



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:15 AM UTC

PDB ID : 1RII / pdb_00001rii
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

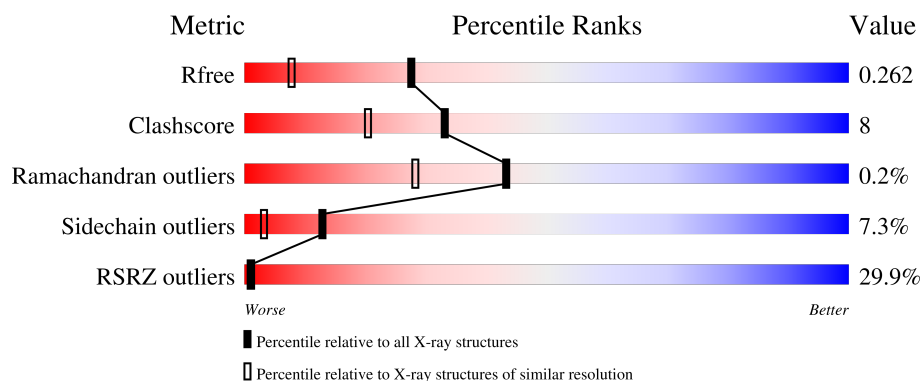
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 $\leq 5\%$. 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	265	28% 74% 16% • 8%
1	B	265	22% 72% 14% • 11%
1	C	265	34% 68% 18% • 11%
1	D	265	23% 72% 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	-

2 Entry composition

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

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

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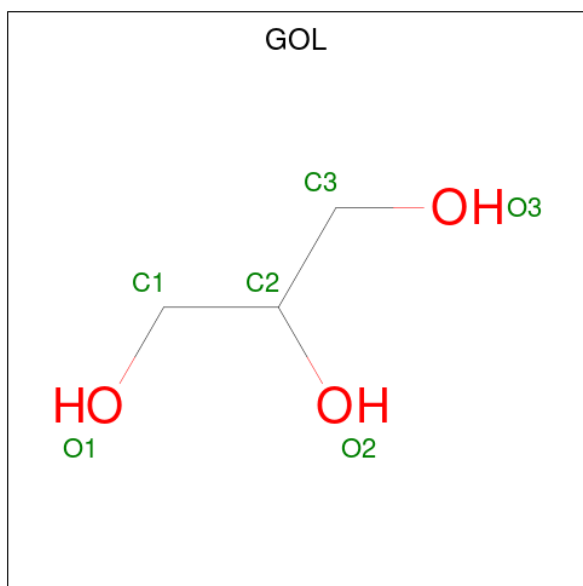
Chain	Residue	Modelled	Actual	Comment	Reference
B	255	ALA	-	cloning artifact	UNP P0A5R6
B	256	ALA	-	cloning artifact	UNP P0A5R6
B	257	ALA	-	cloning artifact	UNP P0A5R6
B	258	LEU	-	cloning artifact	UNP P0A5R6
B	259	GLU	-	cloning artifact	UNP P0A5R6
B	260	HIS	-	cloning artifact	UNP P0A5R6
B	261	HIS	-	cloning 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

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

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

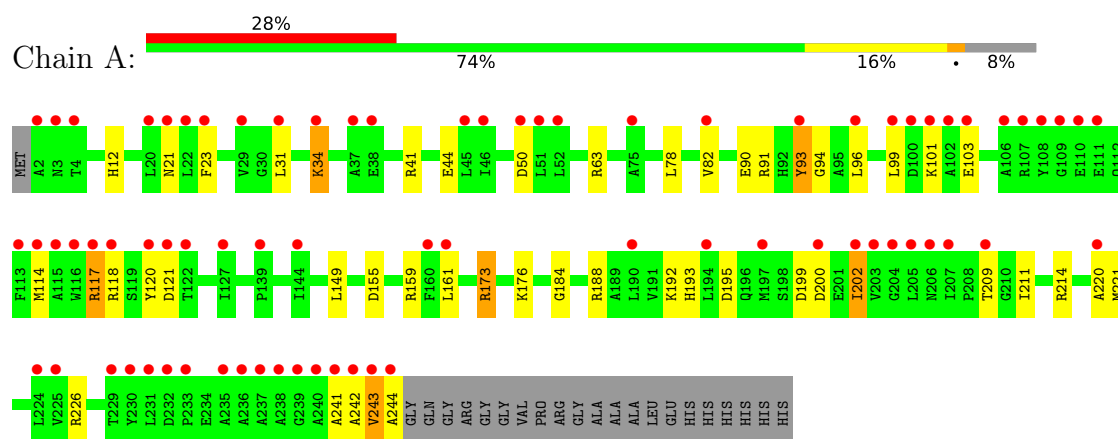
- Molecule 3 is water.

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

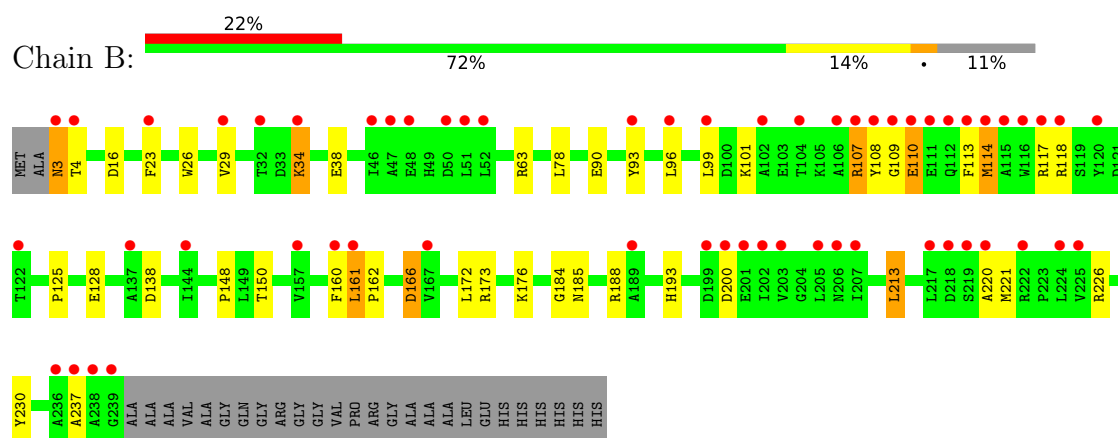
3 Residue-property plots [i](#)

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.

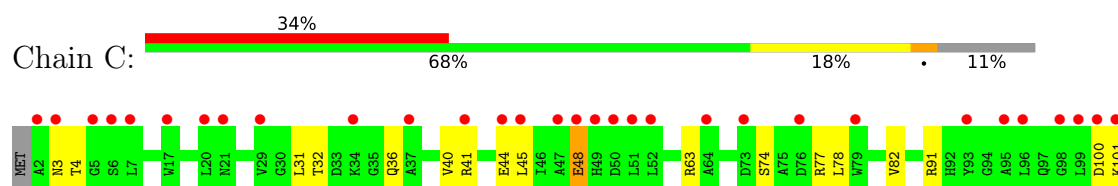
- Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase

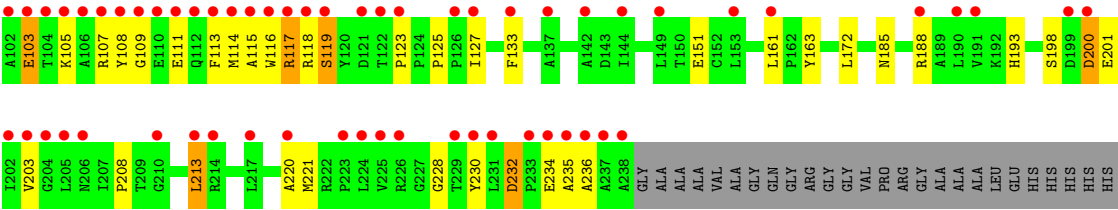


- Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase



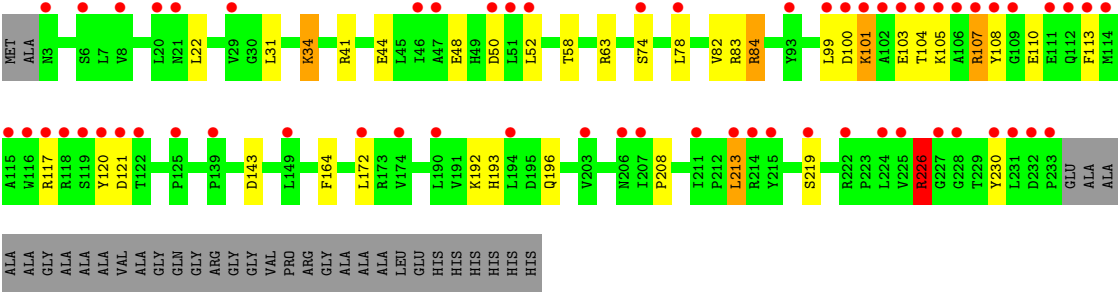
- Molecule 1: 2,3-bisphosphoglycerate-dependent phosphoglycerate mutase





HIS

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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.43	0/1933	1.25	0/2634
1	B	0.44	0/1899	1.27	6/2585 (0.2%)
1	C	0.42	0/1906	1.35	8/2597 (0.3%)
1	D	0.43	0/1899	1.28	4/2584 (0.2%)
All	All	0.43	0/7637	1.29	18/10400 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	PRO	O-C-N	8.84	125.37	121.31
1	B	128	GLU	CA-CB-CG	7.28	128.67	114.10
1	D	52	LEU	CA-C-O	7.22	124.66	119.32
1	D	226	ARG	CD-NE-CZ	7.21	134.49	124.40
1	D	22	LEU	CA-C-O	-6.15	113.97	120.80
1	C	232	ASP	CA-CB-CG	6.06	118.66	112.60
1	B	150	THR	O-C-N	-6.01	117.51	123.46
1	C	163	TYR	CA-C-O	5.94	126.72	120.42
1	C	100	ASP	CA-CB-CG	5.74	118.34	112.60
1	D	164	PHE	CA-CB-CG	-5.49	108.31	113.80
1	C	109	GLY	CA-C-N	5.44	128.02	120.29
1	C	109	GLY	C-N-CA	5.44	128.02	120.29
1	B	160	PHE	CA-C-O	5.31	126.23	120.55
1	B	166	ASP	CA-CB-CG	-5.19	107.41	112.60
1	C	123	PRO	O-C-N	5.11	123.55	121.15
1	B	138	ASP	CA-C-O	5.10	124.90	119.80
1	C	228	GLY	CA-C-O	-5.02	114.73	122.52
1	C	133	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1884	0	1859	32	0
1	B	1854	0	1829	29	0
1	C	1853	0	1816	27	0
1	D	1838	0	1809	28	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	1	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:D:101:LYS:HE2	1:D:105:LYS:HZ1	1.54	0.73
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:B:63:ARG:HH21	2:B:502:GOL:H31	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:101:LYS:HD3	1:D:105:LYS:HZ2	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:176:LYS:NZ	3:B:798:HOH:O	2.50	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

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

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	243/265 (92%)	234 (96%)	8 (3%)	1 (0%)	30	16
1	B	236/265 (89%)	232 (98%)	3 (1%)	1 (0%)	30	16
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%)	43	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	VAL
1	B	237	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	195/208 (94%)	181 (93%)	14 (7%)	13	3
1	B	194/208 (93%)	179 (92%)	15 (8%)	12	2
1	C	194/208 (93%)	181 (93%)	13 (7%)	15	4
1	D	196/208 (94%)	178 (91%)	18 (9%)	8	2
All	All	779/832 (94%)	719 (92%)	60 (8%)	13	2

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	103	GLU
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

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Mol	Chain	Res	Type
1	B	107	ARG
1	B	110	GLU
1	B	114	MET
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	172	LEU
1	C	200	ASP
1	C	213	LEU
1	C	234	GLU
1	D	31	LEU
1	D	34	LYS
1	D	50[A]	ASP
1	D	50[B]	ASP
1	D	74	SER
1	D	78	LEU
1	D	82	VAL
1	D	84[A]	ARG
1	D	84[B]	ARG
1	D	99	LEU
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	219	SER
1	D	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	132	GLN
1	B	185	ASN
1	C	3	ASN
1	C	112	GLN
1	D	36	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 oligosaccharides 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	503	-	5,5,5	0.98	0	5,5,5	1.80	2 (40%)
2	GOL	D	505	-	5,5,5	0.84	0	5,5,5	1.63	1 (20%)
2	GOL	B	502	-	5,5,5	0.92	0	5,5,5	2.17	3 (60%)
2	GOL	A	501	-	5,5,5	0.89	0	5,5,5	1.80	2 (40%)
2	GOL	D	504	-	5,5,5	0.69	0	5,5,5	1.16	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	503	-	-	3/4/4/4	-
2	GOL	D	505	-	-	2/4/4/4	-
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(°)	Ideal(°)
2	B	502	GOL	O1-C1-C2	3.40	125.68	110.38
2	A	501	GOL	O3-C3-C2	3.27	125.10	110.38
2	D	503	GOL	O3-C3-C2	3.16	124.60	110.38
2	D	505	GOL	O1-C1-C2	2.76	122.78	110.38
2	D	503	GOL	O1-C1-C2	2.50	121.61	110.38
2	B	502	GOL	O2-C2-C1	2.35	118.90	109.18
2	B	502	GOL	O3-C3-C2	2.33	120.85	110.38
2	A	501	GOL	O1-C1-C2	2.31	120.79	110.38

There are no chirality outliers.

All (11) 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-O2

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	503	GOL	4	0
2	D	505	GOL	1	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%)	1.62	75 (30%)	1 1	20, 30, 53, 91	2 (0%)
1	B	237/265 (89%)	1.47	58 (24%)	2 2	21, 29, 52, 71	1 (0%)
1	C	237/265 (89%)	1.86	89 (37%)	1 0	24, 34, 57, 80	3 (1%)
1	D	231/265 (87%)	1.54	61 (26%)	1 1	13, 29, 54, 68	5 (2%)
All	All	948/1060 (89%)	1.62	283 (29%)	1 1	13, 30, 55, 91	11 (1%)

All (283) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	VAL	10.4
1	A	244	ALA	9.5
1	C	236	ALA	9.0
1	C	2	ALA	7.8
1	B	238	ALA	7.7
1	B	239	GLY	7.6
1	A	242	ALA	7.4
1	D	233	PRO	7.3
1	A	241	ALA	6.5
1	D	102	ALA	6.1
1	C	237	ALA	5.6
1	B	108	TYR	5.5
1	D	116	TRP	5.2
1	C	238	ALA	5.2
1	B	114	MET	5.1
1	C	235	ALA	5.0
1	C	51	LEU	5.0
1	C	116	TRP	4.9
1	A	116	TRP	4.8
1	A	51	LEU	4.7
1	A	238	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	237	ALA	4.6
1	C	115	ALA	4.6
1	B	3	ASN	4.5
1	B	107	ARG	4.5
1	A	110	GLU	4.4
1	B	200	ASP	4.4
1	A	236	ALA	4.4
1	D	117	ARG	4.4
1	C	233	PRO	4.3
1	A	240	ALA	4.3
1	C	108	TYR	4.3
1	B	106	ALA	4.2
1	D	231	LEU	4.2
1	D	113	PHE	4.2
1	B	109	GLY	4.2
1	C	114	MET	4.2
1	D	114	MET	4.2
1	C	203	VAL	4.2
1	D	3	ASN	4.2
1	D	52	LEU	4.1
1	C	104	THR	4.1
1	C	122	THR	4.1
1	C	113	PHE	4.1
1	A	235	ALA	4.0
1	D	115	ALA	4.0
1	A	93	TYR	4.0
1	A	237	ALA	4.0
1	B	93	TYR	3.9
1	C	109	GLY	3.9
1	D	106	ALA	3.9
1	D	224	LEU	3.9
1	D	230	TYR	3.9
1	D	121	ASP	3.9
1	C	52	LEU	3.9
1	D	101	LYS	3.9
1	D	203	VAL	3.7
1	D	107	ARG	3.7
1	A	160	PHE	3.7
1	A	205	LEU	3.7
1	C	231	LEU	3.7
1	D	51	LEU	3.7
1	B	116	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	106	ALA	3.6
1	B	113	PHE	3.6
1	B	224	LEU	3.6
1	A	206	ASN	3.6
1	C	106	ALA	3.5
1	C	49	HIS	3.5
1	D	104	THR	3.5
1	A	202	ILE	3.4
1	B	225	VAL	3.4
1	A	114	MET	3.4
1	B	220	ALA	3.4
1	D	119	SER	3.4
1	B	52	LEU	3.4
1	D	109	GLY	3.4
1	B	236	ALA	3.3
1	C	102	ALA	3.3
1	D	232	ASP	3.3
1	D	207	ILE	3.3
1	C	204	GLY	3.3
1	A	37	ALA	3.3
1	B	117	ARG	3.3
1	D	118	ARG	3.3
1	C	111	GLU	3.3
1	C	112	GLN	3.3
1	D	190	LEU	3.2
1	C	119	SER	3.2
1	C	110	GLU	3.2
1	A	3	ASN	3.2
1	A	225	VAL	3.2
1	A	108	TYR	3.2
1	B	202	ILE	3.2
1	D	172	LEU	3.2
1	A	115	ALA	3.2
1	C	99	LEU	3.1
1	C	205	LEU	3.1
1	C	133	PHE	3.1
1	A	45	LEU	3.1
1	A	194	LEU	3.1
1	A	2	ALA	3.1
1	B	122	THR	3.1
1	A	203	VAL	3.1
1	C	225	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	127	ILE	3.1
1	A	101	LYS	3.1
1	D	228	GLY	3.0
1	C	3	ASN	3.0
1	D	74	SER	3.0
1	C	48	GLU	3.0
1	C	230	TYR	3.0
1	B	102	ALA	3.0
1	C	50[A]	ASP	3.0
1	D	50[A]	ASP	3.0
1	C	117	ARG	3.0
1	C	93	TYR	3.0
1	D	108	TYR	3.0
1	A	109	GLY	3.0
1	B	205	LEU	2.9
1	C	202	ILE	2.9
1	B	199	ASP	2.9
1	D	225	VAL	2.9
1	C	21	ASN	2.9
1	D	93	TYR	2.9
1	C	45	LEU	2.9
1	A	224	LEU	2.9
1	C	224	LEU	2.9
1	D	111	GLU	2.9
1	B	23	PHE	2.8
1	C	229	THR	2.8
1	C	188	ARG	2.8
1	A	99	LEU	2.8
1	C	149	LEU	2.8
1	C	200	ASP	2.8
1	C	20	LEU	2.8
1	C	217	LEU	2.8
1	C	127	ILE	2.8
1	D	211	ILE	2.8
1	C	105	LYS	2.8
1	B	110	GLU	2.8
1	D	103[A]	GLU	2.8
1	B	222	ARG	2.7
1	C	107	ARG	2.7
1	B	111	GLU	2.7
1	C	103	GLU	2.7
1	A	117	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	210	GLY	2.7
1	D	112	GLN	2.7
1	C	137	ALA	2.7
1	C	34	LYS	2.7
1	C	101	LYS	2.7
1	D	105	LYS	2.7
1	A	50	ASP	2.7
1	C	98	GLY	2.7
1	A	96	LEU	2.7
1	B	51	LEU	2.7
1	C	191	VAL	2.7
1	B	144	ILE	2.7
1	C	47	ALA	2.7
1	A	233	PRO	2.6
1	A	190	LEU	2.6
1	A	231	LEU	2.6
1	B	161	LEU	2.6
1	A	107	ARG	2.6
1	B	4	THR	2.6
1	A	232	ASP	2.6
1	A	113	PHE	2.6
1	B	217	LEU	2.6
1	B	120	TYR	2.6
1	B	167	VAL	2.6
1	D	219	SER	2.6
1	A	102	ALA	2.6
1	C	126	PRO	2.6
1	B	32	THR	2.5
1	A	34[A]	LYS	2.5
1	D	194	LEU	2.5
1	D	213	LEU	2.5
1	A	82	VAL	2.5
1	B	203	VAL	2.5
1	A	144	ILE	2.5
1	B	46	ILE	2.5
1	C	123	PRO	2.5
1	C	73	ASP	2.5
1	B	112	GLN	2.5
1	A	239	GLY	2.5
1	C	214	ARG	2.5
1	C	226	ARG	2.5
1	A	20	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	7	LEU	2.5
1	C	161	LEU	2.5
1	D	149	LEU	2.5
1	A	100	ASP	2.5
1	A	38	GLU	2.5
1	B	99	LEU	2.5
1	C	95	ALA	2.5
1	D	174	VAL	2.5
1	A	197	MET	2.5
1	B	219	SER	2.5
1	A	31	LEU	2.4
1	A	161	LEU	2.4
1	C	213	LEU	2.4
1	C	220	ALA	2.4
1	A	200	ASP	2.4
1	A	118	ARG	2.4
1	B	96	LEU	2.4
1	C	190	LEU	2.4
1	C	223	PRO	2.4
1	A	23	PHE	2.4
1	B	137	ALA	2.4
1	C	118	ARG	2.4
1	D	78	LEU	2.4
1	B	50	ASP	2.4
1	C	44	GLU	2.4
1	A	207	ILE	2.4
1	B	207	ILE	2.4
1	A	29	VAL	2.4
1	C	29	VAL	2.4
1	D	29	VAL	2.4
1	B	201	GLU	2.3
1	B	47	ALA	2.3
1	C	96	LEU	2.3
1	C	79	TRP	2.3
1	B	118	ARG	2.3
1	A	122	THR	2.3
1	D	20	LEU	2.3
1	A	111	GLU	2.3
1	A	204	GLY	2.3
1	A	229	THR	2.3
1	D	122	THR	2.3
1	D	99	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	6	SER	2.3
1	B	115	ALA	2.2
1	C	37	ALA	2.2
1	B	206	ASN	2.2
1	C	153	LEU	2.2
1	C	100	ASP	2.2
1	C	206	ASN	2.2
1	A	75	ALA	2.2
1	B	189	ALA	2.2
1	C	64	ALA	2.2
1	A	121	ASP	2.2
1	C	199	ASP	2.2
1	A	52	LEU	2.2
1	A	103	GLU	2.2
1	A	46	ILE	2.2
1	C	144	ILE	2.2
1	D	46	ILE	2.2
1	D	21	ASN	2.2
1	B	29	VAL	2.2
1	C	76	ASP	2.2
1	C	234	GLU	2.2
1	D	222	ARG	2.2
1	A	230	TYR	2.2
1	A	139	PRO	2.2
1	A	209	THR	2.2
1	D	100	ASP	2.1
1	A	4	THR	2.1
1	A	120	TYR	2.1
1	B	34	LYS	2.1
1	C	17	TRP	2.1
1	B	104	THR	2.1
1	C	41[A]	ARG	2.1
1	A	220	ALA	2.1
1	C	5	GLY	2.1
1	D	227	GLY	2.1
1	B	157	VAL	2.1
1	D	8	VAL	2.1
1	B	218	ASP	2.1
1	B	160	PHE	2.1
1	D	47	ALA	2.0
1	C	121[A]	ASP	2.0
1	D	214[A]	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	22	LEU	2.0
1	D	125	PRO	2.0
1	D	139	PRO	2.0
1	B	48	GLU	2.0
1	A	21	ASN	2.0
1	D	206	ASN	2.0
1	D	120	TYR	2.0
1	D	215	TYR	2.0
1	C	142	ALA	2.0
1	D	6	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	D	504	6/6	0.70	0.22	45,48,50,53	0
2	GOL	D	505	6/6	0.75	0.21	49,53,54,57	0
2	GOL	A	501	6/6	0.86	0.19	32,44,46,46	0
2	GOL	B	502	6/6	0.87	0.19	31,38,41,42	0
2	GOL	D	503	6/6	0.89	0.20	15,23,24,29	6

6.5 Other polymers [i](#)

There are no such residues in this entry.