Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:23 PM UTC

PDB ID	:	7N5K / pdb_00007n5k
Title	:	PCNA from Thermococcus gammatolerans: crystal II, collection 1, 1.98 A, 3.84 MGy
Authors	:	Marin-Tovar, Y.; Rudino-Pinera, E.
Deposited on	:	2021-06-05
Resolution	:	1.98 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:

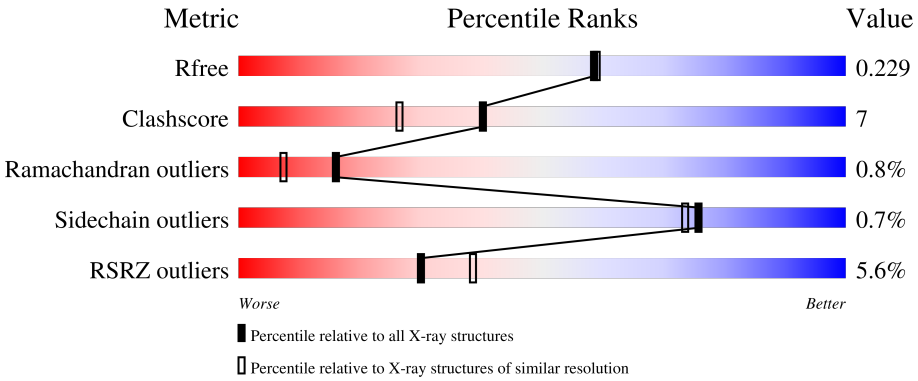
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	265	3% 82% 11% • 6%
1	B	265	7% 82% 11% 7%
1	C	265	4% 80% 12% • 7%
1	D	265	6% 78% 14% • 6%

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	304	-	-	X	-
2	GOL	B	301	-	-	X	-
2	GOL	D	302	-	-	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
1	A	248	Total	C	N	O	S	0	5	0
			2009	1285	315	400	9			
1	B	247	Total	C	N	O	S	0	6	0
			2005	1282	313	401	9			
1	C	247	Total	C	N	O	S	0	6	0
			2007	1283	313	403	8			
1	D	248	Total	C	N	O	S	0	4	0
			2002	1282	314	398	8			

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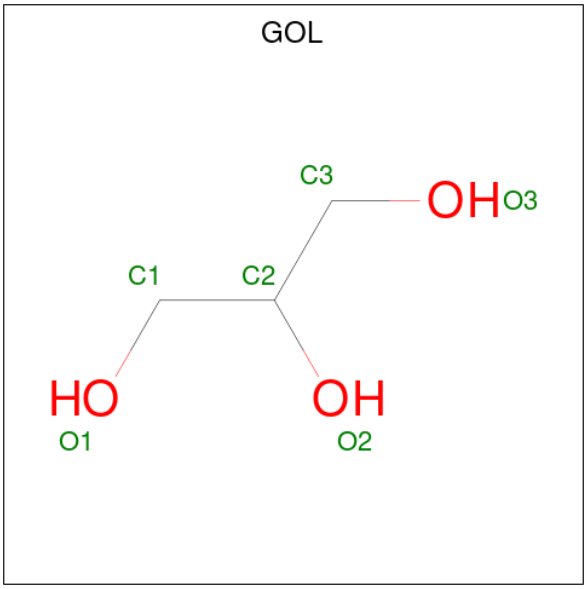
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP C5A5N6

- Molecule 2 is GLYCEROL (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		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

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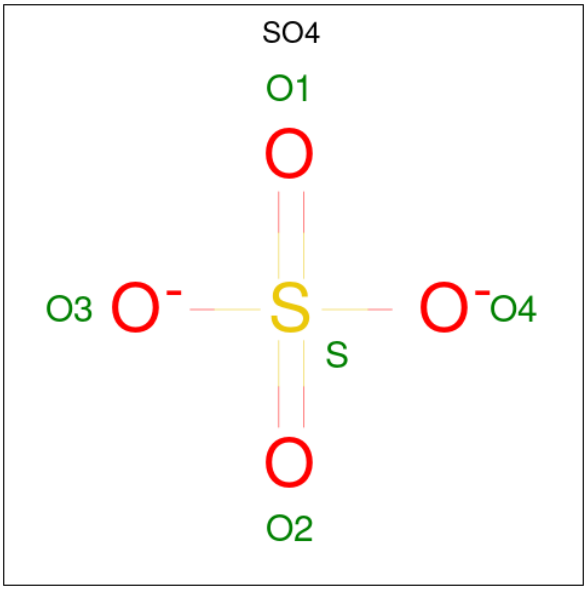
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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 O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

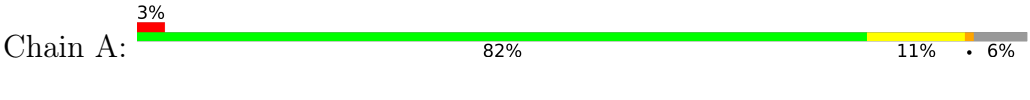
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	91	Total O 91 91	0	0
4	B	80	Total O 80 80	0	0
4	C	75	Total O 75 75	0	0
4	D	74	Total O 74 74	0	0

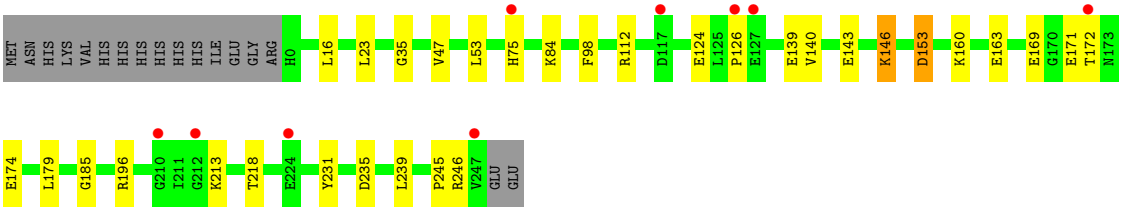
3 Residue-property plots (i)

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

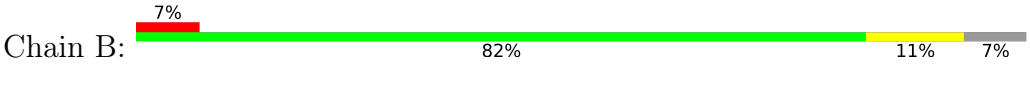
Chain A:

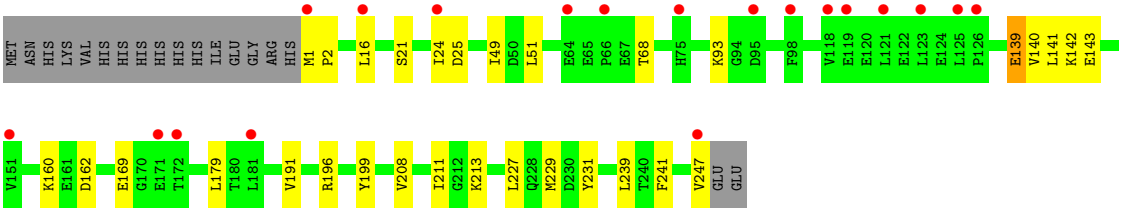




• Molecule 1: DNA polymerase sliding clamp

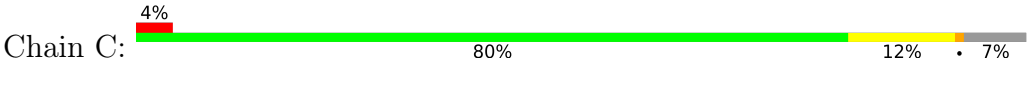
Chain B:

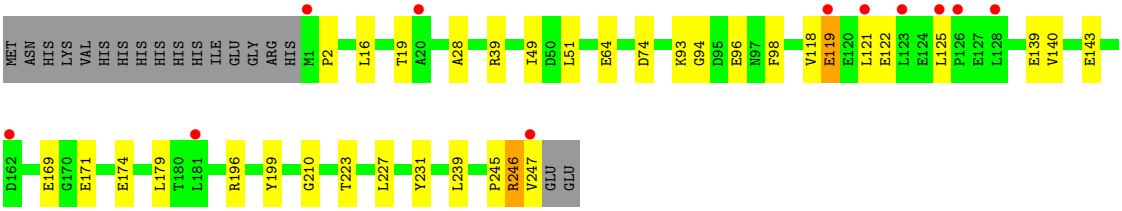




• Molecule 1: DNA polymerase sliding clamp

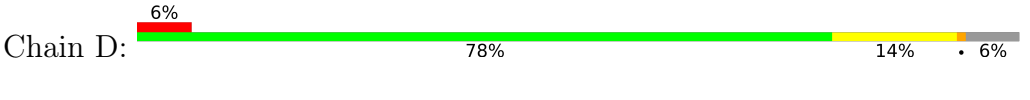
Chain C:

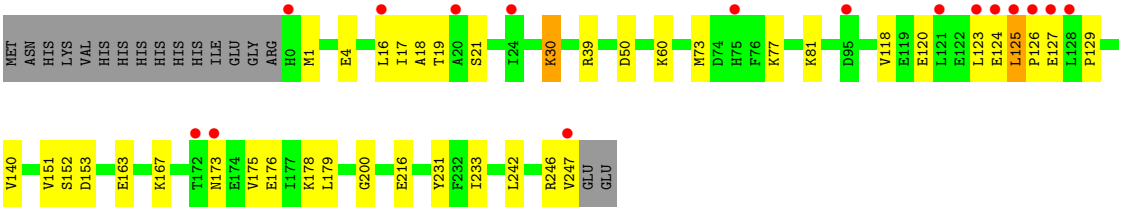




• Molecule 1: DNA polymerase sliding clamp

Chain D:




MET ASN HIS LYS VAL HIS HIS HIS HIS HIS ILE GLU GLY ARG H0 M1 E4 L16 I17 A18 T19 A20 S21 T24 K30 R39 D50 K60 M73 D74 H75 F76 K77 K81 D95 V118 E119 E120 L121 E122 L123 E124 L125 P126 E127 L128 P129
V140 V151 S152 D153 E163 K167 T172 N173 E174 V175 E176 I177 K178 L179 G200 E216 Y231 F232 I233 L242 R246 V247 GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	186.92Å 186.92Å 64.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.12 – 1.98 32.12 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.12-1.98) 99.9 (32.12-1.98)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.190 , 0.228 0.193 , 0.229	Depositor DCC
R_{free} test set	4405 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8541	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.82 % 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 6.4796e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	3/2039 (0.1%)	0.55	0/2746
1	B	0.38	1/2034 (0.0%)	0.52	0/2739
1	C	0.43	3/2036 (0.1%)	0.55	0/2742
1	D	0.45	2/2032 (0.1%)	0.55	0/2737
All	All	0.45	9/8141 (0.1%)	0.54	0/10964

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	GLU	C-O	-7.00	1.16	1.24
1	C	74	ASP	C-O	-6.20	1.17	1.24
1	A	245	PRO	C-O	-5.74	1.16	1.23
1	D	242	LEU	C-O	-5.71	1.17	1.24
1	A	153	ASP	C-O	-5.38	1.17	1.24
1	D	216	GLU	C-O	-5.38	1.17	1.24
1	A	146	LYS	C-O	-5.29	1.18	1.24
1	C	245	PRO	C-O	-5.15	1.16	1.23
1	C	246	ARG	C-O	-5.13	1.17	1.24

There are no bond angle outliers.

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	2009	0	2021	29	0
1	B	2005	0	2018	27	0
1	C	2007	0	2017	25	0
1	D	2002	0	2017	25	0
2	A	30	0	40	13	0
2	B	36	0	48	11	0
2	C	12	0	16	2	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	0	0
3	D	20	0	0	0	0
4	A	91	0	0	1	0
4	B	80	0	0	3	0
4	C	75	0	0	1	0
4	D	74	0	0	2	0
All	All	8541	0	8217	108	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 7.

All (108) 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:146:LYS:NZ	2:A:304:GOL:H31	1.64	1.13
1:A:146:LYS:HZ2	2:A:304:GOL:H31	1.18	0.98
1:B:49:ILE:HD11	1:B:239:LEU:HD11	1.51	0.92
1:C:39:ARG:HH12	1:C:125:LEU:HB2	1.37	0.88
1:D:151:VAL:HG22	1:D:173:ASN:HB3	1.62	0.80
1:A:146:LYS:NZ	2:A:304:GOL:C3	2.43	0.79
1:A:246:ARG:HG2	2:A:302:GOL:H12	1.66	0.77
1:A:146:LYS:HZ1	2:A:304:GOL:H31	1.50	0.75
1:A:169:GLU:HG2	1:A:174:GLU:HG3	1.72	0.71
1:D:151:VAL:HG21	1:D:175[B]:VAL:HG13	1.73	0.68
1:A:146:LYS:HZ1	2:A:304:GOL:C3	2.06	0.66
1:A:213:LYS:H	1:A:213:LYS:HD2	1.61	0.66
1:B:143[A]:GLU:OE2	2:B:303:GOL:O2	2.14	0.66
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.79	0.65
1:D:200:GLY:H	2:D:302:GOL:H11	1.60	0.65
1:A:160:LYS:NZ	2:A:301:GOL:O2	2.29	0.65
1:A:171:GLU:HG2	1:A:172:THR:HG23	1.79	0.65
1:C:39:ARG:NH1	1:C:125:LEU:HB2	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:ARG:HD3	2:D:302:GOL:O2	1.97	0.63
1:C:140:VAL:HG11	1:C:179:LEU:HD11	1.81	0.63
1:D:18:ALA:HA	1:D:77:LYS:HD3	1.81	0.63
1:B:213:LYS:NZ	2:B:306:GOL:O1	2.32	0.62
1:D:30:LYS:NZ	1:D:120:GLU:OE1	2.33	0.62
1:C:64:GLU:O	4:C:401:HOH:O	2.16	0.61
1:C:139:GLU:O	1:C:143[B]:GLU:HB2	2.00	0.60
1:D:167:LYS:HG3	1:D:176:GLU:HG2	1.84	0.59
1:D:16:LEU:HD12	1:D:233:ILE:HG21	1.84	0.59
1:B:2:PRO:HD2	1:B:93:LYS:O	2.03	0.59
1:C:247:VAL:O	1:C:247:VAL:HG22	2.02	0.58
1:C:96:GLU:HG3	1:C:98:PHE:CE2	2.39	0.58
1:B:231:TYR:CE1	1:B:239:LEU:HD23	2.40	0.57
1:A:140:VAL:HG11	1:A:179:LEU:HD11	1.87	0.57
1:B:25:ASP:O	4:B:401:HOH:O	2.17	0.56
1:C:171:GLU:H	1:C:171:GLU:CD	2.13	0.56
1:D:127:GLU:HB2	1:D:129:PRO:HD3	1.87	0.56
1:A:143[B]:GLU:OE1	2:A:304:GOL:O2	2.23	0.56
1:B:142:LYS:NZ	2:B:306:GOL:H2	2.20	0.56
1:A:153:ASP:OD1	1:A:246:ARG:NH1	2.38	0.56
1:C:96:GLU:OE2	1:C:96:GLU:N	2.28	0.56
1:D:163:GLU:OE1	1:D:178:LYS:NZ	2.38	0.55
1:D:77:LYS:NZ	4:D:403:HOH:O	2.38	0.55
1:C:247:VAL:O	1:C:247:VAL:HG13	2.05	0.55
1:C:93:LYS:NZ	1:C:94:GLY:O	2.40	0.54
1:B:68:THR:HG22	2:B:304:GOL:H31	1.89	0.54
1:C:2:PRO:HA	1:C:93:LYS:O	2.08	0.54
1:D:118:VAL:H	2:D:305:GOL:H11	1.72	0.54
1:B:196:ARG:HH22	2:B:301:GOL:H2	1.73	0.53
1:A:84:LYS:HE3	1:B:143[B]:GLU:OE1	2.08	0.53
1:B:49:ILE:HD11	1:B:239:LEU:CD1	2.31	0.53
1:A:218:THR:HG21	2:A:305:GOL:H31	1.90	0.53
1:B:49:ILE:HD13	1:B:241:PHE:CE1	2.44	0.52
1:B:24:ILE:HG13	1:B:49:ILE:HG21	1.90	0.52
2:B:301:GOL:C3	4:B:434:HOH:O	2.59	0.50
1:A:140:VAL:HG21	1:A:185:GLY:HA3	1.92	0.50
1:B:141:LEU:HD21	1:B:229:MET:HE2	1.94	0.50
1:C:246:ARG:HG3	2:C:302:GOL:H2	1.95	0.49
1:B:213:LYS:HG3	2:B:305:GOL:O2	2.12	0.49
2:B:301:GOL:H32	4:B:434:HOH:O	2.12	0.49
1:A:231:TYR:CE1	1:A:239:LEU:HD23	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:VAL:HG11	1:B:179:LEU:HD11	1.95	0.49
1:A:16:LEU:HD21	1:A:53:LEU:HD21	1.95	0.48
1:C:169:GLU:HB3	1:C:174[B]:GLU:HG3	1.95	0.48
1:D:200:GLY:N	2:D:302:GOL:H11	2.29	0.48
1:A:196:ARG:HH22	2:A:301:GOL:H2	1.77	0.48
1:C:28:ALA:HB2	1:C:118:VAL:CG2	2.44	0.47
1:A:160:LYS:HE3	1:A:163:GLU:OE2	2.15	0.47
2:D:305:GOL:H31	4:D:415:HOH:O	2.14	0.47
1:B:162:ASP:OD1	1:B:162:ASP:N	2.46	0.47
1:D:140:VAL:HG11	1:D:179:LEU:HD11	1.97	0.47
1:A:75[B]:HIS:HE1	4:A:482:HOH:O	1.98	0.46
1:A:231:TYR:HE1	1:A:239:LEU:HD23	1.79	0.46
1:B:196:ARG:NH2	2:B:301:GOL:O1	2.47	0.46
1:D:200:GLY:H	2:D:302:GOL:C1	2.28	0.46
1:C:16:LEU:HD11	1:C:51:LEU:HD11	1.98	0.46
1:B:51:LEU:HD13	1:B:239:LEU:HD13	1.98	0.45
1:B:213:LYS:H	2:B:305:GOL:H2	1.82	0.45
1:D:19:THR:HG21	1:D:231:TYR:OH	2.17	0.45
1:B:142:LYS:HZ3	2:B:306:GOL:H2	1.80	0.45
1:C:49:ILE:HD11	1:C:239:LEU:HD11	1.99	0.44
1:D:17:ILE:O	1:D:21:SER:OG	2.20	0.44
1:D:16:LEU:CD1	1:D:233:ILE:HG21	2.48	0.44
1:D:39:ARG:HD2	1:D:50:ASP:OD1	2.18	0.44
1:D:21:SER:HB3	1:D:73:MET:HE3	2.00	0.44
1:A:23:LEU:HD13	1:A:47:VAL:HG11	1.99	0.43
1:C:96:GLU:H	1:C:96:GLU:CD	2.19	0.43
1:C:199:TYR:CZ	1:C:227:LEU:HB2	2.53	0.43
1:A:124:GLU:O	1:A:126:PRO:HD3	2.18	0.43
1:C:119:GLU:CG	1:C:121:LEU:HD11	2.48	0.43
1:A:98:PHE:CD1	1:A:112:ARG:HG3	2.53	0.43
1:C:196:ARG:NH2	2:C:301:GOL:O3	2.52	0.42
1:D:4:GLU:OE1	1:D:60:LYS:NZ	2.52	0.42
1:A:139:GLU:O	1:A:143[A]:GLU:HB2	2.18	0.42
1:C:28:ALA:HB2	1:C:118:VAL:HG21	2.00	0.42
1:D:81:LYS:HD2	1:D:81:LYS:HA	1.70	0.42
1:A:246:ARG:CG	2:A:302:GOL:H12	2.41	0.42
1:A:196:ARG:HH12	2:A:301:GOL:H2	1.85	0.42
1:C:196:ARG:O	1:C:223:THR:HA	2.20	0.42
1:C:19[B]:THR:HG23	1:C:210:GLY:HA3	2.02	0.41
1:B:239:LEU:HA	1:B:239:LEU:HD12	1.84	0.41
1:B:199:TYR:CZ	1:B:227:LEU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:VAL:HA	1:B:211:ILE:HD12	2.02	0.41
1:D:246:ARG:O	1:D:247:VAL:HG13	2.21	0.41
1:B:160:LYS:O	1:B:191:VAL:HG21	2.21	0.41
1:C:231:TYR:CE1	1:C:239:LEU:HD23	2.56	0.41
1:D:125:LEU:HD12	1:D:125:LEU:HA	1.88	0.41
1:A:35:GLY:CA	2:A:303:GOL:H31	2.50	0.40
1:B:231:TYR:HE1	1:B:239:LEU:HD23	1.83	0.40
1:D:152:SER:OG	1:D:153:ASP:N	2.55	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	251/265 (95%)	246 (98%)	4 (2%)	1 (0%)	30 20
1	B	251/265 (95%)	242 (96%)	9 (4%)	0	100 100
1	C	251/265 (95%)	243 (97%)	6 (2%)	2 (1%)	16 7
1	D	250/265 (94%)	237 (95%)	8 (3%)	5 (2%)	6 1
All	All	1003/1060 (95%)	968 (96%)	27 (3%)	8 (1%)	16 7

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ASP
1	D	123	LEU
1	C	122	GLU
1	D	1	MET
1	D	124	GLU
1	D	125	LEU
1	D	126	PRO

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Mol	Chain	Res	Type
1	C	119	GLU

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%)	222 (100%)	0	100 100
1	B	222/233 (95%)	216 (97%)	6 (3%)	39 31
1	C	222/233 (95%)	222 (100%)	0	100 100
1	D	221/233 (95%)	220 (100%)	1 (0%)	81 79
All	All	887/932 (95%)	880 (99%)	7 (1%)	76 71

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	16	LEU
1	B	21[A]	SER
1	B	21[B]	SER
1	B	139	GLU
1	B	169	GLU
1	B	247	VAL
1	D	30	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	97	ASN
1	C	97	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)

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	D	308	-	4,4,4	0.25	0	6,6,6	0.16	0
3	SO4	D	307	-	4,4,4	0.26	0	6,6,6	0.15	0
3	SO4	C	305	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	A	308	-	4,4,4	0.23	0	6,6,6	0.18	0
3	SO4	B	309	-	4,4,4	0.26	0	6,6,6	0.11	0
2	GOL	D	304	-	5,5,5	1.10	0	5,5,5	0.98	0
3	SO4	C	306	-	4,4,4	0.27	0	6,6,6	0.22	0
3	SO4	C	304	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	A	306	-	4,4,4	0.25	0	6,6,6	0.14	0
2	GOL	A	302	-	5,5,5	0.82	0	5,5,5	1.17	1 (20%)
2	GOL	B	304	-	5,5,5	0.94	0	5,5,5	1.06	0
2	GOL	B	306	-	5,5,5	0.77	0	5,5,5	1.17	0
3	SO4	A	309	-	4,4,4	0.25	0	6,6,6	0.16	0
2	GOL	D	302	-	5,5,5	0.65	0	5,5,5	1.18	0
2	GOL	D	305	-	5,5,5	0.88	0	5,5,5	1.18	1 (20%)
3	SO4	B	307	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	D	309	-	4,4,4	0.24	0	6,6,6	0.11	0
2	GOL	A	303	-	5,5,5	0.89	0	5,5,5	0.95	0
3	SO4	A	307	-	4,4,4	0.27	0	6,6,6	0.10	0
2	GOL	C	301	-	5,5,5	1.04	0	5,5,5	1.00	0
2	GOL	C	302	-	5,5,5	0.82	0	5,5,5	1.17	1 (20%)
3	SO4	A	310	-	4,4,4	0.25	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	A	304	-	5,5,5	1.27	1 (20%)	5,5,5	0.79	0
2	GOL	B	301	-	5,5,5	1.07	0	5,5,5	0.95	0
3	SO4	C	303	-	4,4,4	0.26	0	6,6,6	0.12	0
2	GOL	D	301	-	5,5,5	0.91	0	5,5,5	1.13	0
3	SO4	C	307	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	D	306	-	4,4,4	0.28	0	6,6,6	0.04	0
2	GOL	B	302	-	5,5,5	0.93	0	5,5,5	1.21	1 (20%)
2	GOL	B	305	-	5,5,5	1.02	0	5,5,5	1.09	0
2	GOL	A	301	-	5,5,5	1.03	0	5,5,5	0.97	0
2	GOL	D	303	-	5,5,5	0.70	0	5,5,5	1.22	0
3	SO4	B	308	-	4,4,4	0.26	0	6,6,6	0.11	0
2	GOL	B	303	-	5,5,5	1.09	0	5,5,5	0.97	0
3	SO4	B	310	-	4,4,4	0.26	0	6,6,6	0.08	0
2	GOL	A	305	-	5,5,5	1.01	0	5,5,5	1.05	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	303	-	-	4/4/4/4	-
2	GOL	B	302	-	-	4/4/4/4	-
2	GOL	C	301	-	-	2/4/4/4	-
2	GOL	C	302	-	-	3/4/4/4	-
2	GOL	B	305	-	-	0/4/4/4	-
2	GOL	A	302	-	-	4/4/4/4	-
2	GOL	B	304	-	-	1/4/4/4	-
2	GOL	B	306	-	-	0/4/4/4	-
2	GOL	A	301	-	-	2/4/4/4	-
2	GOL	A	304	-	-	2/4/4/4	-
2	GOL	D	302	-	-	2/4/4/4	-
2	GOL	D	303	-	-	0/4/4/4	-
2	GOL	D	304	-	-	2/4/4/4	-
2	GOL	B	301	-	-	2/4/4/4	-
2	GOL	D	305	-	-	2/4/4/4	-
2	GOL	B	303	-	-	1/4/4/4	-
2	GOL	D	301	-	-	2/4/4/4	-
2	GOL	A	305	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	304	GOL	C1-C2	2.29	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	305	GOL	C3-C2-C1	-2.21	103.69	111.80
2	A	302	GOL	C3-C2-C1	-2.08	104.17	111.80
2	C	302	GOL	C3-C2-C1	-2.02	104.41	111.80
2	B	302	GOL	C3-C2-C1	-2.00	104.44	111.80

There are no chirality outliers.

All (35) 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	O1-C1-C2-O2
2	A	303	GOL	C1-C2-C3-O3
2	A	305	GOL	C1-C2-C3-O3
2	B	302	GOL	O1-C1-C2-C3
2	B	302	GOL	C1-C2-C3-O3
2	C	302	GOL	C1-C2-C3-O3
2	D	301	GOL	O1-C1-C2-C3
2	D	304	GOL	O1-C1-C2-C3
2	D	305	GOL	O1-C1-C2-C3
2	B	302	GOL	O1-C1-C2-O2
2	A	301	GOL	O1-C1-C2-C3
2	A	303	GOL	O1-C1-C2-C3
2	A	304	GOL	C1-C2-C3-O3
2	B	301	GOL	O1-C1-C2-C3
2	C	301	GOL	O1-C1-C2-C3
2	D	302	GOL	O1-C1-C2-C3
2	A	304	GOL	O2-C2-C3-O3
2	B	301	GOL	O1-C1-C2-O2
2	C	301	GOL	O1-C1-C2-O2
2	D	301	GOL	O1-C1-C2-O2
2	D	302	GOL	O1-C1-C2-O2
2	D	304	GOL	O1-C1-C2-O2
2	A	302	GOL	O2-C2-C3-O3
2	A	303	GOL	O2-C2-C3-O3
2	A	305	GOL	O2-C2-C3-O3

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

There are no ring outliers.

14 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	GOL	2	0
2	B	304	GOL	1	0
2	B	306	GOL	3	0
2	D	302	GOL	4	0
2	D	305	GOL	2	0
2	A	303	GOL	1	0
2	C	301	GOL	1	0
2	C	302	GOL	1	0
2	A	304	GOL	6	0
2	B	301	GOL	4	0
2	B	305	GOL	2	0
2	A	301	GOL	3	0
2	B	303	GOL	1	0
2	A	305	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, 95^{th} 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%)	0.29	9 (3%)	46	56	17, 41, 65, 88	5 (2%)
1	B	247/265 (93%)	0.52	19 (7%)	19	26	18, 43, 72, 95	6 (2%)
1	C	247/265 (93%)	0.41	11 (4%)	38	47	20, 44, 78, 99	6 (2%)
1	D	248/265 (93%)	0.41	16 (6%)	25	33	21, 43, 76, 111	4 (1%)
All	All	990/1060 (93%)	0.41	55 (5%)	30	38	17, 42, 74, 111	21 (2%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	125	LEU	6.0
1	B	247	VAL	5.8
1	C	125	LEU	5.3
1	C	126	PRO	5.2
1	D	123	LEU	5.1
1	C	247	VAL	4.2
1	D	126	PRO	3.9
1	D	172	THR	3.5
1	D	128	LEU	3.4
1	A	247	VAL	3.3
1	B	1	MET	3.2
1	C	1	MET	3.2
1	C	123	LEU	3.1
1	B	125	LEU	3.0
1	B	75[A]	HIS	2.9
1	B	121	LEU	2.9
1	D	95	ASP	2.9
1	B	172	THR	2.8
1	D	247	VAL	2.8
1	D	121	LEU	2.7
1	C	128	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	126	PRO	2.7
1	A	172	THR	2.7
1	B	24	ILE	2.7
1	D	75[A]	HIS	2.6
1	D	173	ASN	2.6
1	D	0	HIS	2.6
1	A	75[A]	HIS	2.6
1	B	66	PRO	2.6
1	C	20	ALA	2.5
1	B	64	GLU	2.5
1	C	162	ASP	2.4
1	B	95	ASP	2.4
1	D	16	LEU	2.3
1	D	124	GLU	2.3
1	A	117	ASP	2.3
1	B	151	VAL	2.3
1	A	224	GLU	2.3
1	B	118	VAL	2.2
1	B	181	LEU	2.2
1	C	121	LEU	2.2
1	B	119	GLU	2.2
1	D	127	GLU	2.2
1	B	16	LEU	2.1
1	B	98	PHE	2.1
1	A	212	GLY	2.1
1	C	181	LEU	2.1
1	C	119	GLU	2.1
1	B	123	LEU	2.1
1	D	24	ILE	2.0
1	A	210	GLY	2.0
1	D	20	ALA	2.0
1	A	127	GLU	2.0
1	B	171	GLU	2.0
1	A	126	PRO	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, 95^{th} 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	A	301	6/6	0.68	0.16	70,73,75,80	0
3	SO4	A	310	5/5	0.68	0.10	72,82,96,101	0
2	GOL	B	306	6/6	0.69	0.16	63,71,84,85	0
3	SO4	C	307	5/5	0.70	0.09	78,83,103,105	0
2	GOL	A	304	6/6	0.73	0.17	60,65,68,69	0
2	GOL	D	301	6/6	0.75	0.13	71,73,79,82	0
2	GOL	D	303	6/6	0.75	0.14	48,58,68,77	0
3	SO4	A	308	5/5	0.78	0.09	58,78,89,91	0
2	GOL	B	301	6/6	0.78	0.15	70,72,75,78	0
2	GOL	C	301	6/6	0.78	0.13	71,75,82,82	0
2	GOL	D	305	6/6	0.79	0.13	58,71,78,81	0
2	GOL	A	305	6/6	0.80	0.13	56,58,68,74	0
3	SO4	C	305	5/5	0.80	0.10	57,81,92,95	0
2	GOL	B	305	6/6	0.80	0.14	71,73,79,80	0
2	GOL	D	304	6/6	0.81	0.15	62,68,74,76	0
3	SO4	B	307	5/5	0.81	0.08	84,84,91,97	0
2	GOL	D	302	6/6	0.81	0.16	45,53,55,64	0
2	GOL	B	304	6/6	0.81	0.13	64,68,79,80	0
3	SO4	B	308	5/5	0.82	0.11	69,75,97,99	0
3	SO4	B	309	5/5	0.84	0.09	57,68,89,91	0
2	GOL	B	303	6/6	0.84	0.13	54,58,66,71	0
3	SO4	C	306	5/5	0.84	0.11	68,74,92,98	0
2	GOL	A	303	6/6	0.84	0.13	43,52,53,63	0
3	SO4	D	306	5/5	0.84	0.08	77,86,94,98	0
3	SO4	A	307	5/5	0.85	0.11	68,68,83,97	0
3	SO4	C	303	5/5	0.85	0.08	80,82,93,102	0
2	GOL	B	302	6/6	0.86	0.13	41,51,61,62	0
2	GOL	C	302	6/6	0.86	0.13	41,54,55,60	0
3	SO4	D	307	5/5	0.86	0.09	67,81,98,107	0
3	SO4	D	308	5/5	0.87	0.08	64,73,86,89	0
3	SO4	A	306	5/5	0.88	0.07	72,74,86,89	0
3	SO4	B	310	5/5	0.88	0.10	69,77,82,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	302	6/6	0.88	0.13	38,56,60,62	0
3	SO4	A	309	5/5	0.89	0.09	64,77,85,99	0
3	SO4	C	304	5/5	0.90	0.09	74,75,86,97	0
3	SO4	D	309	5/5	0.92	0.09	64,66,75,89	0

6.5 Other polymers (i)

There are no such residues in this entry.