q	B	5002	-	15,15,15	0.69	0	21,21,21	1.39	3 (14%)
3	GOL	B	7002	-	5,5,5	4.54	5 (100%)	5,5,5	5.59	3 (60%)
3	GOL	B	7004	-	5,5,5	4.57	4 (80%)	5,5,5	5.64	3 (60%)
3	GOL	B	7006	-	5,5,5	4.64	5 (100%)	5,5,5	5.78	3 (60%)
2	G6Q	C	5003	-	15,15,15	0.64	0	21,21,21	1.37	3 (14%)
3	GOL	C	7003	-	5,5,5	4.56	5 (100%)	5,5,5	5.69	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
2	G6Q	A	5001	-	-	0/19/20/20	0/0/0/0
3	GOL	A	7001	-	-	0/4/4/4	0/0/0/0
3	GOL	A	7005	-	-	0/4/4/4	0/0/0/0
2	G6Q	B	5002	-	-	0/19/20/20	0/0/0/0
3	GOL	B	7002	-	-	0/4/4/4	0/0/0/0
3	GOL	B	7004	-	-	0/4/4/4	0/0/0/0
3	GOL	B	7006	-	-	0/4/4/4	0/0/0/0
2	G6Q	C	5003	-	-	0/19/20/20	0/0/0/0
3	GOL	C	7003	-	-	0/4/4/4	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	7004	GOL	C3-C2	-7.94	1.19	1.52
3	A	7001	GOL	C3-C2	-7.73	1.20	1.52
3	B	7006	GOL	C3-C2	-7.69	1.20	1.52
3	C	7003	GOL	C3-C2	-7.63	1.20	1.52
3	A	7005	GOL	C3-C2	-7.60	1.20	1.52
3	B	7002	GOL	C3-C2	-7.55	1.21	1.52
3	A	7001	GOL	O1-C1	5.15	1.64	1.42
3	A	7005	GOL	O1-C1	4.44	1.61	1.42
3	C	7003	GOL	O1-C1	4.35	1.61	1.42
3	B	7006	GOL	O1-C1	4.34	1.61	1.42
3	B	7004	GOL	O1-C1	4.25	1.60	1.42
3	B	7002	GOL	O1-C1	4.10	1.60	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	7001	GOL	O3-C3	3.66	1.58	1.42
3	B	7002	GOL	O3-C3	3.53	1.57	1.42
3	B	7006	GOL	C1-C2	-3.42	1.38	1.52
3	B	7006	GOL	O3-C3	3.38	1.57	1.42
3	B	7004	GOL	O3-C3	3.35	1.56	1.42
3	A	7005	GOL	O3-C3	3.26	1.56	1.42
3	C	7003	GOL	O3-C3	3.24	1.56	1.42
3	A	7005	GOL	O2-C2	-3.13	1.33	1.43
3	A	7001	GOL	C1-C2	-3.13	1.39	1.52
3	B	7002	GOL	O2-C2	-3.09	1.33	1.43
3	B	7004	GOL	C1-C2	-3.03	1.39	1.52
3	A	7005	GOL	C1-C2	-3.02	1.39	1.52
3	A	7001	GOL	O2-C2	-2.90	1.34	1.43
3	C	7003	GOL	C1-C2	-2.88	1.40	1.52
3	C	7003	GOL	O2-C2	-2.83	1.34	1.43
3	B	7002	GOL	C1-C2	-2.67	1.41	1.52
3	B	7006	GOL	O2-C2	-2.53	1.35	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7005	GOL	O3-C3-C2	10.41	160.49	109.71
3	B	7006	GOL	O3-C3-C2	10.40	160.45	109.71
3	C	7003	GOL	O3-C3-C2	10.29	159.94	109.71
3	A	7001	GOL	O3-C3-C2	10.23	159.63	109.71
3	B	7004	GOL	O3-C3-C2	10.18	159.40	109.71
3	B	7002	GOL	O3-C3-C2	10.18	159.37	109.71
3	B	7006	GOL	O2-C2-C3	7.00	140.09	108.22
3	A	7005	GOL	O2-C2-C3	6.77	139.08	108.22
3	A	7001	GOL	O2-C2-C3	6.70	138.73	108.22
3	B	7004	GOL	O2-C2-C3	6.66	138.56	108.22
3	C	7003	GOL	O2-C2-C3	6.61	138.31	108.22
3	B	7002	GOL	O2-C2-C3	6.23	136.61	108.22
3	B	7002	GOL	O1-C1-C2	3.65	127.51	109.71
2	A	5001	G6Q	C3-C2-C1	3.49	116.24	111.69
3	A	7005	GOL	O1-C1-C2	3.39	126.23	109.71
3	C	7003	GOL	O1-C1-C2	3.38	126.22	109.71
3	A	7001	GOL	O1-C1-C2	3.29	125.76	109.71
2	C	5003	G6Q	C3-C2-C1	3.11	115.75	111.69
2	B	5002	G6Q	C3-C2-C1	2.99	115.58	111.69
3	B	7006	GOL	O1-C1-C2	2.97	124.19	109.71
3	B	7004	GOL	O1-C1-C2	2.94	124.06	109.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5002	G6Q	C4-C3-C2	2.49	118.11	113.67
2	C	5003	G6Q	C4-C3-C2	2.40	117.95	113.67
2	C	5003	G6Q	O3P-P-O1P	2.09	117.26	110.44
2	B	5002	G6Q	O3P-P-O1P	2.02	117.05	110.44
2	A	5001	G6Q	O3P-P-O1P	2.02	117.04	110.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	564/613 (92%)	0.44	34 (6%) 21 21	9, 15, 32, 42	0
1	B	564/613 (92%)	0.35	24 (4%) 34 34	9, 14, 31, 44	0
1	C	561/613 (91%)	0.48	31 (5%) 24 24	9, 16, 31, 44	0
All	All	1689/1839 (91%)	0.42	89 (5%) 26 25	9, 15, 31, 44	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	606	HIS	8.3
1	C	503	ALA	7.1
1	C	504	GLY	6.3
1	B	504	GLY	6.1
1	A	44	ALA	5.9
1	B	606	HIS	5.8
1	B	502	ALA	5.2
1	B	44	ALA	5.0
1	C	505	GLU	5.0
1	C	312	ASP	4.2
1	B	515	LEU	4.1
1	B	503	ALA	4.0
1	A	504	GLY	3.9
1	A	43	GLY	3.7
1	A	307	LYS	3.7
1	C	582	ARG	3.6
1	C	606	HIS	3.6
1	A	500	LEU	3.6
1	C	508	ALA	3.5
1	B	507	SER	3.5
1	B	505	GLU	3.5
1	A	502	ALA	3.4
1	A	52	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	506	ARG	3.4
1	A	506	ARG	3.4
1	B	499	GLU	3.1
1	A	515	LEU	3.0
1	C	498	ARG	3.0
1	A	503	ALA	2.9
1	B	506	ARG	2.8
1	C	313	GLU	2.8
1	B	45	ASP	2.8
1	B	307	LYS	2.8
1	A	304	GLN	2.8
1	A	420	SER	2.8
1	C	399	TRP	2.7
1	A	312	ASP	2.7
1	C	401	LEU	2.7
1	A	308	GLU	2.7
1	B	313	GLU	2.7
1	C	514	LEU	2.7
1	A	94	LYS	2.7
1	A	309	PHE	2.7
1	C	500	LEU	2.6
1	C	444	PHE	2.6
1	B	68	ASP	2.6
1	C	604	LEU	2.6
1	C	58	GLN	2.6
1	A	496	VAL	2.5
1	A	45	ASP	2.5
1	A	469	ILE	2.5
1	B	468	LYS	2.4
1	A	497	ARG	2.4
1	B	399	TRP	2.4
1	C	361	ALA	2.4
1	A	314	GLU	2.4
1	B	586	ARG	2.4
1	A	118	ARG	2.4
1	A	508	ALA	2.3
1	C	157	ARG	2.3
1	A	292	VAL	2.3
1	A	313	GLU	2.3
1	A	510	LYS	2.3
1	A	401	LEU	2.3
1	C	432	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	511	ILE	2.2
1	C	64	GLU	2.2
1	C	433	PHE	2.2
1	A	422	LYS	2.2
1	C	83	GLN	2.2
1	C	126	ARG	2.1
1	C	46	ALA	2.1
1	A	498	ARG	2.1
1	B	416	TYR	2.1
1	A	529	LEU	2.1
1	C	121	GLU	2.1
1	C	52	SER	2.1
1	B	118	ARG	2.1
1	C	54	ALA	2.1
1	C	309	PHE	2.1
1	C	304	GLN	2.1
1	B	52	SER	2.0
1	A	249	ILE	2.0
1	A	405	LEU	2.0
1	B	398	LEU	2.0
1	B	73	LYS	2.0
1	B	510	LYS	2.0
1	C	311	ILE	2.0
1	A	399	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	B	7006	6/6	0.21	5.12	31,38,39,41	0
3	GOL	A	7001	6/6	0.17	3.76	24,27,28,31	0
3	GOL	B	7004	6/6	0.23	3.32	36,37,37,38	0
3	GOL	C	7003	6/6	0.16	2.81	26,29,30,32	0
2	G6Q	C	5003	16/16	0.13	1.41	17,23,29,29	0
3	GOL	B	7002	6/6	0.14	0.72	23,30,31,34	0
2	G6Q	A	5001	16/16	0.11	0.51	16,21,27,28	0
3	GOL	A	7005	6/6	0.17	0.41	33,35,36,38	0
2	G6Q	B	5002	16/16	0.09	0.15	14,18,25,26	0

6.5 Other polymers

There are no such residues in this entry.