Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 12:26 AM EDT

PDB ID	:	1RII
Title	:	Crystal structure of phosphoglycerate mutase from M. Tuberculosis
Authors	:	Mueller, P.; Sawaya, M.R.; Chan, S.; Wu, Y.; Pashkova, I.; Perry, J.; Eisenberg, D.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2003-11-17
Resolution	:	1.70 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:

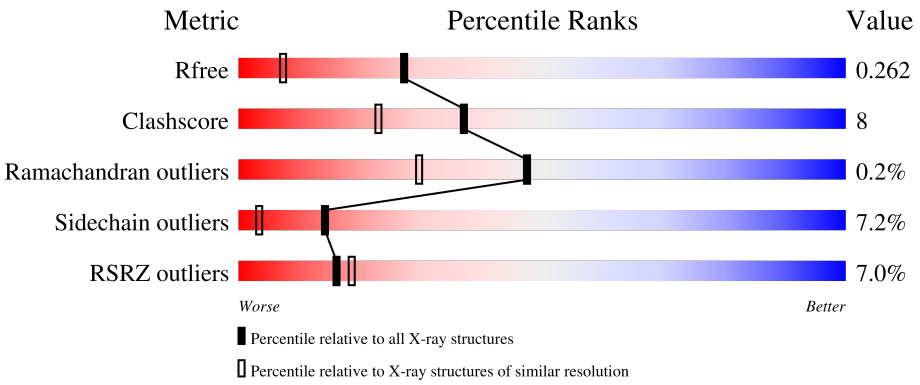
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	265	5% 74% 15% • 8%
1	B	265	6% 74% 13% • 11%
1	C	265	8% 69% 17% • 11%
1	D	265	6% 73% 12% • • 13%

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
2	GOL	A	501	-	-	X	-
2	GOL	B	502	-	-	X	-
2	GOL	D	503	-	X	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7910 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 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1884	1188	338	354	4	0	2	0
1	B	237	1854	1168	334	348	4	0	1	0
1	C	237	1853	1168	331	350	4	0	3	0
1	D	231	1838	1159	331	344	4	0	5	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	GLY	-	cloning artifact	UNP P0A5R6
A	251	VAL	-	cloning artifact	UNP P0A5R6
A	252	PRO	-	cloning artifact	UNP P0A5R6
A	253	ARG	-	cloning artifact	UNP P0A5R6
A	254	GLY	-	cloning artifact	UNP P0A5R6
A	255	ALA	-	cloning artifact	UNP P0A5R6
A	256	ALA	-	cloning artifact	UNP P0A5R6
A	257	ALA	-	cloning artifact	UNP P0A5R6
A	258	LEU	-	cloning artifact	UNP P0A5R6
A	259	GLU	-	cloning artifact	UNP P0A5R6
A	260	HIS	-	cloning artifact	UNP P0A5R6
A	261	HIS	-	cloning artifact	UNP P0A5R6
A	262	HIS	-	cloning artifact	UNP P0A5R6
A	263	HIS	-	cloning artifact	UNP P0A5R6
A	264	HIS	-	cloning artifact	UNP P0A5R6
A	265	HIS	-	cloning artifact	UNP P0A5R6
B	250	GLY	-	cloning artifact	UNP P0A5R6
B	251	VAL	-	cloning artifact	UNP P0A5R6
B	252	PRO	-	cloning artifact	UNP P0A5R6
B	253	ARG	-	cloning artifact	UNP P0A5R6
B	254	GLY	-	cloning artifact	UNP P0A5R6

Continued on next page...

Continued from previous page...

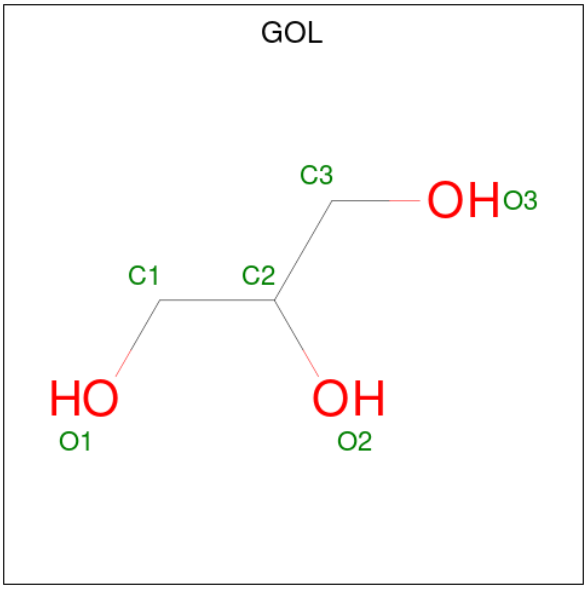
Chain	Residue	Modelled	Actual	Comment	Reference
B	255	ALA	-	cloning artifact	UNP P0A5R6
B	256	ALA	-	cloning artifact	UNP P0A5R6
B	257	ALA	-	cloning artifact	UNP P0A5R6
B	258	LEU	-	cloning artifact	UNP P0A5R6
B	259	GLU	-	cloning artifact	UNP P0A5R6
B	260	HIS	-	cloning artifact	UNP P0A5R6
B	261	HIS	-	cloning artifact	UNP P0A5R6
B	262	HIS	-	cloning artifact	UNP P0A5R6
B	263	HIS	-	cloning artifact	UNP P0A5R6
B	264	HIS	-	cloning artifact	UNP P0A5R6
B	265	HIS	-	cloning artifact	UNP P0A5R6
C	250	GLY	-	cloning artifact	UNP P0A5R6
C	251	VAL	-	cloning artifact	UNP P0A5R6
C	252	PRO	-	cloning artifact	UNP P0A5R6
C	253	ARG	-	cloning artifact	UNP P0A5R6
C	254	GLY	-	cloning artifact	UNP P0A5R6
C	255	ALA	-	cloning artifact	UNP P0A5R6
C	256	ALA	-	cloning artifact	UNP P0A5R6
C	257	ALA	-	cloning artifact	UNP P0A5R6
C	258	LEU	-	cloning artifact	UNP P0A5R6
C	259	GLU	-	cloning artifact	UNP P0A5R6
C	260	HIS	-	cloning artifact	UNP P0A5R6
C	261	HIS	-	cloning artifact	UNP P0A5R6
C	262	HIS	-	cloning artifact	UNP P0A5R6
C	263	HIS	-	cloning artifact	UNP P0A5R6
C	264	HIS	-	cloning artifact	UNP P0A5R6
C	265	HIS	-	cloning artifact	UNP P0A5R6
D	250	GLY	-	cloning artifact	UNP P0A5R6
D	251	VAL	-	cloning artifact	UNP P0A5R6
D	252	PRO	-	cloning artifact	UNP P0A5R6
D	253	ARG	-	cloning artifact	UNP P0A5R6
D	254	GLY	-	cloning artifact	UNP P0A5R6
D	255	ALA	-	cloning artifact	UNP P0A5R6
D	256	ALA	-	cloning artifact	UNP P0A5R6
D	257	ALA	-	cloning artifact	UNP P0A5R6
D	258	LEU	-	cloning artifact	UNP P0A5R6
D	259	GLU	-	cloning artifact	UNP P0A5R6
D	260	HIS	-	cloning artifact	UNP P0A5R6
D	261	HIS	-	cloning artifact	UNP P0A5R6
D	262	HIS	-	cloning artifact	UNP P0A5R6
D	263	HIS	-	cloning artifact	UNP P0A5R6
D	264	HIS	-	cloning artifact	UNP P0A5R6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	265	HIS	-	cloning artifact	UNP P0A5R6

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

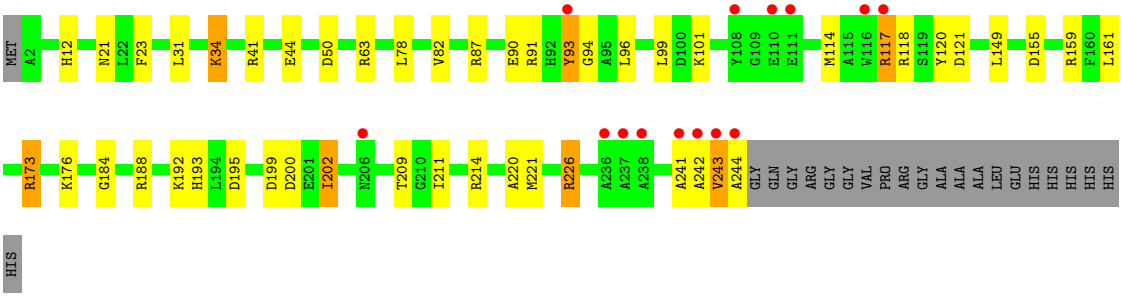
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	112	112	112	0	0
3	B	134	134	134	0	0
3	C	87	87	87	0	0
3	D	118	118	118	0	0

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.

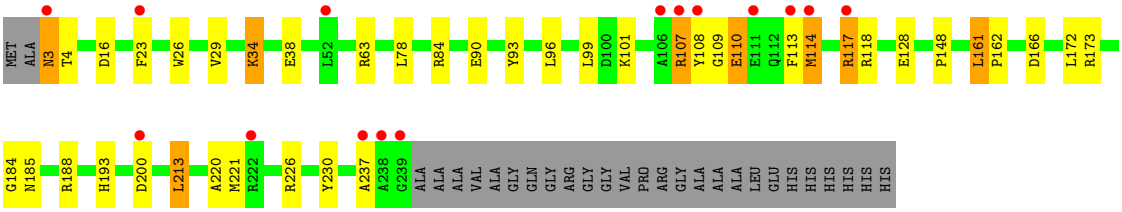
• Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase

Chain A:



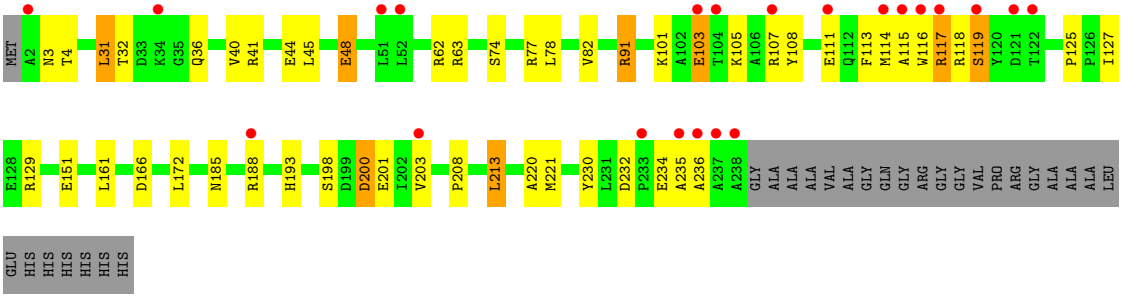
• Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase

Chain B:



• Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase

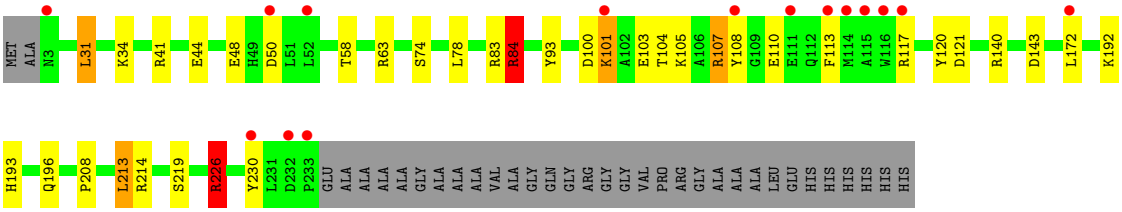
Chain C:



• Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase

Chain D:

6%
73%
12%
13%


MET ALA N3 L31 K34 R41 E44 E48 H49 D50 L51 L52 T58 R63 S74 L78 R83 R84 Y93 D100 K101 A102 E103 T104 K105 A106 R107 Y108 G109 E110 E111 Q112 F113 M114 A115 W116 R117 Y120 D121 R140 D143 L172 K192
H193 Q196 P208 L213 R214 S219 R226 Y230 L231 D232 P233 GLU ALA ALA ALA ALA GLY ALA ALA ALA VAL ALA GLY GLN GLY ARG GLY GLY VAL PRO ARG GLY ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.91Å 136.79Å 65.93Å 90.00° 97.78° 90.00°	Depositor
Resolution (Å)	58.37 – 1.70 58.37 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (58.37-1.70) 94.4 (58.37-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 1.70Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.221 , 0.270 0.216 , 0.262	Depositor DCC
R_{free} test set	2677 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 70.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7910	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.34	0/1933	0.97	2/2634 (0.1%)
1	B	0.35	0/1899	1.01	3/2585 (0.1%)
1	C	0.33	0/1906	1.01	4/2597 (0.2%)
1	D	0.35	0/1899	1.06	7/2584 (0.3%)
All	All	0.35	0/7637	1.01	16/10400 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	84	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	D	226	ARG	CD-NE-CZ	7.78	134.49	123.60
1	D	84[A]	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	D	84[B]	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	84	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	D	226	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	128	GLU	CA-CB-CG	6.94	128.67	113.40
1	C	166	ASP	CB-CG-OD1	6.61	124.25	118.30
1	D	93	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	D	31	LEU	CA-CB-CG	5.83	128.70	115.30
1	D	140	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	91	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	87	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	31	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	226	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	C	62	ARG	NE-CZ-NH1	5.10	122.85	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	1884	0	1859	32	0
1	B	1854	0	1829	28	0
1	C	1853	0	1816	27	0
1	D	1838	0	1809	29	0
2	A	6	0	8	4	0
2	B	6	0	7	5	0
2	D	18	0	22	5	0
3	A	112	0	0	2	0
3	B	134	0	0	0	0
3	C	87	0	0	2	0
3	D	118	0	0	2	0
All	All	7910	0	7350	116	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 8.

All (116) 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:D:83[A]:ARG:HE	2:D:505:GOL:H32	1.40	0.85
1:D:63:ARG:HE	2:D:503:GOL:H32	1.42	0.83
1:A:93:TYR:OH	1:A:117:ARG:HG3	1.85	0.75
1:B:63:ARG:NE	2:B:502:GOL:H12	2.03	0.74
1:B:110:GLU:OE2	1:B:114:MET:HG2	1.87	0.74
1:A:241:ALA:O	1:A:243:VAL:HG22	1.90	0.72
1:D:63:ARG:NE	2:D:503:GOL:H12	2.07	0.69
1:B:173:ARG:HD2	3:C:1044:HOH:O	1.91	0.69
1:D:100:ASP:OD1	1:D:103[B]:GLU:HG2	1.95	0.67
1:C:200:ASP:O	1:C:203:VAL:HG12	1.96	0.66
1:C:213:LEU:HG	1:C:230:TYR:CE1	2.33	0.64
1:D:101:LYS:HE2	1:D:105:LYS:HZ1	1.63	0.64
1:B:63:ARG:HH21	2:B:502:GOL:H31	1.64	0.62
1:B:213:LEU:HG	1:B:230:TYR:CE1	2.34	0.62
1:A:63:ARG:NE	2:A:501:GOL:H12	2.14	0.62
1:B:90:GLU:OE1	1:B:185:ASN:HB2	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:GLU:O	1:D:48:GLU:HG3	1.98	0.62
1:C:103:GLU:O	1:C:103:GLU:HG3	1.97	0.62
1:A:21:ASN:ND2	1:A:101:LYS:HD3	2.15	0.62
1:D:107:ARG:HD2	1:D:108:TYR:CE2	2.36	0.61
1:D:101:LYS:HD3	1:D:105:LYS:HZ2	1.65	0.61
1:A:209:THR:O	1:A:211:ILE:HD12	2.01	0.60
1:C:161:LEU:HD21	1:C:193:HIS:CG	2.37	0.59
1:B:34:LYS:O	1:B:38:GLU:HG3	2.03	0.58
1:C:91:ARG:HD3	1:C:151:GLU:O	2.03	0.58
1:C:118:ARG:O	1:C:203:VAL:HG21	2.04	0.58
1:D:213:LEU:HG	1:D:230:TYR:CE1	2.39	0.57
1:D:58:THR:HG21	1:D:84[A]:ARG:HH21	1.69	0.57
1:B:184:GLY:O	1:B:188:ARG:HG3	2.05	0.57
1:A:184:GLY:O	1:A:188:ARG:HG3	2.05	0.56
1:A:63:ARG:HE	2:A:501:GOL:H32	1.70	0.56
1:B:34:LYS:HD3	1:B:38:GLU:OE2	2.06	0.55
1:B:213:LEU:HG	1:B:230:TYR:CZ	2.42	0.54
1:B:63:ARG:NH2	2:B:502:GOL:H31	2.23	0.53
1:B:114:MET:O	1:B:118:ARG:HB2	2.08	0.53
1:C:101:LYS:HE2	1:C:113:PHE:CE2	2.45	0.51
1:C:213:LEU:HG	1:C:230:TYR:CZ	2.45	0.51
1:A:117:ARG:HH11	1:A:117:ARG:HB3	1.76	0.51
1:C:115:ALA:O	1:C:119:SER:HB3	2.11	0.51
1:B:16:ASP:HB2	1:B:29:VAL:CG1	2.41	0.51
1:D:101:LYS:HG3	1:D:113:PHE:CZ	2.46	0.50
1:C:44:GLU:O	1:C:48:GLU:OE1	2.30	0.50
1:A:242:ALA:O	1:A:243:VAL:O	2.30	0.50
1:D:63:ARG:NE	2:D:503:GOL:H32	2.21	0.49
1:A:117:ARG:NH1	1:A:118:ARG:HD3	2.26	0.49
1:B:3:ASN:OD1	1:B:4:THR:O	2.30	0.49
1:A:23:PHE:HB2	1:A:96:LEU:O	2.13	0.48
1:A:199:ASP:O	1:A:202:ILE:HD12	2.12	0.48
1:D:107:ARG:HB3	1:D:108:TYR:CD2	2.49	0.48
1:B:220:ALA:O	1:B:221:MET:HB2	2.13	0.47
1:C:40:VAL:HG13	1:C:74:SER:OG	2.15	0.47
1:B:113:PHE:HD2	1:B:114:MET:SD	2.38	0.47
1:B:63:ARG:HH21	2:B:502:GOL:C3	2.27	0.47
1:C:220:ALA:O	1:C:221:MET:HB2	2.14	0.47
1:A:12:HIS:CE1	2:A:501:GOL:H32	2.49	0.47
1:D:208:PRO:HD2	1:D:230:TYR:OH	2.14	0.47
1:D:107:ARG:HD2	1:D:108:TYR:CZ	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:THR:O	1:C:36:GLN:HG3	2.15	0.47
1:D:120:TYR:HD2	1:D:121:ASP:OD1	1.98	0.46
1:A:211:ILE:HD11	3:A:830:HOH:O	2.15	0.46
1:A:90:GLU:OE2	2:A:501:GOL:O3	2.29	0.46
1:D:58:THR:CG2	1:D:84[A]:ARG:HH21	2.29	0.45
1:A:243:VAL:O	1:A:244:ALA:HB3	2.17	0.45
1:A:176:LYS:NZ	3:A:774:HOH:O	2.50	0.45
1:B:162:PRO:O	1:B:166:ASP:HB2	2.17	0.45
1:A:195:ASP:O	1:A:226:ARG:NH2	2.50	0.45
1:C:185:ASN:OD1	1:C:188:ARG:NH1	2.50	0.45
1:A:41:ARG:NH1	1:A:44:GLU:OE1	2.50	0.45
1:A:94:GLY:HA2	1:A:149:LEU:O	2.17	0.45
1:C:198:SER:OG	1:C:201:GLU:HG3	2.15	0.45
1:A:155:ASP:O	1:A:159:ARG:HG3	2.17	0.45
1:B:63:ARG:HE	2:B:502:GOL:H12	1.76	0.45
1:C:116:TRP:CH2	1:C:125:PRO:HD3	2.52	0.45
1:D:41:ARG:NH1	1:D:48:GLU:OE2	2.49	0.45
1:A:173:ARG:O	1:A:173:ARG:HG3	2.13	0.44
1:B:173:ARG:NE	1:D:143:ASP:OD1	2.50	0.44
1:C:101:LYS:O	1:C:105:LYS:HG3	2.18	0.44
1:C:232:ASP:O	1:C:235:ALA:O	2.36	0.44
1:A:91:ARG:NH2	1:A:117:ARG:O	2.50	0.43
1:D:41:ARG:NH1	1:D:44:GLU:OE1	2.50	0.43
1:C:208:PRO:HD2	1:C:230:TYR:OH	2.18	0.43
1:D:101:LYS:HE2	1:D:105:LYS:NZ	2.33	0.43
1:B:23:PHE:CD1	1:B:101:LYS:HE2	2.54	0.43
1:A:161:LEU:HD11	1:A:193:HIS:CE1	2.54	0.43
1:B:113:PHE:O	1:B:117:ARG:HG3	2.19	0.43
1:D:107:ARG:NH1	1:D:108:TYR:OH	2.50	0.43
1:C:114:MET:O	1:C:117:ARG:HB3	2.19	0.42
2:D:503:GOL:H31	3:D:636:HOH:O	2.19	0.42
1:D:196:GLN:NE2	1:D:196:GLN:HA	2.34	0.42
1:B:161:LEU:HD21	1:B:193:HIS:CG	2.55	0.42
1:D:41:ARG:HH11	1:D:44:GLU:CB	2.33	0.42
1:C:107:ARG:HD2	1:C:108:TYR:CZ	2.55	0.42
1:C:127:ILE:HD12	3:C:782:HOH:O	2.20	0.42
1:C:161:LEU:HD21	1:C:193:HIS:ND1	2.35	0.42
1:D:34:LYS:HE3	3:D:959:HOH:O	2.19	0.42
1:A:220:ALA:O	1:A:221:MET:HB2	2.20	0.42
1:B:26:TRP:CH2	1:B:148:PRO:HD2	2.55	0.41
1:B:109:GLY:O	1:B:113:PHE:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41[A]:ARG:HH21	1:C:45:LEU:HD21	1.85	0.41
1:D:226:ARG:HG2	1:D:226:ARG:HH11	1.85	0.41
1:D:193:HIS:O	1:D:196:GLN:NE2	2.50	0.41
1:C:208:PRO:HG3	1:C:236:ALA:O	2.21	0.41
1:D:120:TYR:CZ	1:D:192:LYS:HE3	2.56	0.41
1:B:107:ARG:HD2	1:B:108:TYR:CZ	2.55	0.41
1:D:101:LYS:O	1:D:104:THR:N	2.54	0.41
1:A:214:ARG:HH11	1:A:214:ARG:HD3	1.70	0.41
1:A:99:LEU:HD12	1:A:99:LEU:N	2.36	0.41
1:B:34:LYS:NZ	1:B:38:GLU:OE2	2.50	0.41
1:A:120:TYR:CZ	1:A:192:LYS:HE3	2.57	0.40
1:B:118:ARG:HH11	1:B:118:ARG:HD3	1.70	0.40
1:C:3:ASN:ND2	1:C:4:THR:N	2.70	0.40
1:C:63:ARG:HH11	1:C:63:ARG:HD3	1.61	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	243/265 (92%)	234 (96%)	8 (3%)	1 (0%)	34	18
1	B	236/265 (89%)	232 (98%)	3 (1%)	1 (0%)	34	18
1	C	238/265 (90%)	234 (98%)	4 (2%)	0	100	100
1	D	234/265 (88%)	229 (98%)	5 (2%)	0	100	100
All	All	951/1060 (90%)	929 (98%)	20 (2%)	2 (0%)	47	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	237	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	195/208 (94%)	182 (93%)	13 (7%)	16 4
1	B	194/208 (93%)	178 (92%)	16 (8%)	11 2
1	C	194/208 (93%)	180 (93%)	14 (7%)	14 3
1	D	196/208 (94%)	179 (91%)	17 (9%)	10 2
All	All	779/832 (94%)	719 (92%)	60 (8%)	14 3

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	34[A]	LYS
1	A	34[B]	LYS
1	A	50	ASP
1	A	78	LEU
1	A	82	VAL
1	A	93	TYR
1	A	114	MET
1	A	117	ARG
1	A	121	ASP
1	A	173	ARG
1	A	200	ASP
1	A	202	ILE
1	B	3	ASN
1	B	34	LYS
1	B	78	LEU
1	B	93	TYR
1	B	96	LEU
1	B	99	LEU
1	B	107	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	110	GLU
1	B	114	MET
1	B	117	ARG
1	B	161	LEU
1	B	172	LEU
1	B	200	ASP
1	B	213	LEU
1	B	226[A]	ARG
1	B	226[B]	ARG
1	C	31	LEU
1	C	48	GLU
1	C	77	ARG
1	C	78	LEU
1	C	82	VAL
1	C	103	GLU
1	C	111	GLU
1	C	117	ARG
1	C	119	SER
1	C	129	ARG
1	C	172	LEU
1	C	200	ASP
1	C	213	LEU
1	C	234	GLU
1	D	31	LEU
1	D	50[A]	ASP
1	D	50[B]	ASP
1	D	74	SER
1	D	78	LEU
1	D	84[A]	ARG
1	D	84[B]	ARG
1	D	101	LYS
1	D	107	ARG
1	D	110	GLU
1	D	117	ARG
1	D	172	LEU
1	D	213	LEU
1	D	214[A]	ARG
1	D	214[B]	ARG
1	D	219	SER
1	D	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	132	GLN
1	C	3	ASN
1	C	112	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	GOL	D	505	-	5,5,5	0.82	0	5,5,5	1.55	1 (20%)
2	GOL	D	503	-	5,5,5	0.96	0	5,5,5	1.72	2 (40%)
2	GOL	B	502	-	5,5,5	0.89	0	5,5,5	2.07	3 (60%)
2	GOL	A	501	-	5,5,5	0.88	0	5,5,5	1.71	2 (40%)
2	GOL	D	504	-	5,5,5	0.68	0	5,5,5	1.11	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
2	GOL	D	505	-	-	2/4/4/4	-
2	GOL	D	503	-	-	4/4/4/4	-
2	GOL	B	502	-	-	2/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-
2	GOL	D	504	-	-	2/4/4/4	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	GOL	O1-C1-C2	3.23	125.68	110.20
2	A	501	GOL	O3-C3-C2	3.11	125.10	110.20
2	D	503	GOL	O3-C3-C2	3.00	124.60	110.20
2	D	505	GOL	O1-C1-C2	2.62	122.78	110.20
2	D	503	GOL	O1-C1-C2	2.38	121.61	110.20
2	B	502	GOL	O3-C3-C2	2.22	120.85	110.20
2	B	502	GOL	O2-C2-C1	2.22	118.90	109.12
2	A	501	GOL	O1-C1-C2	2.21	120.79	110.20

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	C1-C2-C3-O3
2	A	501	GOL	O2-C2-C3-O3
2	D	503	GOL	C1-C2-C3-O3
2	D	503	GOL	O2-C2-C3-O3
2	D	504	GOL	O1-C1-C2-O2
2	B	502	GOL	O1-C1-C2-C3
2	D	504	GOL	O1-C1-C2-C3
2	D	505	GOL	O1-C1-C2-C3
2	B	502	GOL	O1-C1-C2-O2
2	D	505	GOL	O1-C1-C2-O2
2	D	503	GOL	O1-C1-C2-C3
2	D	503	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	505	GOL	1	0
2	D	503	GOL	4	0
2	B	502	GOL	5	0
2	A	501	GOL	4	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	243/265 (91%)	0.71	14 (5%)	23	25	21, 30, 53, 91	0
1	B	237/265 (89%)	0.73	15 (6%)	20	22	21, 29, 52, 71	0
1	C	237/265 (89%)	0.82	22 (9%)	8	9	24, 34, 57, 80	0
1	D	231/265 (87%)	0.61	15 (6%)	18	21	21, 30, 54, 68	0
All	All	948/1060 (89%)	0.72	66 (6%)	16	18	21, 30, 55, 91	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	10.8
1	A	243	VAL	9.8
1	B	238	ALA	9.4
1	A	244	ALA	8.6
1	A	242	ALA	7.4
1	C	236	ALA	7.1
1	D	233	PRO	6.8
1	C	238	ALA	6.4
1	C	237	ALA	5.5
1	C	235	ALA	5.4
1	D	117	ARG	4.5
1	C	114	MET	4.3
1	C	115	ALA	4.3
1	D	115	ALA	4.2
1	B	107	ARG	4.2
1	B	3	ASN	4.1
1	D	116	TRP	4.0
1	C	119	SER	3.9
1	B	239	GLY	3.8
1	D	114	MET	3.8
1	C	203	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	106	ALA	3.7
1	A	238	ALA	3.6
1	B	200	ASP	3.5
1	D	101	LYS	3.5
1	C	233	PRO	3.2
1	D	3	ASN	3.2
1	B	108	TYR	3.2
1	C	122	THR	3.2
1	B	222	ARG	3.1
1	D	50[A]	ASP	3.0
1	A	237	ALA	2.9
1	C	111	GLU	2.9
1	A	236	ALA	2.9
1	B	237	ALA	2.8
1	D	230	TYR	2.8
1	D	232	ASP	2.8
1	C	34	LYS	2.8
1	B	113	PHE	2.7
1	A	241	ALA	2.6
1	C	116	TRP	2.6
1	A	111	GLU	2.6
1	C	104	THR	2.5
1	B	117	ARG	2.5
1	A	117	ARG	2.4
1	A	206	ASN	2.4
1	B	114	MET	2.4
1	C	107	ARG	2.4
1	D	113	PHE	2.4
1	C	117	ARG	2.4
1	C	121[A]	ASP	2.4
1	B	52	LEU	2.4
1	D	108	TYR	2.4
1	B	23	PHE	2.3
1	A	93	TYR	2.3
1	A	110	GLU	2.3
1	C	51	LEU	2.3
1	A	108	TYR	2.3
1	D	172	LEU	2.3
1	B	111	GLU	2.3
1	D	111	GLU	2.3
1	D	52	LEU	2.2
1	A	116	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	52	LEU	2.1
1	C	103	GLU	2.1
1	C	188	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	D	505	6/6	0.59	0.30	49,53,54,57	0
2	GOL	D	504	6/6	0.67	0.15	45,48,50,53	0
2	GOL	B	502	6/6	0.86	0.19	31,38,41,42	0
2	GOL	A	501	6/6	0.87	0.29	32,44,46,46	0
2	GOL	D	503	6/6	0.92	0.28	15,23,24,29	6

6.5 Other polymers (i)

There are no such residues in this entry.