



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:25 AM UTC

PDB ID : 4B8R / pdb_00004b8r
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 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

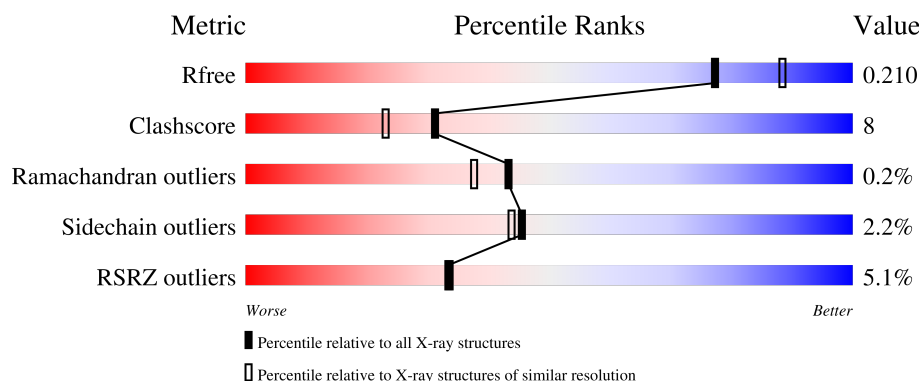
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 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	467	5% 82% 17%

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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TRS	A	1484	-	X	-	-
4	DTT	A	1485	-	-	X	-
7	SO4	A	1498	-	-	X	-
7	SO4	A	1500	-	-	X	-

2 Entry composition [i](#)

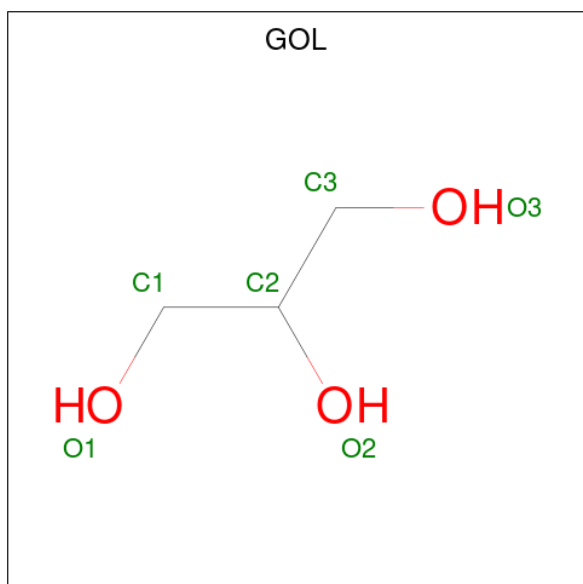
There are 8 unique types of molecules in this entry. The entry contains 4364 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



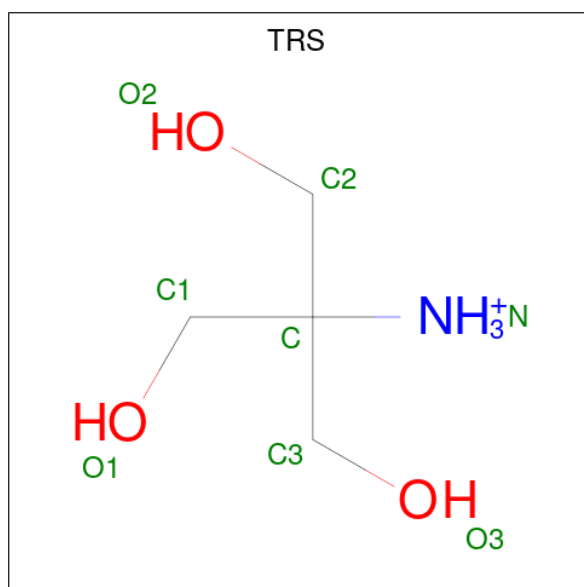
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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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 (CCD ID: TRS) (formula: C₄H₁₂NO₃).



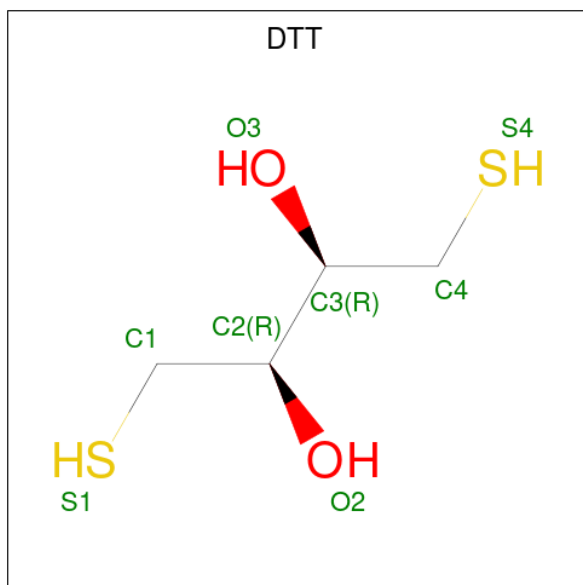
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

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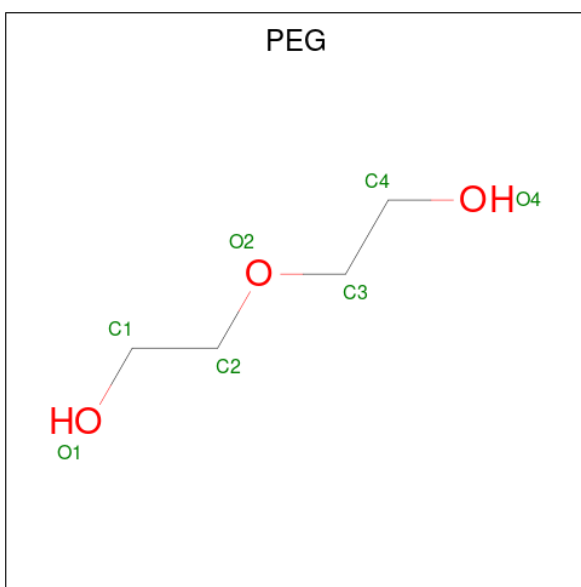
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

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



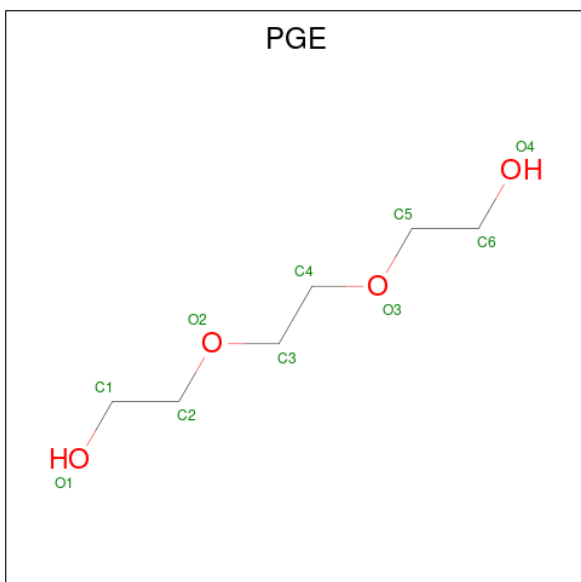
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		
4	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



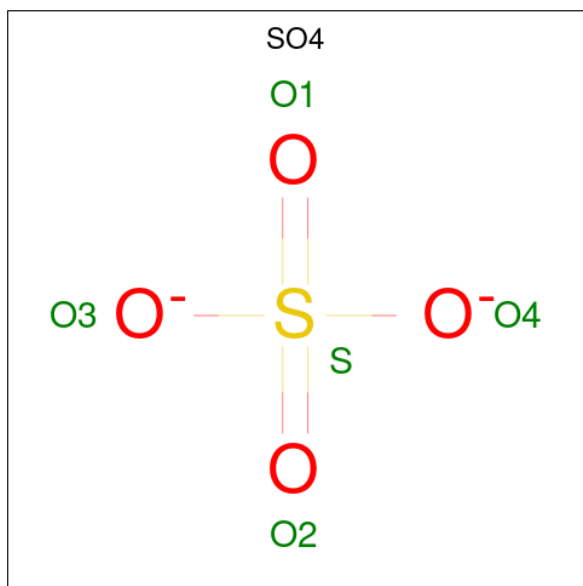
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: 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 (CCD ID: 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		
7	A	1	Total	O	S	0	0
			5	4	1		

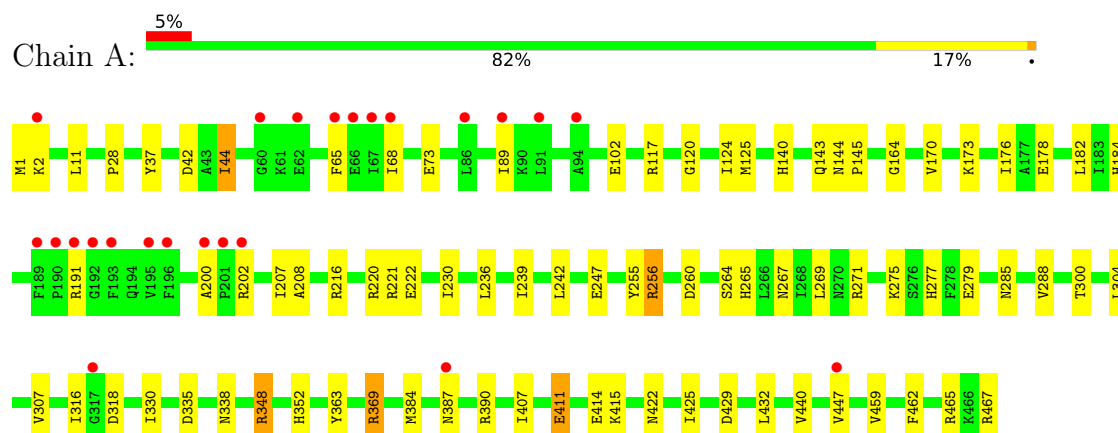
- Molecule 8 is water.

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

3 Residue-property plots

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: 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	2840 reflections (5.04%)	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)	0.37 , 52.9	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

5.1 Standard geometry

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

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	1.56	33/3932 (0.8%)	1.15	8/5307 (0.2%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	HIS	CG-CD2	7.89	1.44	1.35
1	A	143	GLN	N-CA	7.13	1.55	1.46
1	A	184	HIS	ND1-CE1	6.89	1.39	1.32
1	A	265	HIS	CE1-NE2	6.67	1.39	1.32
1	A	318	ASP	CA-C	-6.32	1.44	1.52
1	A	277	HIS	CG-CD2	6.02	1.42	1.35
1	A	173	LYS	N-CA	5.94	1.54	1.46
1	A	260	ASP	N-CA	5.94	1.53	1.46
1	A	145	PRO	N-CA	5.89	1.54	1.47
1	A	242	LEU	N-CA	5.78	1.53	1.46
1	A	239	ILE	C-O	5.76	1.30	1.24
1	A	440	VAL	N-CA	5.76	1.52	1.46
1	A	348	ARG	C-O	5.55	1.30	1.23
1	A	348	ARG	N-CA	5.47	1.52	1.46
1	A	170	VAL	C-O	5.46	1.29	1.23
1	A	176	ILE	CA-CB	5.46	1.59	1.54
1	A	407	ILE	N-CA	5.44	1.52	1.46
1	A	265	HIS	CG-CD2	5.39	1.41	1.35
1	A	144	ASN	CA-C	5.29	1.59	1.53
1	A	184	HIS	CE1-NE2	5.29	1.37	1.32
1	A	369	ARG	CZ-NH1	5.28	1.40	1.32
1	A	279	GLU	CA-CB	5.26	1.59	1.52
1	A	269	LEU	CA-C	5.20	1.59	1.52
1	A	432	LEU	N-CA	5.17	1.52	1.46
1	A	277	HIS	CE1-NE2	5.14	1.37	1.32
1	A	208	ALA	C-O	5.13	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	GLU	CA-CB	5.12	1.60	1.52
1	A	352	HIS	CG-CD2	5.11	1.41	1.35
1	A	230	ILE	N-CA	5.10	1.52	1.46
1	A	307	VAL	CA-CB	5.05	1.60	1.54
1	A	11	LEU	N-CA	-5.05	1.40	1.46
1	A	425	ILE	N-CA	-5.01	1.40	1.46
1	A	338	ASN	CA-C	-5.00	1.46	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ILE	CB-CA-C	-6.28	104.49	110.70
1	A	411	GLU	N-CA-C	5.63	117.42	111.28
1	A	44	ILE	CB-CG1-CD1	-5.38	102.50	113.80
1	A	216	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	A	384	MET	CB-CA-C	-5.24	102.63	110.90
1	A	330	ILE	N-CA-C	5.23	116.58	110.62
1	A	182	LEU	CA-C-N	-5.07	116.91	123.19
1	A	182	LEU	C-N-CA	-5.07	116.91	123.19

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	59	0
2	A	90	0	120	19	0
3	A	16	0	24	0	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	67	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 (67) 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
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:HH11	1:A:271[B]:ARG:CG	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:191:ARG:HH11	1:A:202:ARG:HB2	1.70	0.57
1:A:285:ASN:CB	5:A:1490:PEG:H12	2.34	0.57
1:A:267:ASN:HB2	2:A:1482:GOL:C3	2.37	0.54
1:A:271[B]:ARG:NH1	1:A:271[B]:ARG:CG	2.61	0.54
2:A:1472:GOL:O1	7:A:1498:SO4:O1	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:236:LEU:HD21	1:A:462:PHE:CG	2.51	0.46
1:A:267:ASN:ND2	2:A:1482:GOL:H2	2.30	0.46
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:124[A]:ILE:HG22	1:A:125:MET:HE2	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:73:GLU:H	1:A:73:GLU:CD	2.27	0.42
1:A:89:ILE:HG23	1:A:200:ALA:HB2	2.02	0.41
1:A:222:GLU:OE2	7:A:1500:SO4:O4	2.39	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

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	473/467 (101%)	461 (98%)	11 (2%)	1 (0%)	43	37

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%)	43	40

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

Mol	Chain	Res	Type
1	A	2	LYS
1	A	28	PRO
1	A	256[A]	ARG
1	A	256[C]	ARG
1	A	304	LEU
1	A	387	ASN
1	A	390	ARG
1	A	414	GLU
1	A	447	VAL
1	A	459	VAL

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	18	ASN
1	A	140	HIS
1	A	194	GLN

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Mol	Chain	Res	Type
1	A	199	GLN
1	A	285	ASN
1	A	387	ASN

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](#)

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	$\# Z > 2$
3	TRS	A	1483	-	7,7,7	0.68	0	9,9,9	1.85	2 (22%)
4	DTT	A	1485	-	7,7,7	0.91	0	4,8,8	0.84	0
2	GOL	A	1471	-	5,5,5	0.26	0	5,5,5	1.25	1 (20%)
5	PEG	A	1491	-	6,6,6	0.33	0	5,5,5	0.58	0
6	PGE	A	1494	-	9,9,9	0.43	0	8,8,8	0.72	0
7	SO4	A	1495	-	4,4,4	0.56	0	6,6,6	0.34	0
5	PEG	A	1488	-	6,6,6	1.11	0	5,5,5	1.36	1 (20%)
3	TRS	A	1484	-	7,7,7	0.72	0	9,9,9	2.27	3 (33%)
2	GOL	A	1478	-	5,5,5	0.30	0	5,5,5	0.70	0
7	SO4	A	1498	-	4,4,4	0.46	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	1481	-	5,5,5	0.62	0	5,5,5	0.89	0
7	SO4	A	1499	-	4,4,4	0.26	0	6,6,6	0.73	0
4	DTT	A	1486	-	7,7,7	0.78	0	4,8,8	2.88	2 (50%)
2	GOL	A	1480	-	5,5,5	0.64	0	5,5,5	1.10	1 (20%)
2	GOL	A	1476	-	5,5,5	0.89	0	5,5,5	1.39	1 (20%)
5	PEG	A	1490	-	6,6,6	0.53	0	5,5,5	1.32	1 (20%)
2	GOL	A	1479	-	5,5,5	0.18	0	5,5,5	0.71	0
2	GOL	A	1475	-	5,5,5	0.29	0	5,5,5	0.56	0
6	PGE	A	1492	-	9,9,9	0.55	0	8,8,8	1.03	0
5	PEG	A	1487	-	6,6,6	0.59	0	5,5,5	0.82	0
7	SO4	A	1496	-	4,4,4	0.32	0	6,6,6	0.58	0
7	SO4	A	1500	-	4,4,4	0.43	0	6,6,6	0.50	0
5	PEG	A	1489	-	6,6,6	0.51	0	5,5,5	0.98	0
6	PGE	A	1493	-	9,9,9	0.58	0	8,8,8	1.40	1 (12%)
2	GOL	A	1482	-	5,5,5	0.26	0	5,5,5	0.56	0
2	GOL	A	1469	-	5,5,5	0.70	0	5,5,5	1.48	0
2	GOL	A	1474	-	5,5,5	0.42	0	5,5,5	0.60	0
7	SO4	A	1497	-	4,4,4	0.12	0	6,6,6	0.31	0
2	GOL	A	1473	-	5,5,5	0.73	0	5,5,5	1.53	0
2	GOL	A	1472	-	5,5,5	0.43	0	5,5,5	1.01	1 (20%)
2	GOL	A	1468	-	5,5,5	0.30	0	5,5,5	0.96	0
2	GOL	A	1477	-	5,5,5	0.37	0	5,5,5	1.05	0
2	GOL	A	1470	-	5,5,5	0.51	0	5,5,5	1.14	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	TRS	A	1483	-	-	7/9/9/9	-
4	DTT	A	1485	-	-	4/8/8/8	-
2	GOL	A	1471	-	-	2/4/4/4	-
5	PEG	A	1491	-	-	2/4/4/4	-
6	PGE	A	1494	-	-	5/7/7/7	-
5	PEG	A	1488	-	-	2/4/4/4	-
3	TRS	A	1484	-	-	9/9/9/9	-
2	GOL	A	1478	-	-	0/4/4/4	-
2	GOL	A	1481	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTT	A	1486	-	-	0/8/8/8	-
2	GOL	A	1480	-	-	2/4/4/4	-
2	GOL	A	1476	-	-	0/4/4/4	-
5	PEG	A	1490	-	-	1/4/4/4	-
2	GOL	A	1479	-	-	4/4/4/4	-
2	GOL	A	1475	-	-	1/4/4/4	-
6	PGE	A	1492	-	-	5/7/7/7	-
5	PEG	A	1487	-	-	4/4/4/4	-
5	PEG	A	1489	-	-	3/4/4/4	-
6	PGE	A	1493	-	-	5/7/7/7	-
2	GOL	A	1482	-	-	2/4/4/4	-
2	GOL	A	1469	-	-	4/4/4/4	-
2	GOL	A	1474	-	-	0/4/4/4	-
2	GOL	A	1473	-	-	3/4/4/4	-
2	GOL	A	1472	-	-	4/4/4/4	-
2	GOL	A	1468	-	-	2/4/4/4	-
2	GOL	A	1477	-	-	4/4/4/4	-
2	GOL	A	1470	-	-	3/4/4/4	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1486	DTT	O2-C2-C3	-4.33	100.48	109.57
3	A	1484	TRS	O3-C3-C	-4.23	99.09	110.88
3	A	1483	TRS	O1-C1-C	-3.91	99.99	110.88
3	A	1484	TRS	O1-C1-C	-3.51	101.08	110.88
4	A	1486	DTT	C3-C4-S4	-3.31	105.18	114.43
5	A	1490	PEG	C3-O2-C2	-2.84	100.85	113.26
6	A	1493	PGE	O2-C3-C4	-2.70	98.03	110.35
3	A	1484	TRS	C2-C-N	2.59	114.79	108.17
3	A	1483	TRS	C1-C-N	-2.49	101.83	108.17
2	A	1476	GOL	O1-C1-C2	-2.47	99.26	110.38
2	A	1471	GOL	O2-C2-C1	-2.25	99.87	109.18
2	A	1472	GOL	O3-C3-C2	-2.09	100.95	110.38
5	A	1488	PEG	O2-C3-C4	2.02	119.01	110.11
2	A	1480	GOL	O1-C1-C2	-2.01	101.34	110.38

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1468	GOL	O1-C1-C2-C3
2	A	1469	GOL	C1-C2-C3-O3
2	A	1470	GOL	C1-C2-C3-O3
2	A	1471	GOL	C1-C2-C3-O3
2	A	1472	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	1480	GOL	C1-C2-C3-O3
2	A	1480	GOL	O2-C2-C3-O3
2	A	1481	GOL	C1-C2-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
3	A	1483	TRS	N-C-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
4	A	1485	DTT	C1-C2-C3-O3
4	A	1485	DTT	C1-C2-C3-C4
4	A	1485	DTT	O2-C2-C3-O3
6	A	1493	PGE	C6-C5-O3-C4
2	A	1469	GOL	O1-C1-C2-O2
2	A	1471	GOL	O2-C2-C3-O3
2	A	1479	GOL	O2-C2-C3-O3
2	A	1481	GOL	O2-C2-C3-O3
6	A	1492	PGE	O2-C3-C4-O3
5	A	1489	PEG	O2-C3-C4-O4
2	A	1469	GOL	O1-C1-C2-C3
2	A	1472	GOL	O1-C1-C2-C3
2	A	1479	GOL	O1-C1-C2-C3
2	A	1479	GOL	C1-C2-C3-O3
2	A	1482	GOL	O1-C1-C2-C3
2	A	1482	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	1487	PEG	O1-C1-C2-O2
6	A	1494	PGE	O3-C5-C6-O4
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	1489	PEG	O1-C1-C2-O2
5	A	1491	PEG	O1-C1-C2-O2
6	A	1493	PGE	O3-C5-C6-O4
5	A	1487	PEG	O2-C3-C4-O4
2	A	1468	GOL	O1-C1-C2-O2
2	A	1469	GOL	O2-C2-C3-O3
6	A	1493	PGE	O2-C3-C4-O3
6	A	1492	PGE	O1-C1-C2-O2
2	A	1470	GOL	O1-C1-C2-O2
2	A	1470	GOL	O2-C2-C3-O3
2	A	1479	GOL	O1-C1-C2-O2
6	A	1494	PGE	C4-C3-O2-C2
6	A	1494	PGE	C3-C4-O3-C5
6	A	1493	PGE	C4-C3-O2-C2
5	A	1489	PEG	C4-C3-O2-C2
6	A	1494	PGE	C1-C2-O2-C3
5	A	1487	PEG	C1-C2-O2-C3
2	A	1475	GOL	O1-C1-C2-O2
5	A	1491	PEG	C1-C2-O2-C3
4	A	1485	DTT	S1-C1-C2-O2
2	A	1472	GOL	O1-C1-C2-O2
6	A	1492	PGE	C1-C2-O2-C3
3	A	1484	TRS	N-C-C1-O1
2	A	1473	GOL	O1-C1-C2-C3
5	A	1488	PEG	O2-C3-C4-O4
3	A	1483	TRS	C3-C-C1-O1
5	A	1488	PEG	C4-C3-O2-C2
5	A	1490	PEG	O1-C1-C2-O2
6	A	1493	PGE	C1-C2-O2-C3
6	A	1492	PGE	C6-C5-O3-C4
5	A	1487	PEG	C4-C3-O2-C2

There are no ring outliers.

14 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1485	DTT	5	0
6	A	1494	PGE	1	0
7	A	1498	SO4	2	0
2	A	1481	GOL	3	0
4	A	1486	DTT	3	0
2	A	1480	GOL	1	0
5	A	1490	PEG	2	0
2	A	1479	GOL	2	0
6	A	1492	PGE	4	0
7	A	1500	SO4	2	0
6	A	1493	PGE	3	0
2	A	1482	GOL	11	0
2	A	1473	GOL	1	0
2	A	1472	GOL	1	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	467/467 (100%)	-0.22	24 (5%)	33 33	10, 28, 67, 92	8 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	ALA	3.6
1	A	447	VAL	3.5
1	A	65	PHE	3.1
1	A	191	ARG	3.1
1	A	192	GLY	3.0
1	A	2	LYS	3.0
1	A	387	ASN	2.8
1	A	190	PRO	2.7
1	A	89	ILE	2.7
1	A	196	PHE	2.6
1	A	68	ILE	2.6
1	A	62	GLU	2.5
1	A	94	ALA	2.3
1	A	91	LEU	2.3
1	A	189	PHE	2.3
1	A	195	VAL	2.3
1	A	193	PHE	2.3
1	A	60	GLY	2.3
1	A	317	GLY	2.2
1	A	201	PRO	2.1
1	A	66	GLU	2.1
1	A	67	ILE	2.1
1	A	86	LEU	2.1
1	A	202	ARG	2.1

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($\text{\AA}^2$)	Q<0.9
5	PEG	A	1491	7/7	0.77	0.22	66,73,81,91	0
7	SO4	A	1496	5/5	0.78	0.16	67,98,170,195	0
7	SO4	A	1495	5/5	0.81	0.12	73,89,118,122	0
7	SO4	A	1497	5/5	0.83	0.11	51,74,112,130	0
2	GOL	A	1469	6/6	0.85	0.17	45,52,54,69	0
5	PEG	A	1490	7/7	0.86	0.16	42,50,62,68	0
7	SO4	A	1499	5/5	0.86	0.11	80,93,122,135	0
4	DTT	A	1486	8/8	0.87	0.14	41,55,65,71	0
5	PEG	A	1487	7/7	0.87	0.17	49,62,71,78	0
2	GOL	A	1482	6/6	0.88	0.13	46,65,68,75	0
6	PGE	A	1494	10/10	0.88	0.16	51,67,75,77	0
2	GOL	A	1468	6/6	0.88	0.15	55,65,68,78	0
4	DTT	A	1485	8/8	0.89	0.18	28,65,102,119	0
2	GOL	A	1478	6/6	0.89	0.14	53,59,82,84	0
6	PGE	A	1493	10/10	0.90	0.15	25,57,82,95	0
3	TRS	A	1483	8/8	0.90	0.14	40,55,69,80	0
5	PEG	A	1489	7/7	0.90	0.14	39,62,77,89	0
2	GOL	A	1471	6/6	0.90	0.12	47,55,56,69	0
2	GOL	A	1474	6/6	0.90	0.16	52,57,68,71	0
6	PGE	A	1492	10/10	0.90	0.16	30,58,71,86	0
2	GOL	A	1470	6/6	0.91	0.16	25,59,78,80	0
2	GOL	A	1477	6/6	0.91	0.18	52,64,73,86	0
2	GOL	A	1472	6/6	0.91	0.15	49,56,73,82	0
2	GOL	A	1480	6/6	0.91	0.13	48,54,79,85	0
2	GOL	A	1481	6/6	0.91	0.14	38,55,70,70	0
2	GOL	A	1479	6/6	0.92	0.11	51,61,65,68	0
2	GOL	A	1473	6/6	0.92	0.13	35,39,49,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TRS	A	1484	8/8	0.92	0.13	41,54,65,88	0
2	GOL	A	1475	6/6	0.92	0.11	54,59,63,92	0
7	SO4	A	1498	5/5	0.93	0.13	27,31,43,47	5
5	PEG	A	1488	7/7	0.93	0.13	36,37,60,71	0
2	GOL	A	1476	6/6	0.96	0.12	27,35,37,47	0
7	SO4	A	1500	5/5	0.97	0.12	28,28,36,40	5

6.5 Other polymers [i](#)

There are no such residues in this entry.