



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:29 pm BST

PDB ID : 4B8R
Title : Crystal Structure of Thermococcus litoralis ADP-dependent Glucokinase (GK)
Authors : Herrera-Morande, A.; Rivas-Pardo, J.A.; Fernandez, F.J.; Guixe, V.; Vega, M.C.
Deposited on : 2012-08-30
Resolution : 2.05 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

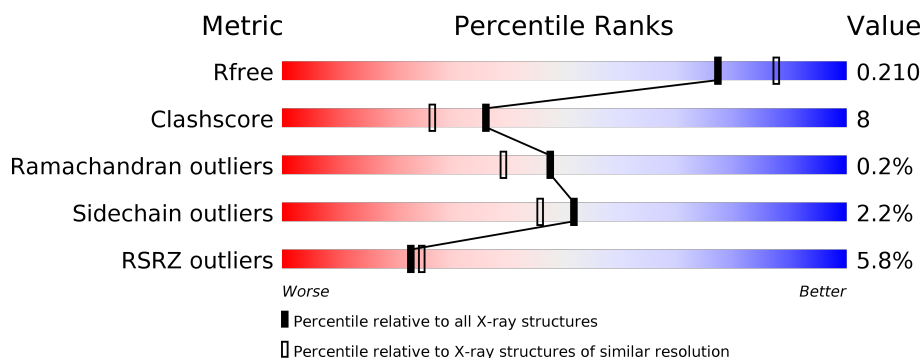
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 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	467	<div> <div>6%</div> <div>85%</div> <div>13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1482	-	-	X	-
3	TRS	A	1484	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DTT	A	1485	-	-	X	-
7	SO4	A	1498	-	-	X	-
7	SO4	A	1500	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4364 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 ADP-DEPENDENT GLUCOKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	8	0
			3854	2461	662	721	10			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



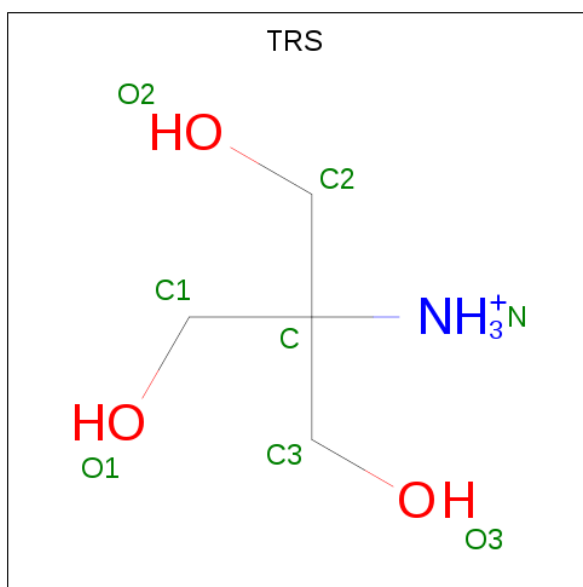
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



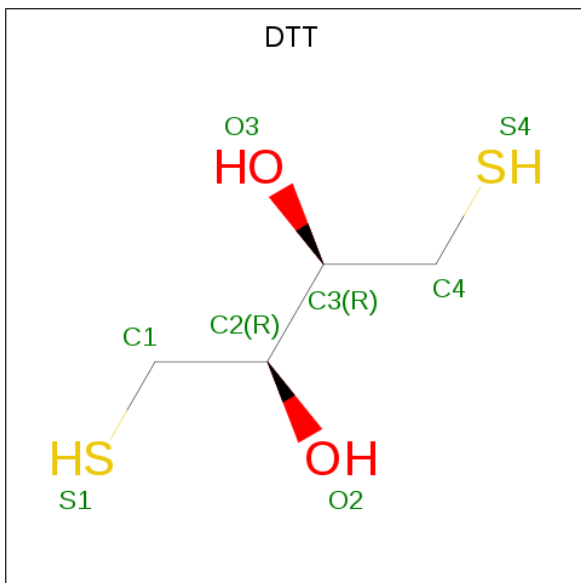
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

Continued on next page...

Continued from previous page...

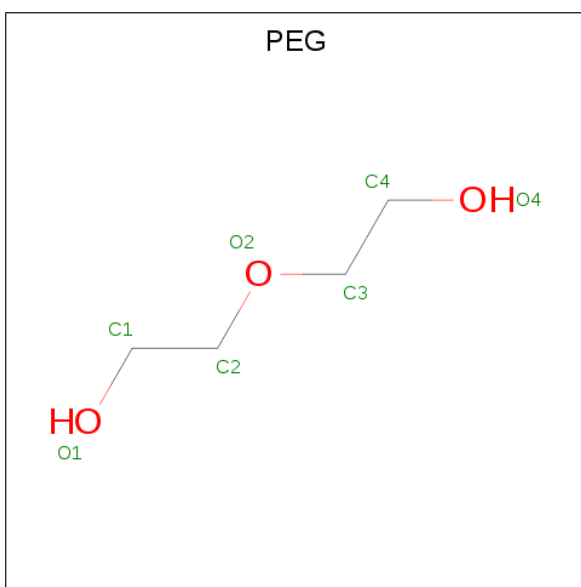
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



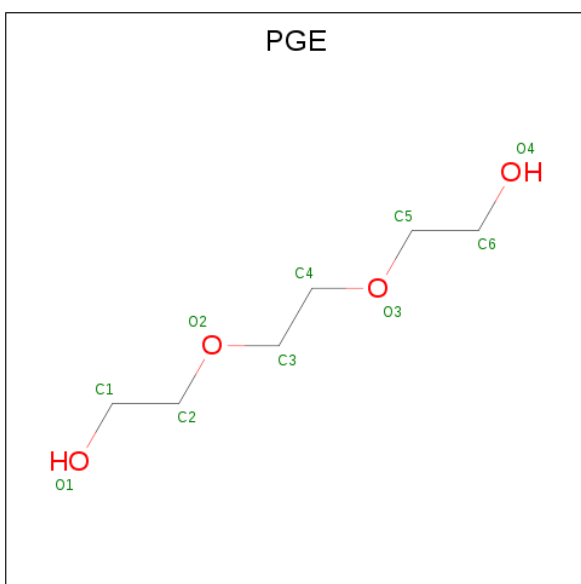
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		
4	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



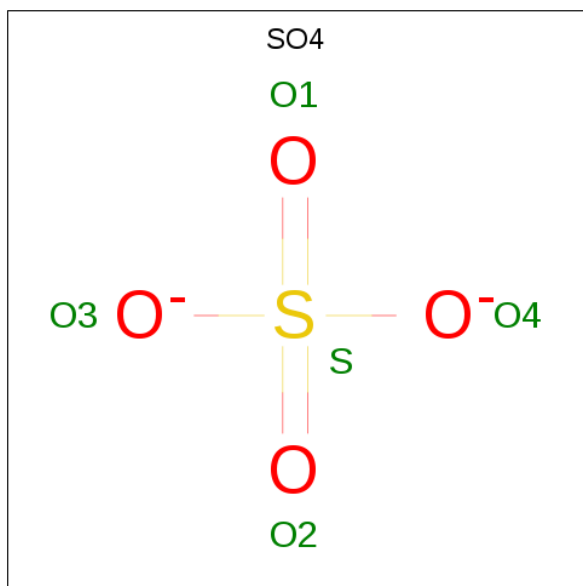
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	A	1	Total	C	O	0	0
			10	6	4		
6	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

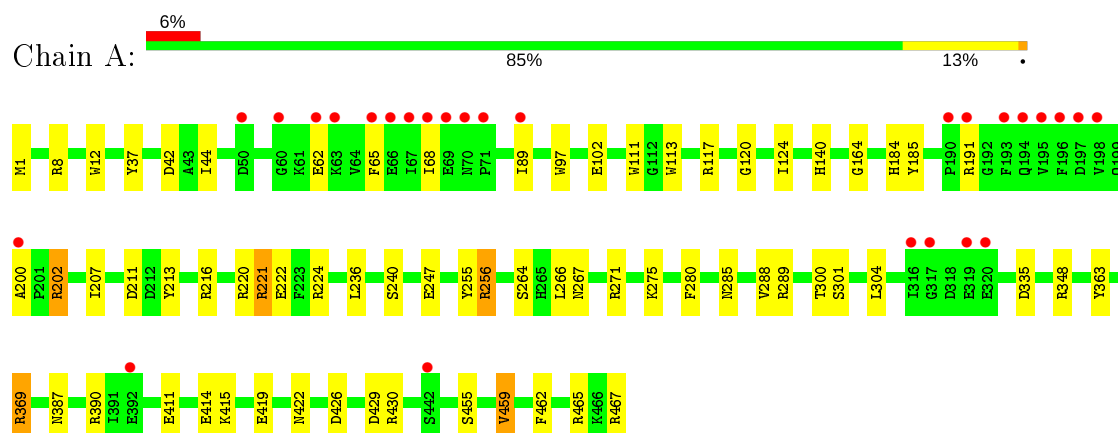
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	293	Total	O	0	0
			293	293		

3 Residue-property plots [i](#)

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

• Molecule 1: ADP-DEPENDENT GLUCOKINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.10Å 109.10Å 129.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.28 – 2.05 39.28 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.28-2.05) 99.2 (39.28-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.170 , 0.211 0.169 , 0.210	Depositor DCC
R_{free} test set	2811 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4364	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PGE, SO4, TRS, PEG, DTT

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	1.21	13/3932 (0.3%)	1.04	11/5307 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	TRP	CD2-CE2	7.02	1.49	1.41
1	A	111	TRP	CD2-CE2	6.75	1.49	1.41
1	A	185	TYR	CB-CG	6.44	1.61	1.51
1	A	455	SER	CB-OG	5.81	1.49	1.42
1	A	301	SER	CB-OG	5.69	1.49	1.42
1	A	419	GLU	CD-OE2	-5.56	1.19	1.25
1	A	369	ARG	CZ-NH1	5.45	1.40	1.33
1	A	419	GLU	CD-OE1	-5.45	1.19	1.25
1	A	240	SER	CB-OG	5.20	1.49	1.42
1	A	97	TRP	CD2-CE2	5.18	1.47	1.41
1	A	184	HIS	CG-CD2	5.17	1.44	1.35
1	A	12	TRP	CD2-CE2	5.15	1.47	1.41
1	A	213	TYR	CE1-CZ	5.14	1.45	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ARG	NE-CZ-NH2	-11.64	114.48	120.30
1	A	216	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A	430	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	266	LEU	CB-CG-CD1	-6.51	99.93	111.00
1	A	369	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	221	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	224	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	459	VAL	CG1-CB-CG2	5.32	119.41	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	426	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	8	ARG	NE-CZ-NH1	5.15	122.87	120.30

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	3854	0	3865	58	0
2	A	90	0	120	19	0
3	A	16	0	24	1	0
4	A	16	0	20	8	0
5	A	35	0	50	2	0
6	A	30	0	42	8	0
7	A	30	0	0	4	0
8	A	293	0	0	13	0
All	All	4364	0	4121	66	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 (66) 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:117[B]:ARG:NH1	8:A:2085:HOH:O	1.75	1.15
1:A:271[B]:ARG:HG2	1:A:271[B]:ARG:HH11	1.10	1.13
1:A:120:GLY:H	4:A:1485:DTT:H11	1.31	0.93
1:A:140:HIS:HE1	1:A:220:ARG:H	1.23	0.87
1:A:429:ASP:OD1	8:A:2270:HOH:O	1.93	0.87
1:A:271[B]:ARG:HG2	1:A:271[B]:ARG:NH1	1.90	0.83
1:A:285:ASN:HB2	5:A:1490:PEG:H12	1.59	0.83
1:A:42:ASP:OD2	4:A:1485:DTT:H12	1.79	0.82
2:A:1473:GOL:H11	8:A:2282:HOH:O	1.82	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335[B]:ASP:OD1	8:A:2220:HOH:O	2.03	0.75
7:A:1498:SO4:O2	8:A:2291:HOH:O	2.07	0.73
1:A:285:ASN:HD22	1:A:288:VAL:H	1.39	0.69
2:A:1481:GOL:H11	8:A:2274:HOH:O	1.91	0.69
1:A:369:ARG:HH22	4:A:1486:DTT:H12	1.59	0.68
1:A:422:ASN:OD1	4:A:1486:DTT:S4	2.52	0.68
1:A:267:ASN:HD22	2:A:1482:GOL:H2	1.60	0.66
1:A:275:LYS:HD3	6:A:1493:PGE:H62	1.77	0.66
1:A:267:ASN:HD22	2:A:1482:GOL:C2	2.09	0.65
1:A:271[B]:ARG:CG	1:A:271[B]:ARG:HH11	1.95	0.65
1:A:42:ASP:OD2	1:A:117[B]:ARG:NH2	2.31	0.64
1:A:247:GLU:OE2	8:A:2174:HOH:O	2.14	0.63
1:A:221:ARG:NH2	2:A:1479:GOL:H32	2.14	0.63
1:A:267:ASN:HD22	2:A:1482:GOL:C3	2.11	0.63
1:A:102:GLU:H	2:A:1480:GOL:H2	1.64	0.61
1:A:37:TYR:O	1:A:140:HIS:HD2	1.83	0.61
1:A:267:ASN:HB2	2:A:1482:GOL:H32	1.83	0.59
6:A:1492:PGE:H4	8:A:2196:HOH:O	2.04	0.57
1:A:285:ASN:CB	5:A:1490:PEG:H12	2.34	0.57
1:A:191:ARG:HH11	1:A:202:ARG:HB2	1.70	0.57
1:A:267:ASN:HB2	2:A:1482:GOL:C3	2.37	0.54
2:A:1472:GOL:O1	7:A:1498:SO4:O1	2.21	0.54
1:A:271[B]:ARG:CG	1:A:271[B]:ARG:NH1	2.61	0.54
1:A:140:HIS:CE1	1:A:220:ARG:H	2.13	0.54
2:A:1481:GOL:C1	8:A:2285:HOH:O	2.56	0.53
1:A:267:ASN:CB	2:A:1482:GOL:H31	2.37	0.53
1:A:207:ILE:HD13	4:A:1485:DTT:H41	1.92	0.52
1:A:191:ARG:HD3	1:A:202:ARG:HA	1.93	0.50
1:A:465:ARG:HH22	6:A:1492:PGE:H62	1.77	0.50
1:A:300:THR:OG1	6:A:1493:PGE:C4	2.60	0.50
1:A:264[B]:SER:HA	2:A:1482:GOL:H32	1.93	0.49
1:A:267:ASN:HB3	2:A:1482:GOL:H31	1.93	0.49
1:A:267:ASN:CB	2:A:1482:GOL:C3	2.91	0.49
1:A:289:ARG:HH22	3:A:1483:TRS:HN1	1.61	0.49
2:A:1481:GOL:H12	8:A:2285:HOH:O	2.12	0.48
1:A:264[A]:SER:HA	2:A:1482:GOL:H32	1.94	0.48
1:A:255:TYR:CE2	1:A:256[A]:ARG:HG2	2.48	0.48
1:A:465:ARG:HH22	6:A:1492:PGE:C6	2.27	0.47
1:A:348:ARG:HD2	1:A:363:TYR:OH	2.15	0.46
1:A:267:ASN:ND2	2:A:1482:GOL:H2	2.30	0.46
1:A:236:LEU:HD21	1:A:462:PHE:CG	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:THR:OG1	6:A:1493:PGE:H4	2.17	0.44
1:A:65:PHE:HA	1:A:68:ILE:HD12	2.00	0.44
1:A:369:ARG:HH22	4:A:1486:DTT:C1	2.29	0.43
1:A:221:ARG:HG2	7:A:1500:SO4:O1	2.18	0.43
1:A:256[A]:ARG:NH1	8:A:2181:HOH:O	2.15	0.43
1:A:221:ARG:HH22	2:A:1479:GOL:H32	1.83	0.43
1:A:1:MET:N	8:A:2001:HOH:O	2.51	0.43
1:A:120:GLY:N	4:A:1485:DTT:H11	2.14	0.42
1:A:465:ARG:HH12	6:A:1492:PGE:H62	1.84	0.42
1:A:222:GLU:OE2	7:A:1500:SO4:O4	2.39	0.41
1:A:89:ILE:HG23	1:A:200:ALA:HB2	2.02	0.41
1:A:124[A]:ILE:HD11	4:A:1485:DTT:S1	2.60	0.41
1:A:411:GLU:O	1:A:415:LYS:HG2	2.21	0.41
6:A:1494:PGE:C3	6:A:1494:PGE:H6	2.46	0.40
1:A:467:ARG:HD2	8:A:2278:HOH:O	2.20	0.40
1:A:44:ILE:HD11	1:A:117[A]:ARG:NE	2.37	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	473/467 (101%)	461 (98%)	11 (2%)	1 (0%)	47 39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	GLY

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	412/404 (102%)	402 (98%)	10 (2%)	49 42

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	202	ARG
1	A	256[A]	ARG
1	A	256[C]	ARG
1	A	280	PHE
1	A	304	LEU
1	A	387	ASN
1	A	390	ARG
1	A	414	GLU
1	A	459	VAL

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

Mol	Chain	Res	Type
1	A	18	ASN
1	A	140	HIS
1	A	194	GLN
1	A	199	GLN
1	A	285	ASN
1	A	387	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

33 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	A	1479	-	5,5,5	0.19	0	5,5,5	0.64	0
7	SO4	A	1496	-	4,4,4	0.35	0	6,6,6	0.57	0
2	GOL	A	1469	-	5,5,5	0.70	0	5,5,5	1.39	0
2	GOL	A	1480	-	5,5,5	0.62	0	5,5,5	1.01	0
3	TRS	A	1484	-	7,7,7	0.65	0	9,9,9	2.00	3 (33%)
3	TRS	A	1483	-	7,7,7	0.64	0	9,9,9	1.62	2 (22%)
5	PEG	A	1491	-	6,6,6	0.33	0	5,5,5	0.59	0
6	PGE	A	1493	-	9,9,9	0.58	0	8,8,8	1.41	1 (12%)
2	GOL	A	1468	-	5,5,5	0.30	0	5,5,5	0.89	0
6	PGE	A	1492	-	9,9,9	0.55	0	8,8,8	1.03	0
2	GOL	A	1472	-	5,5,5	0.42	0	5,5,5	0.93	0
7	SO4	A	1499	-	4,4,4	0.29	0	6,6,6	0.71	0
7	SO4	A	1495	-	4,4,4	0.47	0	6,6,6	0.38	0
2	GOL	A	1470	-	5,5,5	0.50	0	5,5,5	1.06	0
5	PEG	A	1489	-	6,6,6	0.51	0	5,5,5	0.97	0
2	GOL	A	1474	-	5,5,5	0.41	0	5,5,5	0.56	0
7	SO4	A	1497	-	4,4,4	0.18	0	6,6,6	0.39	0
7	SO4	A	1500	-	4,4,4	0.33	0	6,6,6	0.52	0
2	GOL	A	1476	-	5,5,5	0.85	0	5,5,5	1.28	1 (20%)
7	SO4	A	1498	-	4,4,4	0.36	0	6,6,6	0.51	0
4	DTT	A	1486	-	7,7,7	0.76	0	4,8,8	2.91	2 (50%)
2	GOL	A	1481	-	5,5,5	0.58	0	5,5,5	0.83	0
2	GOL	A	1473	-	5,5,5	0.69	0	5,5,5	1.44	0
2	GOL	A	1477	-	5,5,5	0.34	0	5,5,5	0.98	0
5	PEG	A	1487	-	6,6,6	0.59	0	5,5,5	0.83	0
5	PEG	A	1488	-	6,6,6	1.10	0	5,5,5	1.38	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	1471	-	5,5,5	0.26	0	5,5,5	1.18	1 (20%)
2	GOL	A	1478	-	5,5,5	0.29	0	5,5,5	0.66	0
2	GOL	A	1475	-	5,5,5	0.29	0	5,5,5	0.51	0
6	PGE	A	1494	-	9,9,9	0.42	0	8,8,8	0.73	0
2	GOL	A	1482	-	5,5,5	0.25	0	5,5,5	0.55	0
5	PEG	A	1490	-	6,6,6	0.53	0	5,5,5	1.34	1 (20%)
4	DTT	A	1485	-	7,7,7	0.89	0	4,8,8	0.80	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	A	1479	-	-	4/4/4/4	-
2	GOL	A	1469	-	-	4/4/4/4	-
2	GOL	A	1480	-	-	2/4/4/4	-
3	TRS	A	1484	-	-	9/9/9/9	-
3	TRS	A	1483	-	-	6/9/9/9	-
5	PEG	A	1491	-	-	2/4/4/4	-
6	PGE	A	1493	-	-	5/7/7/7	-
2	GOL	A	1468	-	-	2/4/4/4	-
6	PGE	A	1492	-	-	5/7/7/7	-
2	GOL	A	1472	-	-	4/4/4/4	-
2	GOL	A	1470	-	-	3/4/4/4	-
5	PEG	A	1489	-	-	3/4/4/4	-
2	GOL	A	1474	-	-	0/4/4/4	-
2	GOL	A	1476	-	-	0/4/4/4	-
4	DTT	A	1486	-	-	0/8/8/8	-
2	GOL	A	1481	-	-	2/4/4/4	-
2	GOL	A	1473	-	-	3/4/4/4	-
2	GOL	A	1477	-	-	4/4/4/4	-
5	PEG	A	1487	-	-	3/4/4/4	-
5	PEG	A	1488	-	-	2/4/4/4	-
2	GOL	A	1471	-	-	2/4/4/4	-
2	GOL	A	1478	-	-	0/4/4/4	-
2	GOL	A	1475	-	-	1/4/4/4	-
6	PGE	A	1494	-	-	5/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	1482	-	-	2/4/4/4	-
5	PEG	A	1490	-	-	1/4/4/4	-
4	DTT	A	1485	-	-	4/8/8/8	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1486	DTT	O2-C2-C3	-4.50	100.48	109.72
3	A	1484	TRS	O3-C3-C	-3.76	99.09	111.00
3	A	1483	TRS	O1-C1-C	-3.47	99.99	111.00
4	A	1486	DTT	C3-C4-S4	-3.19	105.18	114.47
3	A	1484	TRS	O1-C1-C	-3.13	101.08	111.00
5	A	1490	PEG	C3-O2-C2	-2.87	100.85	113.29
6	A	1493	PGE	O2-C3-C4	-2.74	98.03	110.39
2	A	1476	GOL	O1-C1-C2	-2.28	99.26	110.20
3	A	1484	TRS	C2-C-N	2.28	114.79	107.98
2	A	1471	GOL	O2-C2-C1	-2.10	99.87	109.12
3	A	1483	TRS	C1-C-N	-2.06	101.83	107.98
5	A	1488	PEG	O2-C3-C4	2.04	119.01	110.07

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1469	GOL	C1-C2-C3-O3
2	A	1480	GOL	C1-C2-C3-O3
2	A	1480	GOL	O2-C2-C3-O3
3	A	1484	TRS	C2-C-C1-O1
3	A	1484	TRS	C3-C-C1-O1
3	A	1484	TRS	C1-C-C2-O2
3	A	1484	TRS	C3-C-C2-O2
3	A	1484	TRS	N-C-C2-O2
3	A	1484	TRS	C1-C-C3-O3
3	A	1484	TRS	C2-C-C3-O3
3	A	1484	TRS	N-C-C3-O3
3	A	1483	TRS	C1-C-C2-O2
3	A	1483	TRS	C3-C-C2-O2
3	A	1483	TRS	N-C-C2-O2
3	A	1483	TRS	C1-C-C3-O3
3	A	1483	TRS	C2-C-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1483	TRS	N-C-C3-O3
2	A	1468	GOL	O1-C1-C2-C3
4	A	1485	DTT	C1-C2-C3-O3
4	A	1485	DTT	C1-C2-C3-C4
4	A	1485	DTT	O2-C2-C3-O3
2	A	1472	GOL	C1-C2-C3-O3
2	A	1470	GOL	C1-C2-C3-O3
2	A	1481	GOL	C1-C2-C3-O3
2	A	1473	GOL	C1-C2-C3-O3
2	A	1477	GOL	O1-C1-C2-C3
2	A	1477	GOL	C1-C2-C3-O3
2	A	1477	GOL	O2-C2-C3-O3
2	A	1471	GOL	C1-C2-C3-O3
6	A	1493	PGE	C6-C5-O3-C4
6	A	1492	PGE	O2-C3-C4-O3
2	A	1479	GOL	O2-C2-C3-O3
2	A	1469	GOL	O1-C1-C2-O2
2	A	1481	GOL	O2-C2-C3-O3
2	A	1471	GOL	O2-C2-C3-O3
5	A	1489	PEG	O2-C3-C4-O4
5	A	1487	PEG	O1-C1-C2-O2
6	A	1494	PGE	O3-C5-C6-O4
2	A	1479	GOL	O1-C1-C2-C3
2	A	1479	GOL	C1-C2-C3-O3
2	A	1469	GOL	O1-C1-C2-C3
2	A	1472	GOL	O1-C1-C2-C3
2	A	1482	GOL	O1-C1-C2-C3
2	A	1482	GOL	C1-C2-C3-O3
2	A	1472	GOL	O2-C2-C3-O3
2	A	1473	GOL	O2-C2-C3-O3
2	A	1477	GOL	O1-C1-C2-O2
6	A	1492	PGE	O3-C5-C6-O4
6	A	1494	PGE	C6-C5-O3-C4
5	A	1491	PEG	O1-C1-C2-O2
6	A	1493	PGE	O3-C5-C6-O4
5	A	1489	PEG	O1-C1-C2-O2
5	A	1487	PEG	O2-C3-C4-O4
6	A	1493	PGE	O2-C3-C4-O3
2	A	1469	GOL	O2-C2-C3-O3
2	A	1468	GOL	O1-C1-C2-O2
6	A	1492	PGE	O1-C1-C2-O2
6	A	1494	PGE	C4-C3-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	1493	PGE	C4-C3-O2-C2
5	A	1489	PEG	C4-C3-O2-C2
6	A	1494	PGE	C3-C4-O3-C5
2	A	1479	GOL	O1-C1-C2-O2
2	A	1470	GOL	O1-C1-C2-O2
2	A	1470	GOL	O2-C2-C3-O3
6	A	1494	PGE	C1-C2-O2-C3
5	A	1487	PEG	C1-C2-O2-C3
5	A	1491	PEG	C1-C2-O2-C3
4	A	1485	DTT	S1-C1-C2-O2
2	A	1475	GOL	O1-C1-C2-O2
6	A	1492	PGE	C1-C2-O2-C3
2	A	1472	GOL	O1-C1-C2-O2
5	A	1488	PEG	O2-C3-C4-O4
2	A	1473	GOL	O1-C1-C2-C3
3	A	1484	TRS	N-C-C1-O1
5	A	1490	PEG	O1-C1-C2-O2
5	A	1488	PEG	C4-C3-O2-C2
6	A	1493	PGE	C1-C2-O2-C3
6	A	1492	PGE	C6-C5-O3-C4

There are no ring outliers.

15 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1479	GOL	2	0
2	A	1480	GOL	1	0
3	A	1483	TRS	1	0
6	A	1493	PGE	3	0
6	A	1492	PGE	4	0
2	A	1472	GOL	1	0
7	A	1500	SO4	2	0
7	A	1498	SO4	2	0
4	A	1486	DTT	3	0
2	A	1481	GOL	3	0
2	A	1473	GOL	1	0
6	A	1494	PGE	1	0
2	A	1482	GOL	11	0
5	A	1490	PEG	2	0
4	A	1485	DTT	5	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, 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	467/467 (100%)	-0.06	27 (5%)	23 25	17, 28, 67, 92	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	PHE	4.5
1	A	70	ASN	4.2
1	A	67	ILE	3.9
1	A	196	PHE	3.8
1	A	69	GLU	3.7
1	A	197	ASP	3.4
1	A	198	VAL	3.4
1	A	190	PRO	3.3
1	A	317	GLY	3.2
1	A	193	PHE	3.1
1	A	66	GLU	3.1
1	A	319	GLU	3.1
1	A	191	ARG	3.1
1	A	89	ILE	2.7
1	A	200	ALA	2.7
1	A	194	GLN	2.6
1	A	62	GLU	2.6
1	A	71	PRO	2.5
1	A	68	ILE	2.5
1	A	442	SER	2.4
1	A	316	ILE	2.3
1	A	392	GLU	2.1
1	A	60	GLY	2.1
1	A	63	LYS	2.1
1	A	320	GLU	2.0
1	A	50	ASP	2.0
1	A	195	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
2	GOL	A	1468	6/6	0.80	0.20	55,65,68,78	0
5	PEG	A	1491	7/7	0.83	0.37	66,73,81,91	0
5	PEG	A	1487	7/7	0.84	0.21	49,62,71,78	0
2	GOL	A	1469	6/6	0.85	0.18	45,52,54,69	0
2	GOL	A	1482	6/6	0.85	0.27	46,65,68,75	0
2	GOL	A	1478	6/6	0.88	0.21	53,59,82,84	0
6	PGE	A	1494	10/10	0.89	0.15	51,67,75,77	0
2	GOL	A	1475	6/6	0.89	0.33	54,59,63,92	0
4	DTT	A	1486	8/8	0.90	0.17	41,55,65,71	0
6	PGE	A	1493	10/10	0.90	0.20	25,57,82,95	0
3	TRS	A	1484	8/8	0.90	0.23	41,54,65,88	0
6	PGE	A	1492	10/10	0.90	0.13	30,58,71,86	0
5	PEG	A	1489	7/7	0.90	0.13	39,62,77,89	0
2	GOL	A	1474	6/6	0.90	0.14	52,57,68,71	0
2	GOL	A	1470	6/6	0.91	0.17	25,59,78,80	0
7	SO4	A	1496	5/5	0.91	0.31	67,98,170,195	0
5	PEG	A	1490	7/7	0.91	0.18	42,50,62,68	0
7	SO4	A	1497	5/5	0.92	0.17	51,74,112,130	0
7	SO4	A	1495	5/5	0.92	0.23	73,89,118,122	0
5	PEG	A	1488	7/7	0.93	0.17	36,37,60,71	0
3	TRS	A	1483	8/8	0.93	0.15	40,55,69,80	0
2	GOL	A	1479	6/6	0.93	0.10	51,61,65,68	0
2	GOL	A	1472	6/6	0.94	0.16	49,56,73,82	0
7	SO4	A	1499	5/5	0.94	0.22	80,93,122,135	0
2	GOL	A	1471	6/6	0.94	0.24	47,55,56,69	0
4	DTT	A	1485	8/8	0.94	0.18	28,65,102,119	0
2	GOL	A	1477	6/6	0.95	0.15	52,64,73,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	1481	6/6	0.95	0.19	38,55,70,70	0
2	GOL	A	1473	6/6	0.95	0.13	35,39,49,61	0
2	GOL	A	1476	6/6	0.96	0.09	27,35,37,47	0
7	SO4	A	1498	5/5	0.96	0.22	27,31,43,47	5
2	GOL	A	1480	6/6	0.97	0.11	48,54,79,85	0
7	SO4	A	1500	5/5	0.99	0.21	28,28,36,40	5

6.5 Other polymers [i](#)

There are no such residues in this entry.