



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 10:08 AM EDT

PDB ID : 7N5L
Title : PCNA from *Thermococcus gammatolerans*: crystal II, collection 20, 3.07 Å, 77.0 MGy
Authors : Marin-Tovar, Y.; Rudino-Pinera, E.
Deposited on : 2021-06-05
Resolution : 3.07 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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

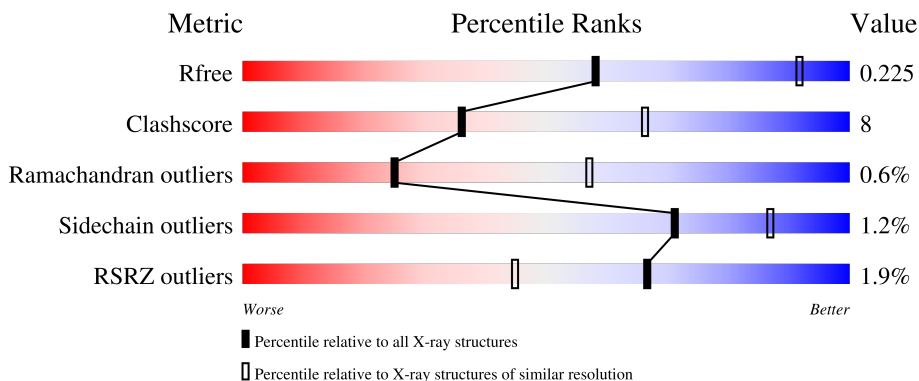
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	74% 20% 6%
1	B	265	72% 21% 7% 1%
1	C	265	76% 17% 7% 2%
1	D	265	76% 17% 6% 4%

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	B	301	-	-	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8541 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 DNA polymerase sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	248	2009	1285	315	400	9	0	5	0
1	B	247	2005	1282	313	401	9	0	6	0
1	C	247	2007	1283	313	403	8	0	6	0
1	D	248	2002	1282	314	398	8	0	4	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP C5A5N6
A	-14	ASN	-	expression tag	UNP C5A5N6
A	-13	HIS	-	expression tag	UNP C5A5N6
A	-12	LYS	-	expression tag	UNP C5A5N6
A	-11	VAL	-	expression tag	UNP C5A5N6
A	-10	HIS	-	expression tag	UNP C5A5N6
A	-9	HIS	-	expression tag	UNP C5A5N6
A	-8	HIS	-	expression tag	UNP C5A5N6
A	-7	HIS	-	expression tag	UNP C5A5N6
A	-6	HIS	-	expression tag	UNP C5A5N6
A	-5	HIS	-	expression tag	UNP C5A5N6
A	-4	ILE	-	expression tag	UNP C5A5N6
A	-3	GLU	-	expression tag	UNP C5A5N6
A	-2	GLY	-	expression tag	UNP C5A5N6
A	-1	ARG	-	expression tag	UNP C5A5N6
A	0	HIS	-	expression tag	UNP C5A5N6
B	-15	MET	-	expression tag	UNP C5A5N6
B	-14	ASN	-	expression tag	UNP C5A5N6
B	-13	HIS	-	expression tag	UNP C5A5N6
B	-12	LYS	-	expression tag	UNP C5A5N6
B	-11	VAL	-	expression tag	UNP C5A5N6

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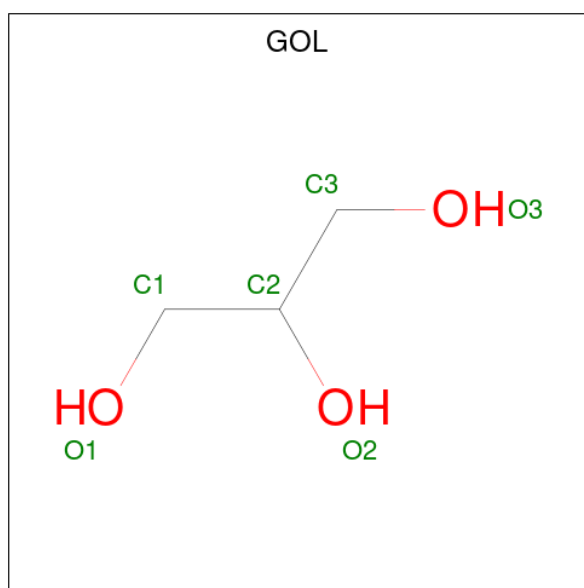
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP C5A5N6
B	-9	HIS	-	expression tag	UNP C5A5N6
B	-8	HIS	-	expression tag	UNP C5A5N6
B	-7	HIS	-	expression tag	UNP C5A5N6
B	-6	HIS	-	expression tag	UNP C5A5N6
B	-5	HIS	-	expression tag	UNP C5A5N6
B	-4	ILE	-	expression tag	UNP C5A5N6
B	-3	GLU	-	expression tag	UNP C5A5N6
B	-2	GLY	-	expression tag	UNP C5A5N6
B	-1	ARG	-	expression tag	UNP C5A5N6
B	0	HIS	-	expression tag	UNP C5A5N6
C	-15	MET	-	expression tag	UNP C5A5N6
C	-14	ASN	-	expression tag	UNP C5A5N6
C	-13	HIS	-	expression tag	UNP C5A5N6
C	-12	LYS	-	expression tag	UNP C5A5N6
C	-11	VAL	-	expression tag	UNP C5A5N6
C	-10	HIS	-	expression tag	UNP C5A5N6
C	-9	HIS	-	expression tag	UNP C5A5N6
C	-8	HIS	-	expression tag	UNP C5A5N6
C	-7	HIS	-	expression tag	UNP C5A5N6
C	-6	HIS	-	expression tag	UNP C5A5N6
C	-5	HIS	-	expression tag	UNP C5A5N6
C	-4	ILE	-	expression tag	UNP C5A5N6
C	-3	GLU	-	expression tag	UNP C5A5N6
C	-2	GLY	-	expression tag	UNP C5A5N6
C	-1	ARG	-	expression tag	UNP C5A5N6
C	0	HIS	-	expression tag	UNP C5A5N6
D	-15	MET	-	expression tag	UNP C5A5N6
D	-14	ASN	-	expression tag	UNP C5A5N6
D	-13	HIS	-	expression tag	UNP C5A5N6
D	-12	LYS	-	expression tag	UNP C5A5N6
D	-11	VAL	-	expression tag	UNP C5A5N6
D	-10	HIS	-	expression tag	UNP C5A5N6
D	-9	HIS	-	expression tag	UNP C5A5N6
D	-8	HIS	-	expression tag	UNP C5A5N6
D	-7	HIS	-	expression tag	UNP C5A5N6
D	-6	HIS	-	expression tag	UNP C5A5N6
D	-5	HIS	-	expression tag	UNP C5A5N6
D	-4	ILE	-	expression tag	UNP C5A5N6
D	-3	GLU	-	expression tag	UNP C5A5N6
D	-2	GLY	-	expression tag	UNP C5A5N6
D	-1	ARG	-	expression tag	UNP C5A5N6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP C5A5N6

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



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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0

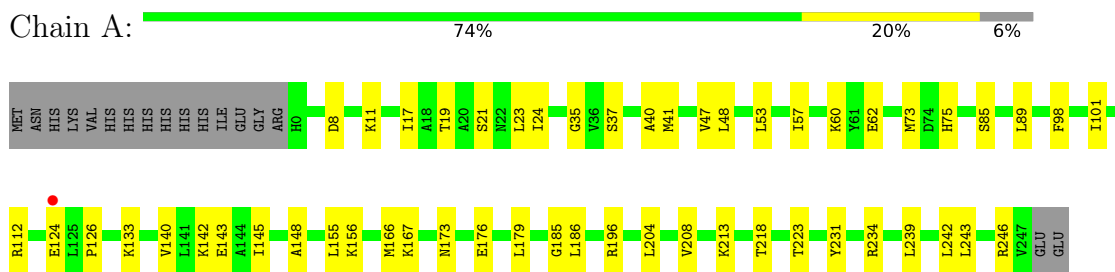
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total 86	O 86	0	0
4	B	79	Total 79	O 79	0	0
4	C	79	Total 79	O 79	0	0
4	D	76	Total 76	O 76	0	0

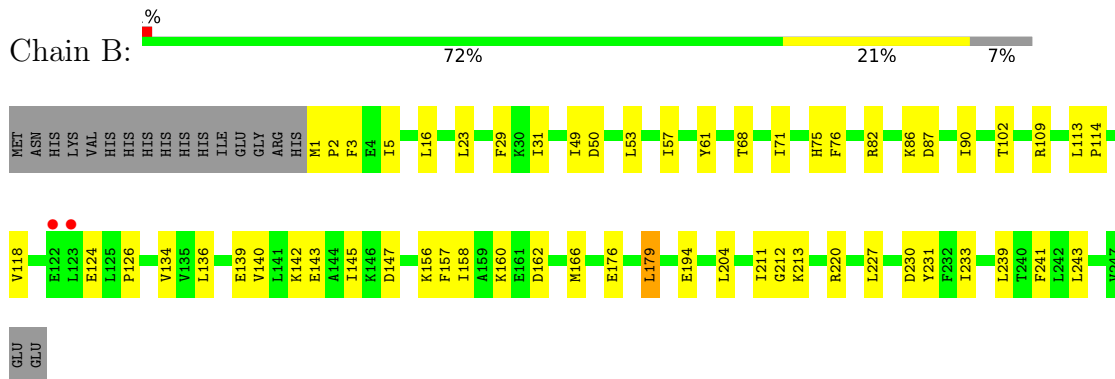
3 Residue-property plots [i](#)

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.

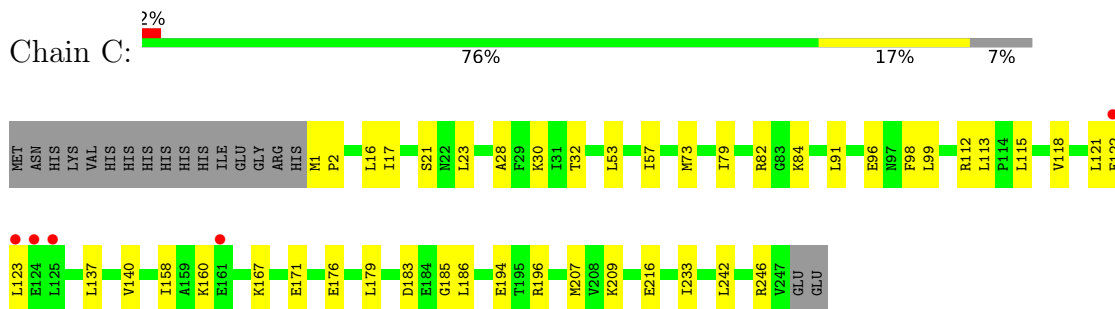
- Molecule 1: DNA polymerase sliding clamp



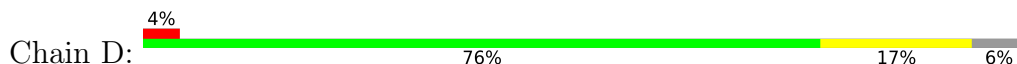
- Molecule 1: DNA polymerase sliding clamp

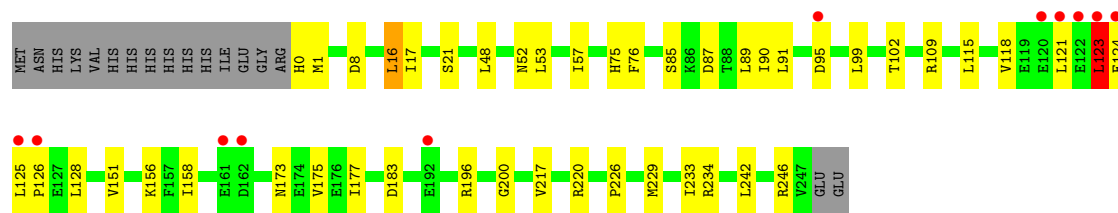


- Molecule 1: DNA polymerase sliding clamp



- Molecule 1: DNA polymerase sliding clamp





4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	187.68Å 187.68Å 64.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.63 – 3.07 44.36 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.63-3.07) 99.9 (44.36-3.07)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.06Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.151 , 0.224 0.154 , 0.225	Depositor DCC
R_{free} test set	1214 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	74.5	Xtrriage
Anisotropy	0.258	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8541	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4693e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, SO4

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	0.52	0/2039	0.67	1/2746 (0.0%)
1	B	0.52	0/2034	0.68	1/2739 (0.0%)
1	C	0.53	0/2036	0.67	0/2742
1	D	0.53	0/2032	0.65	3/2737 (0.1%)
All	All	0.52	0/8141	0.67	5/10964 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	123	LEU	CA-CB-CG	5.83	128.71	115.30
1	B	23	LEU	CA-CB-CG	-5.78	102.00	115.30
1	D	16	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	23	LEU	CA-CB-CG	-5.16	103.44	115.30
1	D	48	LEU	CB-CG-CD2	-5.08	102.36	111.00

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	2009	0	2021	38	0
1	B	2005	0	2018	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2007	0	2017	30	0
1	D	2002	0	2017	30	0
2	A	30	0	40	7	0
2	B	36	0	48	3	0
2	C	12	0	16	1	0
2	D	30	0	40	6	0
3	A	25	0	0	0	0
3	B	20	0	0	0	0
3	C	25	0	0	1	0
3	D	20	0	0	1	0
4	A	86	0	0	3	0
4	B	79	0	0	4	1
4	C	79	0	0	5	1
4	D	76	0	0	3	0
All	All	8541	0	8217	131	1

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 (131) 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:B:143[B]:GLU:OE2	4:B:401:HOH:O	1.99	0.79
1:A:167:LYS:HG3	1:A:176:GLU:HG2	1.67	0.77
1:A:196:ARG:HH12	2:A:301:GOL:H2	1.57	0.68
1:B:176:GLU:OE2	4:B:402:HOH:O	2.11	0.68
1:C:21[A]:SER:OG	4:C:401:HOH:O	2.14	0.66
1:A:145:ILE:HD13	1:A:204:LEU:HB3	1.77	0.66
1:A:142:LYS:HE3	2:A:304:GOL:H32	1.78	0.66
1:D:156:LYS:NZ	4:D:405:HOH:O	2.29	0.65
1:C:28:ALA:HB2	1:C:118:VAL:HG21	1.79	0.63
1:D:196:ARG:NH2	2:D:301:GOL:O1	2.32	0.62
1:B:53:LEU:HB3	1:B:57:ILE:HD11	1.81	0.61
1:A:140:VAL:HG11	1:A:179:LEU:HD11	1.81	0.61
1:B:49:ILE:HD11	1:B:239:LEU:HD11	1.84	0.60
1:D:200:GLY:H	2:D:302:GOL:H11	1.67	0.60
1:A:8[B]:ASP:O	1:A:234:ARG:NH2	2.32	0.59
1:D:17:ILE:O	1:D:21:SER:OG	2.21	0.58
1:D:128:LEU:HD11	1:D:242:LEU:HD11	1.86	0.58
1:B:16:LEU:HD12	1:B:233:ILE:HD12	1.85	0.58
1:B:124:GLU:O	1:B:126:PRO:HD3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ILE:HB	1:B:102:THR:HB	1.86	0.57
1:B:139:GLU:HB2	1:B:213:LYS:HB3	1.86	0.57
1:B:145:ILE:HD13	1:B:204:LEU:HB3	1.86	0.57
1:B:160:LYS:HG2	1:B:194:GLU:HG3	1.87	0.56
1:D:85:SER:N	3:D:308:SO4:O2	2.32	0.56
1:A:143[B]:GLU:OE1	2:A:304:GOL:O2	2.19	0.56
1:D:16:LEU:HD12	1:D:233:ILE:HG21	1.88	0.55
1:D:53:LEU:HB3	1:D:57:ILE:HD11	1.88	0.55
1:D:183:ASP:OD2	4:D:401:HOH:O	2.18	0.55
1:A:8[A]:ASP:O	1:A:234:ARG:NH2	2.36	0.55
1:B:118:VAL:HG22	2:B:304:GOL:H32	1.87	0.55
1:C:17:ILE:HG23	1:C:73:MET:HE3	1.90	0.54
1:A:24:ILE:HG13	1:A:73:MET:HG3	1.90	0.54
1:C:53:LEU:HB3	1:C:57:ILE:HD11	1.89	0.53
1:C:137:LEU:HD12	1:C:185:GLY:HA2	1.91	0.53
1:C:121:LEU:O	1:C:123:LEU:N	2.40	0.53
1:A:231:TYR:HE1	1:A:239:LEU:HD23	1.74	0.53
1:A:196:ARG:O	1:A:223:THR:HA	2.08	0.53
1:D:220:ARG:NH1	4:D:409:HOH:O	2.39	0.52
1:A:11:LYS:HB2	1:A:85:SER:HA	1.90	0.52
1:A:231:TYR:CE1	1:A:239:LEU:HD23	2.45	0.52
1:A:213:LYS:H	1:A:213:LYS:HD2	1.75	0.51
1:A:196:ARG:NH2	2:A:301:GOL:O1	2.42	0.50
1:D:8:ASP:O	1:D:234:ARG:NH2	2.38	0.50
1:A:35:GLY:HA3	2:A:303:GOL:H31	1.94	0.50
1:C:171:GLU:H	1:C:171:GLU:CD	2.14	0.50
1:D:151:VAL:HG21	1:D:175[B]:VAL:HG13	1.93	0.50
1:D:95:ASP:OD1	1:D:95:ASP:N	2.36	0.50
1:A:75[B]:HIS:CE1	4:B:456:HOH:O	2.65	0.49
1:A:145:ILE:HD12	1:A:208:VAL:HG21	1.92	0.49
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.92	0.49
1:C:140:VAL:HG11	1:C:179:LEU:HD11	1.94	0.49
1:B:220:ARG:NH1	1:B:230:ASP:OD2	2.45	0.49
1:D:90:ILE:HB	1:D:102:THR:HB	1.93	0.49
1:A:133:LYS:HE3	2:A:305:GOL:H12	1.95	0.49
1:D:89:LEU:HD11	1:D:91:LEU:HD21	1.94	0.49
1:B:140:VAL:HG11	1:B:179:LEU:HD21	1.95	0.48
1:C:96:GLU:HG3	1:C:98:PHE:CE2	2.47	0.48
1:A:19[A]:THR:HG23	4:A:417:HOH:O	2.12	0.48
1:C:1:MET:H2	1:C:2:PRO:HD3	1.78	0.48
1:A:60:LYS:HE2	1:A:62:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ILE:HG23	1:C:196:ARG:HG2	1.97	0.47
1:C:216[A]:GLU:OE2	1:C:216[A]:GLU:N	2.47	0.47
1:B:212:GLY:HA3	2:B:305:GOL:H2	1.96	0.47
1:A:246:ARG:NH2	4:A:407:HOH:O	2.48	0.47
1:B:162:ASP:N	1:B:162:ASP:OD1	2.48	0.47
1:D:151:VAL:HG13	1:D:173:ASN:HB3	1.97	0.47
1:B:68:THR:HG22	2:B:304:GOL:H31	1.98	0.46
1:B:143[A]:GLU:HG3	1:B:147:ASP:OD2	2.16	0.46
1:A:218:THR:HG21	2:A:305:GOL:H31	1.98	0.45
1:B:49:ILE:HD13	1:B:241:PHE:CD1	2.51	0.45
1:D:52:ASN:OD1	2:D:303:GOL:H32	2.16	0.45
1:A:47:VAL:HG22	1:A:243:LEU:HD13	1.99	0.45
1:B:134:VAL:HG12	1:B:136:LEU:HD22	1.99	0.45
1:C:28:ALA:HB2	1:C:118:VAL:CG2	2.46	0.45
1:D:99:LEU:HB2	1:D:115:LEU:HD21	1.97	0.45
1:D:196:ARG:HH22	2:D:301:GOL:H31	1.81	0.45
1:B:227:LEU:HB3	1:B:243:LEU:HB3	1.99	0.45
1:C:16:LEU:HD13	1:C:233:ILE:HG13	1.98	0.45
1:B:113:LEU:HD12	1:B:114:PRO:HD2	1.98	0.44
1:D:121:LEU:HB3	1:D:123:LEU:HD23	1.98	0.44
1:A:148:ALA:CB	1:A:155:LEU:HD13	2.48	0.44
1:B:29:PHE:CD1	1:B:71:ILE:HD12	2.53	0.44
1:B:86:LYS:HB2	4:B:405:HOH:O	2.16	0.44
1:A:98:PHE:CD1	1:A:112:ARG:HG3	2.53	0.43
1:A:140:VAL:HG21	1:A:185:GLY:HA3	1.99	0.43
1:B:49:ILE:HD13	1:B:241:PHE:CE1	2.53	0.43
1:C:91:LEU:HA	1:C:91:LEU:HD23	1.74	0.43
1:A:19[B]:THR:HG23	4:A:417:HOH:O	2.17	0.43
1:B:75[A]:HIS:HB3	1:B:113:LEU:HD11	2.00	0.43
1:D:226:PRO:HB2	1:D:242:LEU:HD22	2.01	0.43
1:A:48:LEU:HB3	1:A:242:LEU:HB3	2.00	0.43
1:D:177:ILE:HD12	1:D:177:ILE:N	2.34	0.43
1:D:118:VAL:O	2:D:305:GOL:O1	2.36	0.43
1:B:142:LYS:NZ	1:B:211:ILE:O	2.34	0.43
1:B:3:PHE:CE2	1:B:31:ILE:HD13	2.54	0.42
1:C:179:LEU:HD22	1:C:186:LEU:HB2	2.01	0.42
1:A:124:GLU:O	1:A:126:PRO:HD3	2.19	0.42
1:B:49:ILE:HD12	1:B:50:ASP:H	1.84	0.42
1:D:158:ILE:HG23	1:D:196:ARG:HG2	2.01	0.42
1:B:157:PHE:C	1:B:158:ILE:HG13	2.39	0.42
1:A:156:LYS:O	1:A:166:MET:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LEU:HD12	1:C:242:LEU:HA	1.80	0.42
1:D:246:ARG:HD3	2:D:302:GOL:O2	2.20	0.42
1:A:40:ALA:O	1:A:48:LEU:HD12	2.20	0.42
1:A:41[B]:MET:SD	1:A:48:LEU:HD13	2.60	0.42
1:C:79:ILE:HD12	1:C:113:LEU:HD13	2.00	0.42
1:C:96:GLU:HG2	4:C:429:HOH:O	2.20	0.42
1:C:23:LEU:HD11	1:C:207:MET:HG3	2.02	0.42
1:C:99:LEU:HB2	1:C:115:LEU:HD21	2.01	0.42
1:A:148:ALA:HB2	1:A:155:LEU:HD13	2.02	0.42
1:C:246:ARG:HG3	2:C:302:GOL:H2	2.02	0.42
1:A:89:LEU:HD11	1:A:101:ILE:HG23	2.01	0.41
1:B:5:ILE:HG23	1:B:61:TYR:CD1	2.55	0.41
1:A:17:ILE:HD13	1:A:17:ILE:HA	1.82	0.41
1:D:87:ASP:OD2	1:D:109:ARG:NH2	2.51	0.41
1:C:209:LYS:HA	4:C:451:HOH:O	2.20	0.41
1:C:30:LYS:HE3	1:C:32:THR:HG22	2.01	0.41
1:B:156:LYS:O	1:B:166:MET:HA	2.20	0.41
1:D:217:VAL:CG1	1:D:229:MET:HG3	2.51	0.41
1:A:179:LEU:HB3	1:A:186:LEU:HD22	2.03	0.41
1:B:87:ASP:OD2	1:B:109:ARG:NH2	2.54	0.41
1:C:82:ARG:HD2	4:C:457:HOH:O	2.20	0.41
1:D:16:LEU:HD11	1:D:233:ILE:HD13	2.02	0.41
1:C:167:LYS:HG3	1:C:176:GLU:HG2	2.02	0.40
1:D:16:LEU:CD1	1:D:233:ILE:HD13	2.52	0.40
1:A:53:LEU:HB3	1:A:57:ILE:HD11	2.02	0.40
1:C:84:LYS:HB3	3:C:305:SO4:O3	2.20	0.40
1:D:242:LEU:HD23	1:D:242:LEU:HA	1.82	0.40
1:C:98:PHE:CE1	1:C:112:ARG:HG2	2.55	0.40
1:C:160:LYS:HG2	1:C:194:GLU:OE1	2.22	0.40
1:C:183:ASP:HA	4:C:455:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:468:HOH:O	4:C:478:HOH:O[1_556]	2.11	0.09

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	251/265 (95%)	237 (94%)	14 (6%)	0	100	100
1	B	251/265 (95%)	240 (96%)	11 (4%)	0	100	100
1	C	251/265 (95%)	237 (94%)	13 (5%)	1 (0%)	34	66
1	D	250/265 (94%)	230 (92%)	15 (6%)	5 (2%)	7	29
All	All	1003/1060 (95%)	944 (94%)	53 (5%)	6 (1%)	25	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	124	GLU
1	D	123	LEU
1	C	122	GLU
1	D	126	PRO
1	D	1	MET
1	D	125	LEU

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	222/233 (95%)	219 (99%)	3 (1%)	67	84
1	B	222/233 (95%)	218 (98%)	4 (2%)	59	80
1	C	222/233 (95%)	222 (100%)	0	100	100
1	D	221/233 (95%)	217 (98%)	4 (2%)	59	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	887/932 (95%)	876 (99%)	11 (1%)	71	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	37	SER
1	A	173	ASN
1	B	76	PHE
1	B	82	ARG
1	B	179	LEU
1	B	231	TYR
1	D	0	HIS
1	D	75[A]	HIS
1	D	75[B]	HIS
1	D	76	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

36 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	SO4	A	310	-	4,4,4	0.23	0	6,6,6	0.25	0
2	GOL	A	305	-	5,5,5	1.12	1 (20%)	5,5,5	0.87	0
2	GOL	B	305	-	5,5,5	0.86	0	5,5,5	1.14	0
3	SO4	C	304	-	4,4,4	0.19	0	6,6,6	0.22	0
2	GOL	B	301	-	5,5,5	1.26	1 (20%)	5,5,5	0.80	0
3	SO4	C	306	-	4,4,4	0.20	0	6,6,6	0.31	0
3	SO4	A	306	-	4,4,4	0.16	0	6,6,6	0.27	0
2	GOL	D	301	-	5,5,5	0.82	0	5,5,5	1.17	0
3	SO4	C	303	-	4,4,4	0.22	0	6,6,6	0.15	0
2	GOL	D	305	-	5,5,5	0.70	0	5,5,5	1.10	0
2	GOL	B	304	-	5,5,5	0.90	0	5,5,5	1.02	0
2	GOL	B	306	-	5,5,5	0.65	0	5,5,5	1.13	0
3	SO4	B	307	-	4,4,4	0.17	0	6,6,6	0.24	0
3	SO4	B	310	-	4,4,4	0.25	0	6,6,6	0.25	0
3	SO4	D	307	-	4,4,4	0.17	0	6,6,6	0.16	0
2	GOL	D	304	-	5,5,5	1.37	2 (40%)	5,5,5	0.89	0
3	SO4	B	308	-	4,4,4	0.21	0	6,6,6	0.20	0
3	SO4	A	307	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	D	309	-	4,4,4	0.20	0	6,6,6	0.28	0
2	GOL	A	304	-	5,5,5	1.17	1 (20%)	5,5,5	0.92	0
3	SO4	C	305	-	4,4,4	0.20	0	6,6,6	0.23	0
2	GOL	A	303	-	5,5,5	1.39	0	5,5,5	0.74	0
3	SO4	A	309	-	4,4,4	0.23	0	6,6,6	0.16	0
2	GOL	C	302	-	5,5,5	1.11	1 (20%)	5,5,5	1.12	0
3	SO4	A	308	-	4,4,4	0.21	0	6,6,6	0.12	0
2	GOL	C	301	-	5,5,5	1.04	0	5,5,5	0.91	0
3	SO4	D	306	-	4,4,4	0.19	0	6,6,6	0.21	0
2	GOL	B	303	-	5,5,5	1.22	0	5,5,5	0.82	0
2	GOL	B	302	-	5,5,5	0.76	0	5,5,5	1.22	0
2	GOL	A	301	-	5,5,5	0.95	0	5,5,5	0.96	0
2	GOL	D	302	-	5,5,5	0.96	0	5,5,5	0.98	0
3	SO4	B	309	-	4,4,4	0.26	0	6,6,6	0.16	0
3	SO4	C	307	-	4,4,4	0.16	0	6,6,6	0.14	0
3	SO4	D	308	-	4,4,4	0.16	0	6,6,6	0.22	0
2	GOL	D	303	-	5,5,5	1.13	0	5,5,5	1.12	0
2	GOL	A	302	-	5,5,5	0.88	0	5,5,5	1.10	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	C	301	-	-	2/4/4/4	-
2	GOL	A	305	-	-	0/4/4/4	-
2	GOL	D	305	-	-	0/4/4/4	-
2	GOL	B	304	-	-	0/4/4/4	-
2	GOL	B	305	-	-	1/4/4/4	-
2	GOL	A	304	-	-	4/4/4/4	-
2	GOL	B	301	-	-	0/4/4/4	-
2	GOL	B	302	-	-	3/4/4/4	-
2	GOL	A	301	-	-	0/4/4/4	-
2	GOL	B	303	-	-	0/4/4/4	-
2	GOL	B	306	-	-	1/4/4/4	-
2	GOL	D	302	-	-	2/4/4/4	-
2	GOL	D	303	-	-	1/4/4/4	-
2	GOL	A	303	-	-	4/4/4/4	-
2	GOL	D	304	-	-	2/4/4/4	-
2	GOL	C	302	-	-	4/4/4/4	-
2	GOL	D	301	-	-	1/4/4/4	-
2	GOL	A	302	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	302	GOL	C3-C2	2.22	1.60	1.51
2	D	304	GOL	C3-C2	2.16	1.60	1.51
2	D	304	GOL	C1-C2	2.16	1.60	1.51
2	B	301	GOL	C3-C2	2.14	1.60	1.51
2	A	304	GOL	C1-C2	2.07	1.60	1.51
2	A	305	GOL	C1-C2	2.02	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	GOL	O1-C1-C2-C3
2	A	302	GOL	C1-C2-C3-O3
2	A	303	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	304	GOL	O1-C1-C2-O2
2	A	304	GOL	O1-C1-C2-C3
2	C	301	GOL	O1-C1-C2-C3
2	C	302	GOL	C1-C2-C3-O3
2	D	303	GOL	O1-C1-C2-C3
2	D	304	GOL	O1-C1-C2-C3
2	A	302	GOL	O1-C1-C2-O2
2	A	303	GOL	O1-C1-C2-C3
2	B	302	GOL	O1-C1-C2-C3
2	B	306	GOL	C1-C2-C3-O3
2	C	302	GOL	O1-C1-C2-C3
2	D	301	GOL	O1-C1-C2-C3
2	A	302	GOL	O2-C2-C3-O3
2	A	303	GOL	O1-C1-C2-O2
2	C	301	GOL	O1-C1-C2-O2
2	C	302	GOL	O2-C2-C3-O3
2	A	303	GOL	O2-C2-C3-O3
2	A	304	GOL	O2-C2-C3-O3
2	C	302	GOL	O1-C1-C2-O2
2	D	302	GOL	O2-C2-C3-O3
2	D	304	GOL	O1-C1-C2-O2
2	D	302	GOL	O1-C1-C2-C3
2	B	305	GOL	O1-C1-C2-O2
2	A	304	GOL	C1-C2-C3-O3
2	B	302	GOL	O1-C1-C2-O2
2	B	302	GOL	O2-C2-C3-O3

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	305	GOL	2	0
2	B	305	GOL	1	0
2	D	301	GOL	2	0
2	D	305	GOL	1	0
2	B	304	GOL	2	0
2	A	304	GOL	2	0
3	C	305	SO4	1	0
2	A	303	GOL	1	0
2	C	302	GOL	1	0
2	A	301	GOL	2	0
2	D	302	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	308	SO4	1	0
2	D	303	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

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	248/265 (93%)	-0.47	1 (0%) 92 84	43, 70, 108, 126	0
1	B	247/265 (93%)	-0.47	2 (0%) 86 71	46, 71, 113, 139	0
1	C	247/265 (93%)	-0.36	5 (2%) 65 43	48, 73, 116, 137	0
1	D	248/265 (93%)	-0.29	11 (4%) 34 17	43, 73, 116, 145	0
All	All	990/1060 (93%)	-0.40	19 (1%) 66 45	43, 72, 114, 145	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	GLU	5.6
1	D	123	LEU	4.3
1	D	124	GLU	4.1
1	D	161	GLU	3.7
1	C	125	LEU	3.6
1	B	122	GLU	3.6
1	A	124	GLU	3.5
1	C	161	GLU	3.3
1	C	124	GLU	3.3
1	C	123	LEU	3.1
1	D	162	ASP	2.9
1	D	126	PRO	2.9
1	D	95	ASP	2.9
1	C	122	GLU	2.3
1	D	125	LEU	2.2
1	D	121	LEU	2.2
1	D	192	GLU	2.1
1	B	123	LEU	2.1
1	D	120	GLU	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	B	301	6/6	0.73	0.43	92,96,106,108	0
2	GOL	D	304	6/6	0.75	0.27	90,105,115,119	0
2	GOL	C	301	6/6	0.78	0.37	91,99,109,115	0
3	SO4	B	307	5/5	0.80	0.20	119,120,142,155	0
2	GOL	B	303	6/6	0.82	0.69	90,109,112,114	0
2	GOL	A	305	6/6	0.83	0.42	80,101,109,114	0
2	GOL	A	304	6/6	0.83	0.47	105,108,117,128	0
3	SO4	C	307	5/5	0.84	0.35	120,126,149,153	0
2	GOL	D	305	6/6	0.85	0.45	84,94,106,114	0
3	SO4	A	310	5/5	0.85	0.32	127,131,153,171	0
2	GOL	A	301	6/6	0.86	0.25	96,99,106,107	0
2	GOL	D	301	6/6	0.86	0.35	101,106,115,119	0
2	GOL	D	303	6/6	0.86	0.34	73,89,99,104	0
2	GOL	B	304	6/6	0.86	0.34	96,99,108,122	0
2	GOL	B	305	6/6	0.87	0.28	99,107,121,121	0
2	GOL	A	303	6/6	0.89	0.32	84,89,97,103	0
2	GOL	B	306	6/6	0.89	0.40	110,115,118,127	0
3	SO4	D	307	5/5	0.90	0.36	112,114,144,148	0
3	SO4	A	309	5/5	0.91	0.46	90,114,137,160	0
3	SO4	D	306	5/5	0.91	0.19	117,125,142,147	0
3	SO4	C	306	5/5	0.91	0.38	102,103,134,142	0
3	SO4	C	305	5/5	0.92	0.29	108,117,140,140	0
3	SO4	C	303	5/5	0.93	0.22	115,122,130,145	0
3	SO4	B	310	5/5	0.94	0.47	95,103,138,154	0
3	SO4	A	306	5/5	0.94	0.18	98,112,130,141	0
3	SO4	A	308	5/5	0.94	0.27	106,107,132,142	0
2	GOL	C	302	6/6	0.94	0.31	67,87,92,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	302	6/6	0.94	0.19	61,73,83,85	0
2	GOL	D	302	6/6	0.94	0.23	68,76,77,91	0
3	SO4	B	308	5/5	0.94	0.33	105,111,126,150	0
3	SO4	D	308	5/5	0.94	0.21	117,121,131,136	0
3	SO4	D	309	5/5	0.94	0.30	91,94,114,142	0
3	SO4	C	304	5/5	0.95	0.24	99,103,119,137	0
3	SO4	A	307	5/5	0.95	0.39	98,106,125,140	0
2	GOL	B	302	6/6	0.96	0.20	70,86,96,108	0
3	SO4	B	309	5/5	0.96	0.13	105,115,130,141	0

6.5 Other polymers [i](#)

There are no such residues in this entry.