Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 02:07 PM JST

PDB ID	:	6JAE
Title	:	Crystal structure of Trypanosoma brucei gambiense glycerol kinase complex with Pi (pyrophosphatase reaction)
Authors	:	Balogun, E.O.; Chishima, T.; Ichinose, M.; Inaoka, D.K.; Kido, Y.; Ibrahim, B.; Bringaud, F.; de Koning, H.; McKerrow, J.H.; Watanabe, Y.; Nozaki, T.; Michels, P.A.M.; Harada, S.; Kita, K.; Shiba, T.
Deposited on	:	2019-01-24
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

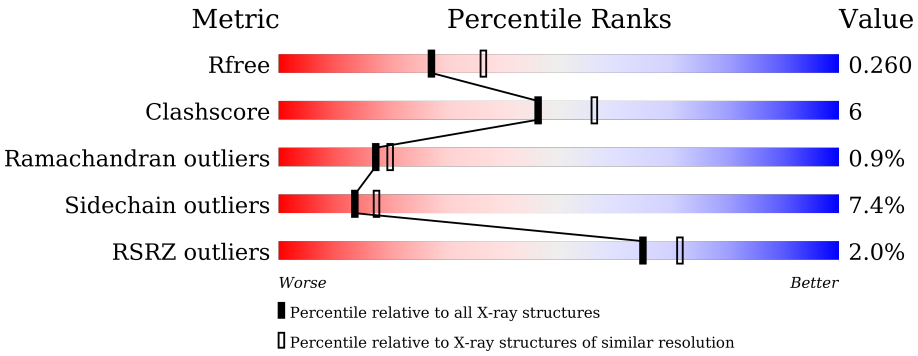
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	518	4% 80% 16%
1	B	518	85% 12%
1	C	518	3% 82% 13%
1	D	518	% 86% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15913 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	B	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	C	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	D	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			

There are 24 discrepancies between the modelled and reference sequences:

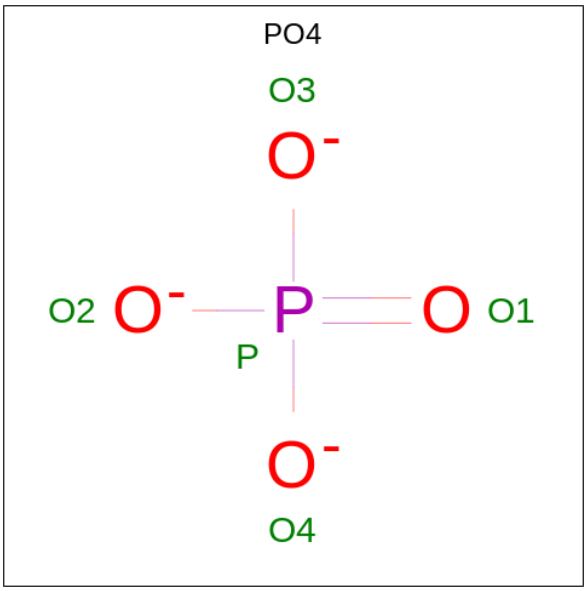
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP D3KVM3
A	-4	ILE	-	expression tag	UNP D3KVM3
A	-3	ASP	-	expression tag	UNP D3KVM3
A	-2	PRO	-	expression tag	UNP D3KVM3
A	-1	PHE	-	expression tag	UNP D3KVM3
A	0	THR	-	expression tag	UNP D3KVM3
B	-5	GLY	-	expression tag	UNP D3KVM3
B	-4	ILE	-	expression tag	UNP D3KVM3
B	-3	ASP	-	expression tag	UNP D3KVM3
B	-2	PRO	-	expression tag	UNP D3KVM3
B	-1	PHE	-	expression tag	UNP D3KVM3
B	0	THR	-	expression tag	UNP D3KVM3
C	-5	GLY	-	expression tag	UNP D3KVM3
C	-4	ILE	-	expression tag	UNP D3KVM3
C	-3	ASP	-	expression tag	UNP D3KVM3
C	-2	PRO	-	expression tag	UNP D3KVM3
C	-1	PHE	-	expression tag	UNP D3KVM3
C	0	THR	-	expression tag	UNP D3KVM3
D	-5	GLY	-	expression tag	UNP D3KVM3
D	-4	ILE	-	expression tag	UNP D3KVM3
D	-3	ASP	-	expression tag	UNP D3KVM3

Continued on next page...

Continued from previous page...

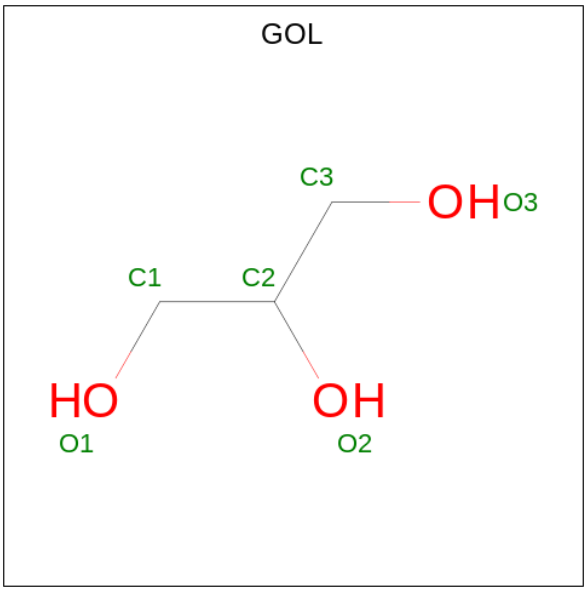
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PRO	-	expression tag	UNP D3KVM3
D	-1	PHE	-	expression tag	UNP D3KVM3
D	0	THR	-	expression tag	UNP D3KVM3

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

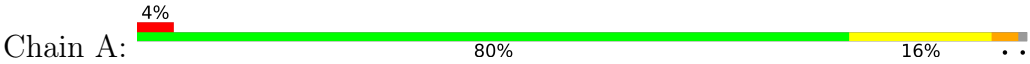
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	11	Total O 11 11	0	0
4	B	13	Total O 13 13	0	0
4	C	13	Total O 13 13	0	0
4	D	14	Total O 14 14	0	0

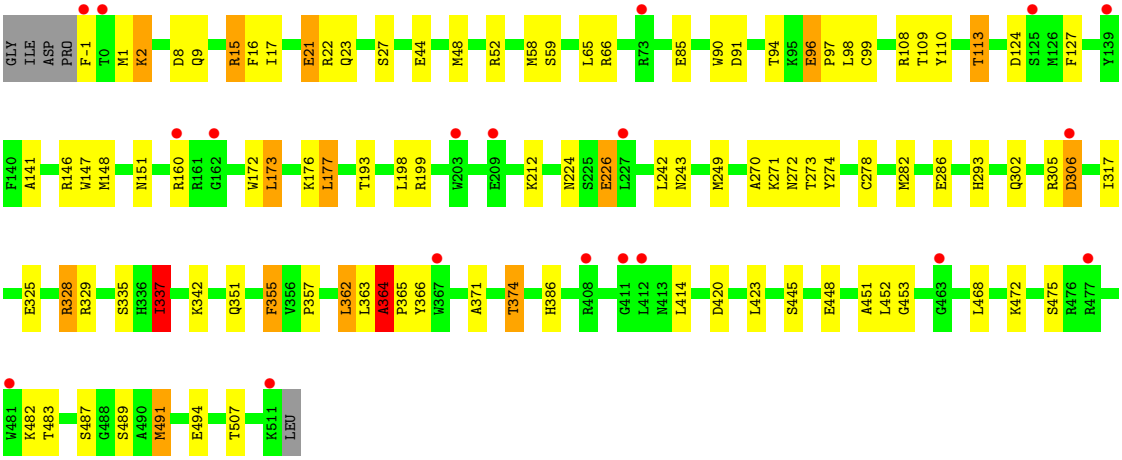
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glycerol kinase

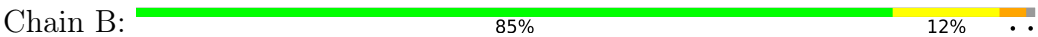
Chain A:

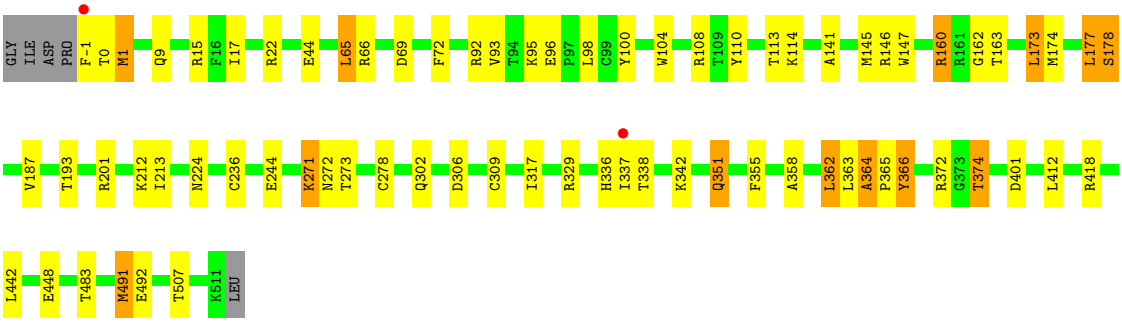




• Molecule 1: Glycerol kinase

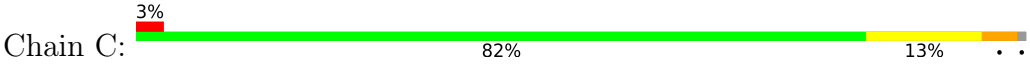
Chain B:

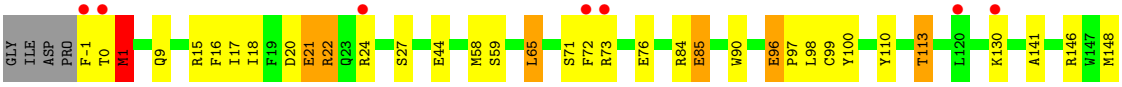


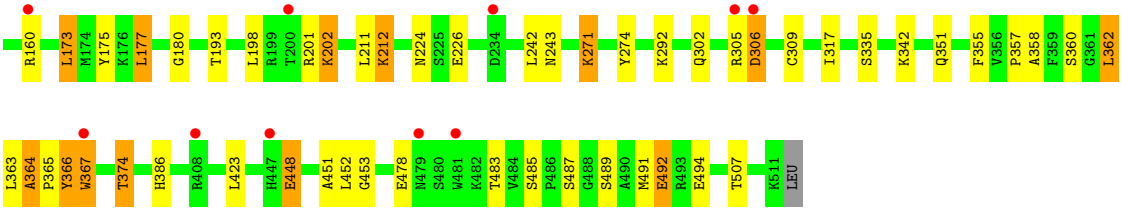


• Molecule 1: Glycerol kinase

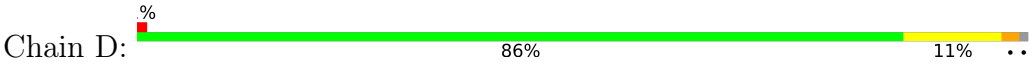
Chain C:

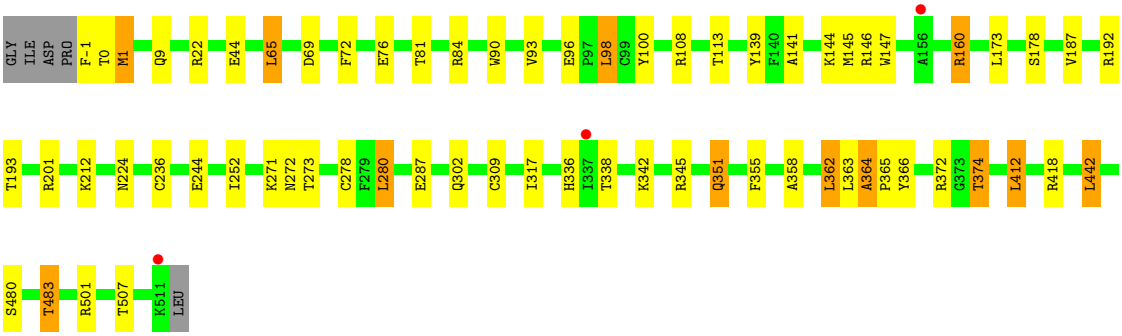






• Molecule 1: Glycerol kinase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.31Å 122.23Å 155.96Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	19.84 – 2.30 19.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.84-2.30) 98.9 (19.84-2.30)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.209 , 0.265 0.211 , 0.260	Depositor DCC
R_{free} test set	5183 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 28.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15913	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, 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	0.69	0/4039	0.85	4/5465 (0.1%)
1	B	0.76	0/4039	0.87	2/5465 (0.0%)
1	C	0.69	0/4039	0.84	1/5465 (0.0%)
1	D	0.76	0/4039	0.87	5/5465 (0.1%)
All	All	0.73	0/16156	0.86	12/21860 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	3
1	D	0	1
All	All	0	7

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	22	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	D	22	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	15	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	22	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	364	ALA	N-CA-C	-5.55	96.00	111.00
1	C	22	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	8	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	D	345	ARG	NE-CZ-NH2	5.22	122.91	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	192	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	D	412	LEU	CA-CB-CG	5.14	127.13	115.30
1	D	345	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	337	ILE	CB-CA-C	-5.02	101.56	111.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	ASP	Peptide
1	A	363	LEU	Peptide
1	B	363	LEU	Peptide
1	C	305	ARG	Peptide
1	C	306	ASP	Peptide
1	C	363	LEU	Peptide
1	D	363	LEU	Peptide

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	3957	0	3970	61	0
1	B	3957	0	3970	48	0
1	C	3957	0	3970	48	0
1	D	3957	0	3970	42	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	2	0
3	C	6	0	8	2	0
3	D	6	0	8	3	0
4	A	11	0	0	0	0
4	B	13	0	0	1	0
4	C	13	0	0	0	0
4	D	14	0	0	0	0
All	All	15913	0	15912	199	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 6.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE1	1:A:21:GLU:CG	1.97	0.93
1:C:110:TYR:O	1:C:113:THR:HG22	1.70	0.91
1:A:1:MET:CE	1:A:21:GLU:CG	2.49	0.89
1:A:328:ARG:HH12	1:A:337:ILE:HD13	1.41	0.83
1:A:1:MET:HE1	1:A:21:GLU:HG3	1.59	0.82
1:A:1:MET:HE1	1:A:21:GLU:HG2	1.60	0.82
1:A:1:MET:CE	1:A:21:GLU:HG3	2.13	0.77
1:B:0:THR:O	1:B:1:MET:HB2	1.83	0.77
1:A:1:MET:CE	1:A:21:GLU:HG2	2.13	0.76
1:D:-1:PHE:O	1:D:0:THR:OG1	2.06	0.72
1:B:364:ALA:HB1	1:B:365:PRO:CD	2.18	0.72
1:B:374:THR:HG23	1:B:507:THR:HG22	1.72	0.72
1:B:44:GLU:HG2	1:B:100:TYR:HB3	1.73	0.71
1:B:224:ASN:HD22	1:B:302:GLN:H	1.35	0.71
1:A:110:TYR:O	1:A:113:THR:HG22	1.89	0.71
1:A:364:ALA:HB1	1:A:365:PRO:HD2	1.73	0.70
1:A:351:GLN:HG2	1:A:386:HIS:CD2	2.25	0.70
1:D:374:THR:HG23	1:D:507:THR:HG22	1.74	0.70
1:B:160:ARG:HH11	1:B:160:ARG:HG2	1.58	0.69
1:C:224:ASN:HD22	1:C:302:GLN:H	1.40	0.69
1:C:364:ALA:CB	1:C:365:PRO:CD	2.72	0.68
1:D:224:ASN:HD22	1:D:302:GLN:H	1.42	0.68
1:B:160:ARG:HH11	1:B:160:ARG:CG	2.07	0.68
1:A:364:ALA:HB1	1:A:365:PRO:CD	2.23	0.68
1:A:224:ASN:HD22	1:A:302:GLN:H	1.42	0.67
1:C:84:ARG:HE	3:C:602:GOL:H31	1.59	0.67
1:B:374:THR:CG2	1:B:507:THR:HG22	2.24	0.67
1:D:44:GLU:HG2	1:D:100:TYR:HB3	1.78	0.66
1:B:364:ALA:HB1	1:B:365:PRO:HD2	1.77	0.66
1:B:0:THR:O	1:B:1:MET:CB	2.44	0.66
1:A:1:MET:HE1	1:A:21:GLU:H	1.61	0.65
1:A:96:GLU:HG3	1:A:97:PRO:HD2	1.77	0.65
1:D:336:HIS:HD2	1:D:338:THR:OG1	1.79	0.65
1:A:99:CYS:SG	1:A:148:MET:HE2	2.38	0.64
1:A:1:MET:HE3	1:A:21:GLU:CG	2.26	0.64
1:C:351:GLN:HG2	1:C:386:HIS:CD2	2.33	0.64
1:D:364:ALA:HB1	1:D:365:PRO:CD	2.26	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:CYS:SG	1:C:148:MET:CE	2.87	0.63
1:D:374:THR:CG2	1:D:507:THR:HG22	2.28	0.63
1:D:0:THR:O	1:D:1:MET:CB	2.47	0.63
1:D:372:ARG:O	1:D:374:THR:HG22	1.99	0.62
1:A:99:CYS:SG	1:A:148:MET:CE	2.87	0.62
1:A:364:ALA:CB	1:A:365:PRO:HD2	2.29	0.62
1:B:104:TRP:CZ2	3:B:701:GOL:H32	2.35	0.62
1:B:372:ARG:O	1:B:374:THR:HG22	1.99	0.62
1:C:366:TYR:O	1:C:367:TRP:C	2.38	0.62
1:C:90:TRP:HA	1:C:98:LEU:HD22	1.82	0.61
1:B:364:ALA:CB	1:B:365:PRO:CD	2.78	0.61
1:C:99:CYS:SG	1:C:148:MET:HE2	2.40	0.61
1:A:362:LEU:HD22	1:A:371:ALA:CB	2.30	0.61
1:A:374:THR:HG21	1:A:507:THR:HA	1.82	0.61
1:A:364:ALA:CB	1:A:365:PRO:CD	2.78	0.61
1:C:364:ALA:HB1	1:C:365:PRO:HD3	1.84	0.60
1:D:0:THR:O	1:D:1:MET:HB2	2.02	0.60
1:B:44:GLU:HG2	1:B:100:TYR:CB	2.32	0.59
1:D:146:ARG:NH1	1:D:212:LYS:O	2.35	0.59
1:D:160:ARG:HG2	1:D:160:ARG:HH11	1.69	0.58
1:B:364:ALA:CB	1:B:365:PRO:HD2	2.34	0.57
1:C:364:ALA:HB1	1:C:365:PRO:CD	2.34	0.57
1:D:336:HIS:CD2	1:D:338:THR:OG1	2.57	0.57
1:A:328:ARG:NH1	1:A:337:ILE:HD13	2.17	0.57
1:B:173:LEU:O	1:B:177:LEU:HB2	2.04	0.57
1:D:44:GLU:HG2	1:D:100:TYR:CB	2.34	0.57
1:B:65:LEU:HD22	1:B:69:ASP:HB3	1.86	0.56
1:D:374:THR:HG21	1:D:507:THR:HA	1.86	0.56
1:C:16:PHE:CD2	1:C:58:MET:HA	2.40	0.56
1:B:146:ARG:NH1	1:B:212:LYS:O	2.38	0.56
1:C:358:ALA:HB2	1:C:362:LEU:HD13	1.87	0.56
1:A:90:TRP:HA	1:A:98:LEU:HD22	1.89	0.55
1:D:84:ARG:HE	3:D:701:GOL:C1	2.20	0.55
1:D:364:ALA:CB	1:D:365:PRO:CD	2.84	0.55
1:A:44:GLU:HG3	1:A:108:ARG:HH22	1.71	0.54
1:C:17:ILE:HD12	1:C:451:ALA:CB	2.36	0.54
1:C:20:ASP:OD2	1:C:22:ARG:NH1	2.39	0.54
1:B:272:ASN:HD21	1:B:278:CYS:HB3	1.73	0.54
1:D:84:ARG:HE	3:D:701:GOL:H11	1.72	0.53
1:D:65:LEU:HD22	1:D:69:ASP:HB3	1.89	0.53
1:C:374:THR:HG21	1:C:507:THR:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ARG:HH11	1:D:160:ARG:CG	2.22	0.53
1:B:306:ASP:O	1:D:212:LYS:HE3	2.09	0.53
1:C:99:CYS:SG	1:C:148:MET:HE3	2.48	0.53
1:D:364:ALA:HB1	1:D:365:PRO:HD2	1.90	0.53
1:C:201:ARG:HD3	1:C:309:CYS:SG	2.49	0.52
1:A:146:ARG:NH1	1:A:212:LYS:O	2.42	0.52
1:C:96:GLU:HG3	1:C:97:PRO:HD2	1.92	0.52
1:D:273:THR:O	1:D:278:CYS:HA	2.09	0.52
1:B:160:ARG:HB2	1:B:160:ARG:NH1	2.24	0.52
1:B:374:THR:HG21	1:B:507:THR:HA	1.90	0.52
1:C:202:LYS:HE3	1:C:202:LYS:HA	1.92	0.52
1:A:48:MET:O	1:A:52:ARG:HG3	2.10	0.52
1:A:325:GLU:O	1:A:329:ARG:HG2	2.10	0.52
1:B:92:ARG:HD3	1:B:163:THR:HA	1.92	0.51
1:D:139:TYR:O	1:D:144:LYS:HE2	2.10	0.51
1:C:85:GLU:OE1	3:C:602:GOL:H32	2.11	0.51
1:B:351:GLN:CG	1:B:351:GLN:O	2.59	0.51
1:C:44:GLU:HG2	1:C:100:TYR:HB3	1.93	0.50
1:D:351:GLN:O	1:D:351:GLN:CG	2.60	0.50
1:D:84:ARG:HB2	3:D:701:GOL:H11	1.94	0.50
1:A:99:CYS:SG	1:A:148:MET:HE3	2.52	0.49
1:B:65:LEU:HD13	1:B:72:PHE:CG	2.47	0.49
1:A:16:PHE:CD2	1:A:58:MET:HA	2.46	0.49
1:B:160:ARG:NH1	1:B:160:ARG:CB	2.75	0.49
1:D:272:ASN:HD21	1:D:278:CYS:HB3	1.76	0.49
1:A:141:ALA:HB3	1:A:193:THR:HA	1.93	0.49
1:C:-1:PHE:O	1:C:0:THR:HG23	2.11	0.49
1:A:355:PHE:O	1:A:357:PRO:HD3	2.13	0.49
1:A:23:GLN:HE22	1:A:475:SER:HB2	1.77	0.48
1:B:273:THR:O	1:B:278:CYS:HA	2.13	0.48
1:B:160:ARG:HH11	1:B:160:ARG:CB	2.26	0.48
1:C:1:MET:SD	1:C:21:GLU:CG	3.01	0.48
1:A:374:THR:HG23	1:A:507:THR:HG22	1.95	0.48
1:A:374:THR:CG2	1:A:507:THR:HG22	2.44	0.48
1:D:201:ARG:HD3	1:D:309:CYS:SG	2.54	0.48
1:C:146:ARG:NH1	1:C:212:LYS:HB3	2.28	0.47
1:A:172:TRP:CH2	1:A:176:LYS:HD3	2.50	0.47
1:B:160:ARG:HB2	1:B:160:ARG:CZ	2.45	0.47
1:D:364:ALA:CB	1:D:365:PRO:HD2	2.45	0.47
1:A:274:TYR:HB3	1:A:423:LEU:HB2	1.97	0.47
1:B:92:ARG:NH1	1:B:162:GLY:O	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ALA:CB	1:B:362:LEU:HD13	2.45	0.46
1:C:364:ALA:HB3	1:C:365:PRO:HD2	1.97	0.46
1:C:351:GLN:HG3	1:C:351:GLN:O	2.15	0.46
1:A:351:GLN:O	1:A:351:GLN:HG3	2.15	0.46
1:D:65:LEU:HD13	1:D:72:PHE:CG	2.51	0.46
1:A:226:GLU:O	1:A:249:MET:HA	2.15	0.46
1:A:270:ALA:HB3	1:A:414:LEU:HD11	1.97	0.46
1:B:65:LEU:HD22	1:B:69:ASP:CB	2.46	0.45
3:B:701:GOL:C1	4:B:801:HOH:O	2.64	0.45
1:B:141:ALA:HB3	1:B:193:THR:HA	1.97	0.45
1:D:160:ARG:CZ	1:D:160:ARG:HB2	2.45	0.45
1:C:141:ALA:HB3	1:C:193:THR:HA	1.99	0.45
1:C:364:ALA:HB3	1:C:365:PRO:CD	2.46	0.45
1:D:141:ALA:O	1:D:145:MET:HG3	2.17	0.45
1:B:17:ILE:CD1	1:B:448:GLU:HG2	2.47	0.45
1:D:272:ASN:HB2	1:D:280:LEU:HD22	1.99	0.45
1:A:109:THR:O	1:A:113:THR:HB	2.17	0.44
1:C:71:SER:O	1:C:72:PHE:C	2.54	0.44
1:A:242:LEU:O	1:A:243:ASN:HB3	2.18	0.44
1:C:17:ILE:HD13	1:C:448:GLU:HG2	1.99	0.44
1:D:65:LEU:HD13	1:D:72:PHE:CD2	2.53	0.44
1:A:173:LEU:O	1:A:177:LEU:HB2	2.18	0.44
1:A:489:SER:C	1:A:491:MET:N	2.71	0.44
1:B:358:ALA:HB2	1:B:362:LEU:HD13	2.00	0.44
1:D:358:ALA:CB	1:D:362:LEU:HD13	2.48	0.43
1:C:274:TYR:HB3	1:C:423:LEU:HB2	2.00	0.43
1:A:270:ALA:HB2	1:A:282:MET:HG3	2.00	0.43
1:B:110:TYR:CE1	1:B:114:LYS:HE2	2.53	0.43
1:B:201:ARG:HD3	1:B:309:CYS:SG	2.58	0.43
1:A:15:ARG:NH1	1:A:448:GLU:OE1	2.52	0.43
1:C:18:ILE:HG21	1:C:65:LEU:HD12	2.01	0.43
1:C:173:LEU:O	1:C:177:LEU:HB2	2.18	0.43
1:B:374:THR:HG21	1:B:507:THR:HG22	2.01	0.43
1:C:202:LYS:HA	1:C:202:LYS:CE	2.47	0.43
1:A:1:MET:HE3	1:A:21:GLU:CD	2.39	0.43
1:C:146:ARG:HD3	1:C:211:LEU:O	2.18	0.43
1:B:271:LYS:HD2	1:B:271:LYS:C	2.39	0.43
1:C:374:THR:HG23	1:C:507:THR:HG22	2.00	0.43
1:D:90:TRP:HA	1:D:98:LEU:HD22	2.00	0.43
1:B:366:TYR:OH	1:B:401:ASP:OD1	2.29	0.43
1:D:442:LEU:HD12	1:D:483:THR:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:THR:HA	1:D:252:ILE:O	2.18	0.42
1:B:174:MET:O	1:B:178:SER:HB2	2.18	0.42
1:A:273:THR:O	1:A:278:CYS:HA	2.19	0.42
1:C:146:ARG:NH1	1:C:212:LYS:O	2.52	0.42
1:A:124:ASP:O	1:A:127:PHE:HB3	2.20	0.42
1:B:351:GLN:O	1:B:351:GLN:HG3	2.20	0.42
1:A:44:GLU:HG3	1:A:108:ARG:NH2	2.34	0.42
1:A:452:LEU:O	1:A:453:GLY:C	2.58	0.42
1:B:491:MET:HG3	1:B:492:GLU:N	2.34	0.42
1:C:489:SER:OG	1:C:492:GLU:HB2	2.19	0.42
1:D:108:ARG:HD3	1:D:147:TRP:CE2	2.55	0.42
1:D:141:ALA:HB3	1:D:193:THR:HA	2.02	0.42
1:A:90:TRP:CA	1:A:98:LEU:HD22	2.50	0.41
1:A:146:ARG:NH1	1:A:212:LYS:HB3	2.35	0.41
1:C:24:ARG:NH2	1:C:478:GLU:O	2.53	0.41
1:D:65:LEU:HD22	1:D:69:ASP:CB	2.49	0.41
1:B:336:HIS:HD2	1:B:338:THR:OG1	2.04	0.41
1:C:175:TYR:CE1	1:C:180:GLY:HA2	2.56	0.41
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.87	0.41
1:A:468:LEU:O	1:A:472:LYS:HG3	2.20	0.41
1:C:355:PHE:O	1:C:357:PRO:HD3	2.20	0.41
1:A:1:MET:HE2	1:A:2:LYS:N	2.35	0.41
1:C:1:MET:SD	1:C:21:GLU:HG2	2.60	0.41
1:A:91:ASP:HB3	1:A:94:THR:OG1	2.20	0.41
1:C:90:TRP:CA	1:C:98:LEU:HD22	2.49	0.41
1:C:374:THR:CG2	1:C:507:THR:HG22	2.51	0.41
1:C:452:LEU:O	1:C:453:GLY:C	2.58	0.41
1:C:271:LYS:HD2	1:C:271:LYS:C	2.41	0.41
1:A:17:ILE:HD12	1:A:451:ALA:CB	2.50	0.40
1:A:147:TRP:O	1:A:151:ASN:OD1	2.39	0.40
1:A:273:THR:HA	1:A:420:ASP:OD2	2.21	0.40
1:A:293:HIS:O	1:A:365:PRO:HA	2.21	0.40
1:B:141:ALA:O	1:B:145:MET:HG3	2.21	0.40
1:B:108:ARG:HD3	1:B:147:TRP:CE2	2.56	0.40
1:B:212:LYS:HD3	1:B:212:LYS:HA	2.01	0.40
1:C:242:LEU:O	1:C:243:ASN:HB3	2.21	0.40
1:A:272:ASN:HD21	1:A:278:CYS:HB3	1.87	0.40
1:B:65:LEU:HD13	1:B:72:PHE:CD2	2.57	0.40
1:D:160:ARG:CG	1:D:160:ARG:NH1	2.84	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	511/518 (99%)	482 (94%)	24 (5%)	5 (1%)	15	17
1	B	511/518 (99%)	492 (96%)	16 (3%)	3 (1%)	25	31
1	C	511/518 (99%)	483 (94%)	21 (4%)	7 (1%)	11	11
1	D	511/518 (99%)	491 (96%)	17 (3%)	3 (1%)	25	31
All	All	2044/2072 (99%)	1948 (95%)	78 (4%)	18 (1%)	17	20

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA
1	B	1	MET
1	B	236	CYS
1	B	364	ALA
1	C	1	MET
1	C	306	ASP
1	C	364	ALA
1	D	1	MET
1	D	364	ALA
1	A	226	GLU
1	A	306	ASP
1	C	367	TRP
1	C	487	SER
1	A	487	SER
1	D	236	CYS
1	A	85	GLU
1	C	85	GLU
1	C	226	GLU

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	421/425 (99%)	388 (92%)	33 (8%)	12	16
1	B	421/425 (99%)	390 (93%)	31 (7%)	13	17
1	C	421/425 (99%)	388 (92%)	33 (8%)	12	16
1	D	421/425 (99%)	393 (93%)	28 (7%)	16	21
All	All	1684/1700 (99%)	1559 (93%)	125 (7%)	13	17

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	PHE
1	A	2	LYS
1	A	9	GLN
1	A	15	ARG
1	A	21	GLU
1	A	27	SER
1	A	59	SER
1	A	65	LEU
1	A	66	ARG
1	A	96	GLU
1	A	113	THR
1	A	160	ARG
1	A	173	LEU
1	A	177	LEU
1	A	198	LEU
1	A	199	ARG
1	A	271	LYS
1	A	286	GLU
1	A	305	ARG
1	A	317	ILE
1	A	328	ARG
1	A	335	SER
1	A	337	ILE
1	A	342	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	355	PHE
1	A	362	LEU
1	A	366	TYR
1	A	374	THR
1	A	445	SER
1	A	482	LYS
1	A	483	THR
1	A	491	MET
1	A	494	GLU
1	B	-1	PHE
1	B	9	GLN
1	B	65	LEU
1	B	66	ARG
1	B	93	VAL
1	B	95	LYS
1	B	96	GLU
1	B	98	LEU
1	B	113	THR
1	B	160	ARG
1	B	173	LEU
1	B	177	LEU
1	B	178	SER
1	B	187	VAL
1	B	213	ILE
1	B	244	GLU
1	B	271	LYS
1	B	317	ILE
1	B	329	ARG
1	B	337	ILE
1	B	342	LYS
1	B	351	GLN
1	B	355	PHE
1	B	362	LEU
1	B	366	TYR
1	B	374	THR
1	B	412	LEU
1	B	418	ARG
1	B	442	LEU
1	B	483	THR
1	B	491	MET
1	C	1	MET
1	C	9	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	15	ARG
1	C	21	GLU
1	C	27	SER
1	C	59	SER
1	C	65	LEU
1	C	73	ARG
1	C	76	GLU
1	C	96	GLU
1	C	113	THR
1	C	130	LYS
1	C	160	ARG
1	C	173	LEU
1	C	177	LEU
1	C	198	LEU
1	C	202	LYS
1	C	212	LYS
1	C	271	LYS
1	C	292	LYS
1	C	317	ILE
1	C	335	SER
1	C	342	LYS
1	C	360	SER
1	C	362	LEU
1	C	366	TYR
1	C	374	THR
1	C	448	GLU
1	C	483	THR
1	C	485	SER
1	C	491	MET
1	C	492	GLU
1	C	494	GLU
1	D	9	GLN
1	D	65	LEU
1	D	76	GLU
1	D	93	VAL
1	D	96	GLU
1	D	98	LEU
1	D	113	THR
1	D	160	ARG
1	D	173	LEU
1	D	178	SER
1	D	187	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	244	GLU
1	D	271	LYS
1	D	280	LEU
1	D	287	GLU
1	D	317	ILE
1	D	342	LYS
1	D	351	GLN
1	D	355	PHE
1	D	362	LEU
1	D	366	TYR
1	D	374	THR
1	D	412	LEU
1	D	418	ARG
1	D	442	LEU
1	D	480	SER
1	D	483	THR
1	D	501	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	151	ASN
1	A	224	ASN
1	A	272	ASN
1	A	302	GLN
1	A	336	HIS
1	A	351	GLN
1	A	393	GLN
1	B	23	GLN
1	B	151	ASN
1	B	224	ASN
1	B	272	ASN
1	B	302	GLN
1	B	336	HIS
1	B	351	GLN
1	B	413	ASN
1	B	447	HIS
1	C	23	GLN
1	C	151	ASN
1	C	224	ASN
1	C	272	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	336	HIS
1	C	351	GLN
1	D	23	GLN
1	D	224	ASN
1	D	272	ASN
1	D	336	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

6 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	PO4	C	601	-	4,4,4	0.67	0	6,6,6	0.77	0
3	GOL	A	602	-	5,5,5	0.53	0	5,5,5	0.40	0
3	GOL	C	602	-	5,5,5	0.77	0	5,5,5	1.09	0
3	GOL	B	701	-	5,5,5	0.58	0	5,5,5	0.93	0
3	GOL	D	701	-	5,5,5	0.53	0	5,5,5	1.01	0
2	PO4	A	601	-	4,4,4	0.84	0	6,6,6	0.90	0

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	D	701	-	-	2/4/4/4	-
3	GOL	A	602	-	-	0/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
3	GOL	B	701	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	GOL	C1-C2-C3-O3
3	C	602	GOL	C1-C2-C3-O3
3	D	701	GOL	C1-C2-C3-O3
3	C	602	GOL	O2-C2-C3-O3
3	D	701	GOL	O2-C2-C3-O3
3	B	701	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	GOL	2	0
3	B	701	GOL	2	0
3	D	701	GOL	3	0

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^{th} 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	513/518 (99%)	0.20	19 (3%) 41 48	40, 60, 85, 108	1 (0%)
1	B	513/518 (99%)	-0.02	2 (0%) 92 95	37, 51, 70, 97	1 (0%)
1	C	513/518 (99%)	0.22	17 (3%) 46 53	40, 59, 85, 110	1 (0%)
1	D	513/518 (99%)	-0.04	3 (0%) 89 92	36, 50, 71, 98	1 (0%)
All	All	2052/2072 (99%)	0.09	41 (1%) 65 71	36, 55, 80, 110	4 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-1	PHE	6.5
1	A	306	ASP	5.5
1	C	0	THR	4.6
1	A	-1	PHE	3.9
1	C	306	ASP	3.8
1	A	162	GLY	3.5
1	A	408	ARG	3.3
1	D	337	ILE	3.1
1	A	0	THR	3.1
1	A	367	TRP	3.0
1	C	120	LEU	3.0
1	D	156	ALA	2.9
1	B	-1	PHE	2.8
1	C	200	THR	2.8
1	A	463	GLY	2.7
1	C	447	HIS	2.7
1	C	73	ARG	2.7
1	C	481	TRP	2.5
1	A	209	GLU	2.5
1	A	411	GLY	2.5
1	C	305	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	24	ARG	2.4
1	D	511	LYS	2.4
1	C	408	ARG	2.4
1	A	203	TRP	2.4
1	C	72	PHE	2.4
1	A	227	LEU	2.3
1	A	481	TRP	2.3
1	A	511	LYS	2.3
1	A	160	ARG	2.3
1	A	477	ARG	2.3
1	A	73	ARG	2.2
1	C	160	ARG	2.2
1	C	234	ASP	2.2
1	C	479	ASN	2.1
1	C	130	LYS	2.1
1	A	139	TYR	2.1
1	B	337	ILE	2.0
1	C	367	TRP	2.0
1	A	412	LEU	2.0
1	A	125	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	D	701	6/6	0.85	0.20	58,69,73,81	0
3	GOL	C	602	6/6	0.87	0.19	44,62,69,76	0
3	GOL	B	701	6/6	0.88	0.19	57,67,76,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	602	6/6	0.93	0.10	41,42,48,53	0
2	PO4	A	601	5/5	0.94	0.12	55,67,75,80	0
2	PO4	C	601	5/5	0.95	0.14	66,68,79,82	0

6.5 Other polymers (i)

There are no such residues in this entry.