



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 04:16 am GMT

PDB ID : 5M86  
Title : Crystal Structure of the Thermoplasma acidophilum Protein Ta1207  
Authors : Pathare, G.R.; Nagy, I.; Bracher, A.  
Deposited on : 2016-10-28  
Resolution : 2.40 Å(reported)

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The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

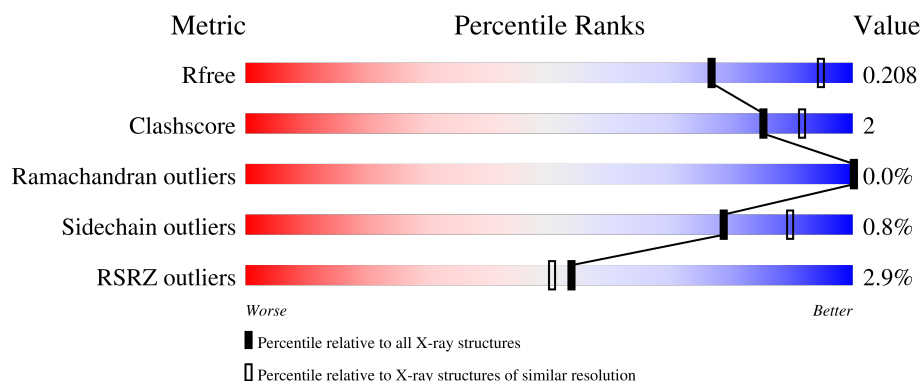
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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  $\geq 3$ , 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	333	<div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	B	333	<div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	C	333	<div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	D	333	<div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	E	333	<div> <div>92%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	333	<div><div></div><div>2%</div><div>92%</div><div>6%</div><div></div><div></div></div>
1	G	333	<div><div></div><div>4%</div><div>90%</div><div>6%</div><div></div><div></div></div>
1	H	333	<div><div></div><div>3%</div><div>91%</div><div>5%</div><div></div><div></div></div>
1	I	333	<div><div></div><div>3%</div><div>91%</div><div>5%</div><div></div><div></div></div>
1	J	333	<div><div></div><div>3%</div><div>91%</div><div>5%</div><div></div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 53263 atoms, of which 26080 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 Ta1207.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	321	Total	C	H	N	O	Se	0	0	0
			5235	1712	2600	423	491	9			
1	B	321	Total	C	H	N	O	Se	0	0	0
			5234	1712	2599	423	491	9			
1	C	321	Total	C	H	N	O	Se	0	0	0
			5235	1712	2600	423	491	9			
1	D	321	Total	C	H	N	O	Se	0	0	0
			5235	1712	2600	423	491	9			
1	E	321	Total	C	H	N	O	Se	0	0	0
			5235	1712	2600	423	491	9			
1	F	321	Total	C	H	N	O	Se	0	0	0
			5235	1712	2600	423	491	9			
1	G	321	Total	C	H	N	O	Se	0	0	0
			5235	1712	2600	423	491	9			
1	H	321	Total	C	H	N	O	Se	0	0	0
			5235	1712	2600	423	491	9			
1	I	321	Total	C	H	N	O	Se	0	0	0
			5236	1712	2601	423	491	9			
1	J	321	Total	C	H	N	O	Se	0	0	0
			5235	1712	2600	423	491	9			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	-	expression tag	UNP Q9HIW9
A	326	LEU	-	expression tag	UNP Q9HIW9
A	327	GLU	-	expression tag	UNP Q9HIW9
A	328	HIS	-	expression tag	UNP Q9HIW9
A	329	HIS	-	expression tag	UNP Q9HIW9
A	330	HIS	-	expression tag	UNP Q9HIW9
A	331	HIS	-	expression tag	UNP Q9HIW9
A	332	HIS	-	expression tag	UNP Q9HIW9
A	333	HIS	-	expression tag	UNP Q9HIW9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	325	ALA	-	expression tag	UNP Q9HIW9
B	326	LEU	-	expression tag	UNP Q9HIW9
B	327	GLU	-	expression tag	UNP Q9HIW9
B	328	HIS	-	expression tag	UNP Q9HIW9
B	329	HIS	-	expression tag	UNP Q9HIW9
B	330	HIS	-	expression tag	UNP Q9HIW9
B	331	HIS	-	expression tag	UNP Q9HIW9
B	332	HIS	-	expression tag	UNP Q9HIW9
B	333	HIS	-	expression tag	UNP Q9HIW9
C	325	ALA	-	expression tag	UNP Q9HIW9
C	326	LEU	-	expression tag	UNP Q9HIW9
C	327	GLU	-	expression tag	UNP Q9HIW9
C	328	HIS	-	expression tag	UNP Q9HIW9
C	329	HIS	-	expression tag	UNP Q9HIW9
C	330	HIS	-	expression tag	UNP Q9HIW9
C	331	HIS	-	expression tag	UNP Q9HIW9
C	332	HIS	-	expression tag	UNP Q9HIW9
C	333	HIS	-	expression tag	UNP Q9HIW9
D	325	ALA	-	expression tag	UNP Q9HIW9
D	326	LEU	-	expression tag	UNP Q9HIW9
D	327	GLU	-	expression tag	UNP Q9HIW9
D	328	HIS	-	expression tag	UNP Q9HIW9
D	329	HIS	-	expression tag	UNP Q9HIW9
D	330	HIS	-	expression tag	UNP Q9HIW9
D	331	HIS	-	expression tag	UNP Q9HIW9
D	332	HIS	-	expression tag	UNP Q9HIW9
D	333	HIS	-	expression tag	UNP Q9HIW9
E	325	ALA	-	expression tag	UNP Q9HIW9
E	326	LEU	-	expression tag	UNP Q9HIW9
E	327	GLU	-	expression tag	UNP Q9HIW9
E	328	HIS	-	expression tag	UNP Q9HIW9
E	329	HIS	-	expression tag	UNP Q9HIW9
E	330	HIS	-	expression tag	UNP Q9HIW9
E	331	HIS	-	expression tag	UNP Q9HIW9
E	332	HIS	-	expression tag	UNP Q9HIW9
E	333	HIS	-	expression tag	UNP Q9HIW9
F	325	ALA	-	expression tag	UNP Q9HIW9
F	326	LEU	-	expression tag	UNP Q9HIW9
F	327	GLU	-	expression tag	UNP Q9HIW9
F	328	HIS	-	expression tag	UNP Q9HIW9
F	329	HIS	-	expression tag	UNP Q9HIW9
F	330	HIS	-	expression tag	UNP Q9HIW9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	331	HIS	-	expression tag	UNP Q9HIW9
F	332	HIS	-	expression tag	UNP Q9HIW9
F	333	HIS	-	expression tag	UNP Q9HIW9
G	325	ALA	-	expression tag	UNP Q9HIW9
G	326	LEU	-	expression tag	UNP Q9HIW9
G	327	GLU	-	expression tag	UNP Q9HIW9
G	328	HIS	-	expression tag	UNP Q9HIW9
G	329	HIS	-	expression tag	UNP Q9HIW9
G	330	HIS	-	expression tag	UNP Q9HIW9
G	331	HIS	-	expression tag	UNP Q9HIW9
G	332	HIS	-	expression tag	UNP Q9HIW9
G	333	HIS	-	expression tag	UNP Q9HIW9
H	325	ALA	-	expression tag	UNP Q9HIW9
H	326	LEU	-	expression tag	UNP Q9HIW9
H	327	GLU	-	expression tag	UNP Q9HIW9
H	328	HIS	-	expression tag	UNP Q9HIW9
H	329	HIS	-	expression tag	UNP Q9HIW9
H	330	HIS	-	expression tag	UNP Q9HIW9
H	331	HIS	-	expression tag	UNP Q9HIW9
H	332	HIS	-	expression tag	UNP Q9HIW9
H	333	HIS	-	expression tag	UNP Q9HIW9
I	325	ALA	-	expression tag	UNP Q9HIW9
I	326	LEU	-	expression tag	UNP Q9HIW9
I	327	GLU	-	expression tag	UNP Q9HIW9
I	328	HIS	-	expression tag	UNP Q9HIW9
I	329	HIS	-	expression tag	UNP Q9HIW9
I	330	HIS	-	expression tag	UNP Q9HIW9
I	331	HIS	-	expression tag	UNP Q9HIW9
I	332	HIS	-	expression tag	UNP Q9HIW9
I	333	HIS	-	expression tag	UNP Q9HIW9
J	325	ALA	-	expression tag	UNP Q9HIW9
J	326	LEU	-	expression tag	UNP Q9HIW9
J	327	GLU	-	expression tag	UNP Q9HIW9
J	328	HIS	-	expression tag	UNP Q9HIW9
J	329	HIS	-	expression tag	UNP Q9HIW9
J	330	HIS	-	expression tag	UNP Q9HIW9
J	331	HIS	-	expression tag	UNP Q9HIW9
J	332	HIS	-	expression tag	UNP Q9HIW9
J	333	HIS	-	expression tag	UNP Q9HIW9

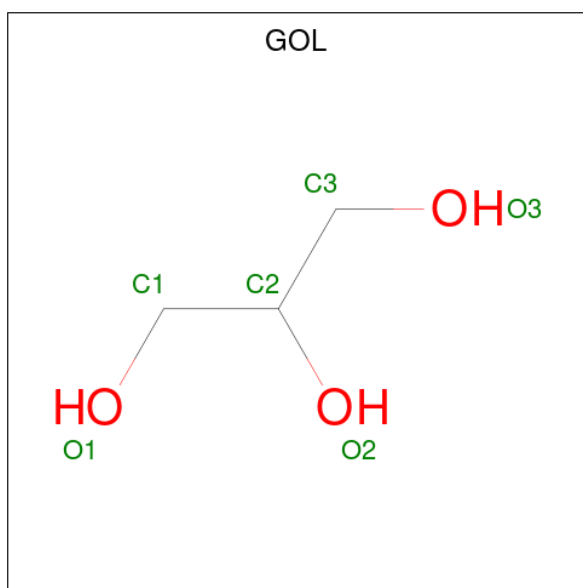
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0
3	G	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	I	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		
4	I	1	Total	C	H	O	0	0
			14	3	8	3		
4	J	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	77	Total	O	0	0
			77	77		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	74	Total 74	O 74	0	0
5	C	69	Total 69	O 69	0	0
5	D	128	Total 128	O 128	0	0
5	E	70	Total 70	O 70	0	0
5	F	79	Total 79	O 79	0	0
5	G	89	Total 89	O 89	0	0
5	H	44	Total 44	O 44	0	0
5	I	41	Total 41	O 41	0	0
5	J	82	Total 82	O 82	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: Ta1207



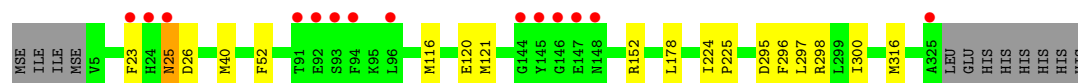
- Molecule 1: Ta1207



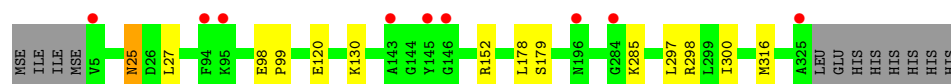
- Molecule 1: Ta1207



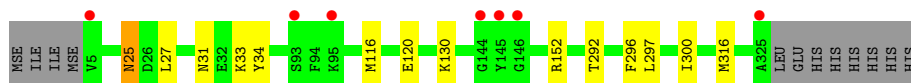
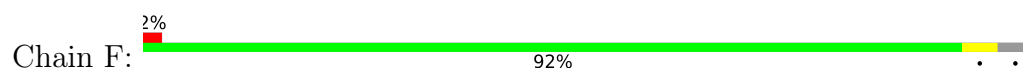
- Molecule 1: Ta1207



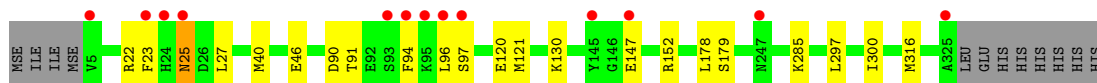
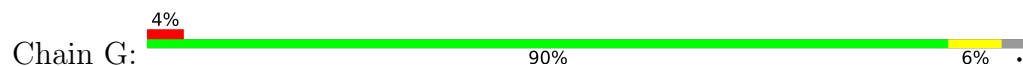
- Molecule 1: Ta1207



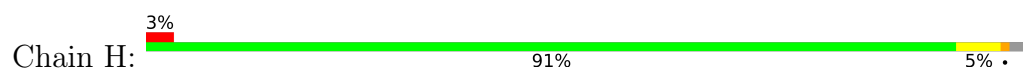
- Molecule 1: Ta1207



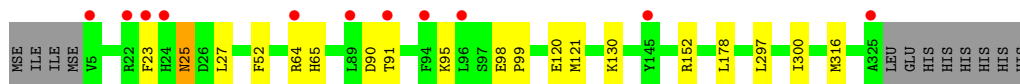
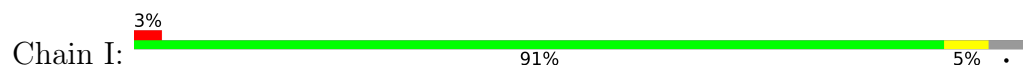
• Molecule 1: Ta1207



• Molecule 1: Ta1207



• Molecule 1: Ta1207



• Molecule 1: Ta1207



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	228.64Å 112.82Å 221.33Å 90.00° 118.70° 90.00°	Depositor
Resolution (Å)	29.66 – 2.40 29.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.66-2.40) 98.9 (29.66-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.176 , 0.203 0.186 , 0.208	Depositor DCC
$R_{free}$ test set	9570 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	53263	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL, GOL, CA

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	0.27	0/2691	0.49	0/3625
1	B	0.26	0/2691	0.46	0/3625
1	C	0.26	0/2691	0.48	0/3625
1	D	0.27	0/2691	0.50	0/3625
1	E	0.25	0/2691	0.47	0/3625
1	F	0.25	0/2691	0.46	0/3625
1	G	0.27	0/2691	0.47	0/3625
1	H	0.29	0/2691	0.48	1/3625 (0.0%)
1	I	0.26	0/2691	0.48	0/3625
1	J	0.27	0/2691	0.48	0/3625
All	All	0.26	0/26910	0.48	1/36250 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	23	PHE	CB-CG-CD2	5.27	124.49	120.80

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2635	2600	2600	12	2
1	B	2635	2599	2600	10	2
1	C	2635	2600	2600	13	0
1	D	2635	2600	2600	11	0
1	E	2635	2600	2600	10	0
1	F	2635	2600	2600	7	0
1	G	2635	2600	2600	13	0
1	H	2635	2600	2600	13	0
1	I	2635	2601	2600	11	0
1	J	2635	2600	2600	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	6	8	8	0	0
4	B	6	8	8	0	0
4	C	6	8	8	0	0
4	D	6	8	8	0	0
4	E	6	8	8	0	0
4	F	6	8	8	0	0
4	G	6	8	8	0	0
4	H	6	8	8	0	0
4	I	6	8	8	0	0
4	J	6	8	8	0	0
5	A	77	0	0	0	0
5	B	74	0	0	0	0
5	C	69	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	128	0	0	0	0
5	E	70	0	0	1	0
5	F	79	0	0	0	0
5	G	89	0	0	0	0
5	H	44	0	0	0	0
5	I	41	0	0	0	0
5	J	82	0	0	0	0
All	All	27183	26080	26080	111	2

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 2.

All (111) 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:28:THR:HA	1:A:116:MSE:HE1	1.77	0.65
1:G:120:GLU:OE1	1:G:152:ARG:NH1	2.30	0.64
1:C:23:PHE:HB2	1:C:95:LYS:HE2	1.81	0.63
1:J:267:MSE:HE3	1:J:296:PHE:CD1	2.35	0.62
1:G:22:ARG:HB2	1:G:147:GLU:HG2	1.81	0.61
1:C:120:GLU:OE1	1:C:152:ARG:NH1	2.34	0.60
1:G:94:PHE:CZ	1:G:96:LEU:HB2	2.37	0.60
1:J:120:GLU:OE1	1:J:152:ARG:NH1	2.34	0.60
1:H:46:GLU:HG3	1:H:47:LYS:HD2	1.84	0.59
1:G:40:MSE:HE1	1:G:121:MSE:SE	2.52	0.59
1:D:120:GLU:OE1	1:D:152:ARG:NH1	2.36	0.59
1:B:22:ARG:NH2	1:B:32:GLU:OE1	2.32	0.58
1:D:25:ASN:OD1	1:D:26:ASP:N	2.36	0.58
1:I:90:ASP:OD1	1:I:91:THR:N	2.35	0.58
1:A:25:ASN:OD1	1:A:27:LEU:N	2.36	0.58
1:B:120:GLU:OE1	1:B:152:ARG:NH1	2.36	0.58
1:H:120:GLU:OE1	1:H:152:ARG:NH1	2.38	0.57
1:A:120:GLU:OE1	1:A:152:ARG:NH1	2.39	0.56
1:I:120:GLU:OE1	1:I:152:ARG:NH1	2.39	0.56
1:A:116:MSE:CE	1:A:119:GLY:HA2	2.37	0.55
1:J:40:MSE:SE	1:J:121:MSE:HG2	2.57	0.55
1:F:25:ASN:OD1	1:F:27:LEU:N	2.40	0.54
1:J:267:MSE:HE2	1:J:274:TYR:N	2.23	0.54
1:J:292:THR:HG21	1:J:296:PHE:CD2	2.42	0.54
1:D:295:ASP:OD1	1:D:296:PHE:N	2.40	0.54
1:F:120:GLU:OE1	1:F:152:ARG:NH1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:ASN:OD1	1:H:27:LEU:N	2.38	0.53
1:H:109:ILE:HG23	1:H:125:VAL:CG2	2.38	0.53
1:J:267:MSE:HE2	1:J:273:TYR:HA	1.90	0.52
1:E:179:SER:HB2	1:E:285:LYS:CE	2.39	0.52
1:C:34:TYR:CE1	1:C:65:HIS:CD2	2.98	0.52
1:H:23:PHE:CE2	1:H:25:ASN:HB2	2.45	0.52
1:J:267:MSE:HE1	1:J:274:TYR:HD2	1.74	0.52
1:A:100:PHE:CZ	1:A:121:MSE:HE1	2.45	0.52
1:I:64:ARG:HE	1:I:65:HIS:CE1	2.28	0.52
1:B:292:THR:HG21	1:B:296:PHE:CD2	2.44	0.51
1:J:25:ASN:OD1	1:J:27:LEU:N	2.43	0.51
1:G:25:ASN:OD1	1:G:27:LEU:N	2.41	0.51
1:B:192:GLU:HB2	1:B:229:ILE:HD12	1.92	0.51
1:I:25:ASN:OD1	1:I:27:LEU:N	2.38	0.51
1:D:23:PHE:CZ	1:D:116:MSE:HE1	2.46	0.51
1:E:25:ASN:OD1	1:E:27:LEU:N	2.41	0.50
1:E:120:GLU:OE1	1:E:152:ARG:NH1	2.43	0.50
1:F:292:THR:HG21	1:F:296:PHE:CD2	2.47	0.50
1:G:90:ASP:OD1	1:G:91:THR:N	2.39	0.49
1:A:292:THR:HG21	1:A:296:PHE:CD2	2.46	0.49
1:J:267:MSE:HE3	1:J:296:PHE:CE1	2.47	0.49
1:E:285:LYS:NZ	5:E:502:HOH:O	2.46	0.48
1:B:25:ASN:OD1	1:B:27:LEU:N	2.44	0.48
1:C:33:LYS:HE3	1:C:34:TYR:CZ	2.49	0.48
1:D:178:LEU:HD13	1:D:316:MSE:HE2	1.96	0.47
1:H:23:PHE:CE2	1:H:25:ASN:CB	2.98	0.47
1:H:98:GLU:HG3	1:H:99:PRO:HD3	1.96	0.47
1:A:25:ASN:OD1	1:A:25:ASN:C	2.53	0.47
1:B:98:GLU:HG3	1:B:99:PRO:HD3	1.97	0.47
1:I:98:GLU:HG3	1:I:99:PRO:HD3	1.97	0.46
1:C:25:ASN:C	1:C:25:ASN:OD1	2.54	0.46
1:G:179:SER:HB2	1:G:285:LYS:CE	2.46	0.46
1:I:25:ASN:OD1	1:I:25:ASN:C	2.55	0.46
1:H:25:ASN:OD1	1:H:25:ASN:C	2.55	0.45
1:D:23:PHE:HE1	1:D:25:ASN:HD22	1.64	0.45
1:H:178:LEU:HD13	1:H:316:MSE:HE2	1.97	0.45
1:E:298:ARG:NH1	1:J:120:GLU:OE2	2.49	0.45
1:J:267:MSE:HE1	1:J:274:TYR:CD2	2.52	0.45
1:C:23:PHE:CB	1:C:95:LYS:HE2	2.46	0.45
1:G:178:LEU:HD13	1:G:316:MSE:HE2	1.99	0.45
1:H:109:ILE:HG23	1:H:125:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:MSE:SE	1:A:121:MSE:HG3	2.68	0.44
1:B:297:LEU:HA	1:B:300:ILE:HD12	1.99	0.44
1:C:120:GLU:OE2	1:D:298:ARG:NH1	2.51	0.44
1:J:96:LEU:CD2	1:J:147:GLU:OE1	2.66	0.44
1:B:25:ASN:OD1	1:B:25:ASN:C	2.56	0.44
1:D:40:MSE:HE1	1:D:121:MSE:HG3	1.99	0.44
1:G:25:ASN:OD1	1:G:25:ASN:C	2.56	0.44
1:F:25:ASN:OD1	1:F:25:ASN:C	2.56	0.43
1:D:52:PHE:CZ	1:D:121:MSE:HE1	2.52	0.43
1:E:25:ASN:OD1	1:E:25:ASN:C	2.56	0.43
1:D:224:ILE:HB	1:D:225:PRO:HD3	2.01	0.43
1:A:297:LEU:HA	1:A:300:ILE:HD12	1.99	0.43
1:H:23:PHE:CE1	1:H:95:LYS:HG2	2.53	0.43
1:H:297:LEU:HA	1:H:300:ILE:HD12	2.00	0.42
1:G:23:PHE:CG	1:G:94:PHE:CE1	3.07	0.42
1:I:52:PHE:CZ	1:I:121:MSE:HE1	2.54	0.42
1:I:297:LEU:HA	1:I:300:ILE:HD12	2.01	0.42
1:F:297:LEU:HA	1:F:300:ILE:HD12	2.02	0.42
1:G:179:SER:HB2	1:G:285:LYS:HE3	2.02	0.42
1:I:98:GLU:CG	1:I:99:PRO:HD3	2.50	0.41
1:I:178:LEU:HD13	1:I:316:MSE:HE2	2.01	0.41
1:A:178:LEU:HD13	1:A:316:MSE:HE2	2.02	0.41
1:B:120:GLU:OE2	1:C:298:ARG:NH1	2.53	0.41
1:E:178:LEU:HD13	1:E:316:MSE:HE2	2.02	0.41
1:E:179:SER:HB2	1:E:285:LYS:HE3	2.02	0.41
1:E:98:GLU:N	1:E:99:PRO:HD2	2.35	0.41
1:J:297:LEU:HA	1:J:300:ILE:HD12	2.02	0.41
1:C:153:TYR:CE1	1:C:158:LYS:HE3	2.55	0.41
1:C:297:LEU:HA	1:C:300:ILE:HD12	2.02	0.41
1:E:297:LEU:HA	1:E:300:ILE:HD12	2.01	0.41
1:F:31:ASN:CB	1:F:116:MSE:HE3	2.51	0.41
1:H:224:ILE:HB	1:H:225:PRO:HD3	2.02	0.41
1:F:33:LYS:HE3	1:F:34:TYR:CZ	2.56	0.41
1:G:297:LEU:HA	1:G:300:ILE:HD12	2.03	0.41
1:J:98:GLU:N	1:J:99:PRO:HD2	2.36	0.41
1:B:274:TYR:CB	1:B:292:THR:HG22	2.52	0.41
1:C:34:TYR:CE1	1:C:65:HIS:CG	3.08	0.41
1:G:91:THR:HG23	1:G:97:SER:HB3	2.02	0.41
1:C:98:GLU:N	1:C:99:PRO:HD2	2.35	0.40
1:C:98:GLU:H	1:C:99:PRO:HD2	1.86	0.40
1:D:297:LEU:HA	1:D:300:ILE:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HB3	1:A:222:HIS:CE1	2.56	0.40
1:I:23:PHE:CE1	1:I:95:LYS:HB3	2.56	0.40
1:A:98:GLU:HG3	1:A:98:GLU:O	2.22	0.40

All (2) 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)
1:A:67:GLU:OE2	1:B:95:LYS:HZ2[4_546]	1.54	0.06
1:A:67:GLU:OE2	1:B:95:LYS:NZ[4_546]	2.18	0.02

## 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	319/333 (96%)	310 (97%)	9 (3%)	0	100	100
1	B	319/333 (96%)	311 (98%)	8 (2%)	0	100	100
1	C	319/333 (96%)	312 (98%)	7 (2%)	0	100	100
1	D	319/333 (96%)	310 (97%)	9 (3%)	0	100	100
1	E	319/333 (96%)	310 (97%)	9 (3%)	0	100	100
1	F	319/333 (96%)	311 (98%)	8 (2%)	0	100	100
1	G	319/333 (96%)	310 (97%)	9 (3%)	0	100	100
1	H	319/333 (96%)	309 (97%)	10 (3%)	0	100	100
1	I	319/333 (96%)	311 (98%)	8 (2%)	0	100	100
1	J	319/333 (96%)	311 (98%)	7 (2%)	1 (0%)	37	51
All	All	3190/3330 (96%)	3105 (97%)	84 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	25	ASN

### 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	290/291 (100%)	288 (99%)	2 (1%)	81	91
1	B	290/291 (100%)	287 (99%)	3 (1%)	73	86
1	C	290/291 (100%)	288 (99%)	2 (1%)	81	91
1	D	290/291 (100%)	289 (100%)	1 (0%)	91	96
1	E	290/291 (100%)	288 (99%)	2 (1%)	81	91
1	F	290/291 (100%)	287 (99%)	3 (1%)	73	86
1	G	290/291 (100%)	287 (99%)	3 (1%)	73	86
1	H	290/291 (100%)	288 (99%)	2 (1%)	81	91
1	I	290/291 (100%)	288 (99%)	2 (1%)	81	91
1	J	290/291 (100%)	288 (99%)	2 (1%)	81	91
All	All	2900/2910 (100%)	2878 (99%)	22 (1%)	79	90

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	130	LYS
1	B	25	ASN
1	B	51	SER
1	B	130	LYS
1	C	25	ASN
1	C	130	LYS
1	D	25	ASN
1	E	25	ASN
1	E	130	LYS
1	F	25	ASN
1	F	130	LYS
1	F	316	MSE

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Mol	Chain	Res	Type
1	G	25	ASN
1	G	46	GLU
1	G	130	LYS
1	H	25	ASN
1	H	130	LYS
1	I	25	ASN
1	I	130	LYS
1	J	25	ASN
1	J	130	LYS

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	60	GLN
1	A	65	HIS
1	B	222	HIS
1	D	65	HIS
1	I	65	HIS
1	J	65	HIS

### 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](#)

Of 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 for Mogul analysis.

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	$\# Z  > 2$
4	GOL	F	403	-	5,5,5	0.36	0	5,5,5	0.22	0
4	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.28	0
4	GOL	C	403	-	5,5,5	0.40	0	5,5,5	0.17	0
4	GOL	A	403	-	5,5,5	0.38	0	5,5,5	0.32	0
4	GOL	I	403	-	5,5,5	0.40	0	5,5,5	0.22	0
4	GOL	J	403	-	5,5,5	0.37	0	5,5,5	0.36	0
4	GOL	G	403	-	5,5,5	0.38	0	5,5,5	0.16	0
4	GOL	H	403	-	5,5,5	0.39	0	5,5,5	0.20	0
4	GOL	E	403	-	5,5,5	0.37	0	5,5,5	0.24	0
4	GOL	D	403	-	5,5,5	0.36	0	5,5,5	0.26	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
4	GOL	F	403	-	-	2/4/4/4	-
4	GOL	B	403	-	-	0/4/4/4	-
4	GOL	C	403	-	-	4/4/4/4	-
4	GOL	A	403	-	-	2/4/4/4	-
4	GOL	I	403	-	-	1/4/4/4	-
4	GOL	J	403	-	-	0/4/4/4	-
4	GOL	G	403	-	-	4/4/4/4	-
4	GOL	H	403	-	-	2/4/4/4	-
4	GOL	E	403	-	-	0/4/4/4	-
4	GOL	D	403	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	403	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	403	GOL	C1-C2-C3-O3
4	F	403	GOL	O1-C1-C2-C3
4	G	403	GOL	O1-C1-C2-C3
4	G	403	GOL	C1-C2-C3-O3
4	C	403	GOL	O2-C2-C3-O3
4	A	403	GOL	O1-C1-C2-C3
4	H	403	GOL	C1-C2-C3-O3
4	C	403	GOL	O1-C1-C2-O2
4	F	403	GOL	O1-C1-C2-O2
4	G	403	GOL	O1-C1-C2-O2
4	H	403	GOL	O2-C2-C3-O3
4	A	403	GOL	O1-C1-C2-O2
4	G	403	GOL	O2-C2-C3-O3
4	I	403	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	312/333 (93%)	-0.43	2 (0%) 85 83	38, 55, 86, 130	0
1	B	312/333 (93%)	-0.29	8 (2%) 57 54	38, 60, 103, 135	0
1	C	312/333 (93%)	-0.25	8 (2%) 57 54	35, 59, 102, 138	0
1	D	312/333 (93%)	-0.37	14 (4%) 39 36	30, 48, 107, 159	0
1	E	312/333 (93%)	-0.24	9 (2%) 54 50	40, 60, 91, 137	0
1	F	312/333 (93%)	-0.31	7 (2%) 62 59	37, 56, 99, 137	0
1	G	312/333 (93%)	-0.30	13 (4%) 41 38	36, 53, 102, 156	0
1	H	312/333 (93%)	-0.11	9 (2%) 54 50	43, 64, 108, 145	0
1	I	312/333 (93%)	-0.10	11 (3%) 47 44	39, 64, 110, 148	0
1	J	312/333 (93%)	-0.34	9 (2%) 54 50	37, 54, 93, 157	0
All	All	3120/3330 (93%)	-0.28	90 (2%) 54 50	30, 58, 101, 159	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	94	PHE	7.0
1	H	23	PHE	6.1
1	I	23	PHE	5.8
1	J	5	VAL	5.0
1	J	94	PHE	4.8
1	B	5	VAL	4.7
1	C	325	ALA	4.6
1	G	325	ALA	4.5
1	G	23	PHE	4.5
1	J	96	LEU	4.4
1	D	23	PHE	4.2
1	G	96	LEU	4.2
1	J	92	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	147	GLU	4.1
1	J	93	SER	4.1
1	A	325	ALA	4.0
1	B	325	ALA	4.0
1	D	94	PHE	4.0
1	I	325	ALA	3.9
1	D	146	GLY	3.9
1	J	97	SER	3.9
1	F	325	ALA	3.9
1	D	24	HIS	3.8
1	C	95	LYS	3.6
1	D	325	ALA	3.6
1	D	96	LEU	3.6
1	H	93	SER	3.6
1	F	5	VAL	3.6
1	I	89	LEU	3.5
1	B	24	HIS	3.4
1	H	94	PHE	3.4
1	F	93	SER	3.3
1	I	5	VAL	3.3
1	E	95	LYS	3.3
1	G	247	ASN	3.1
1	H	325	ALA	3.1
1	D	93	SER	3.1
1	C	24	HIS	3.1
1	H	22	ARG	3.1
1	E	146	GLY	3.1
1	E	5	VAL	3.0
1	D	148	ASN	3.0
1	I	24	HIS	3.0
1	F	145	TYR	3.0
1	C	93	SER	3.0
1	H	95	LYS	3.0
1	J	325	ALA	3.0
1	B	95	LYS	2.9
1	E	145	TYR	2.9
1	I	94	PHE	2.9
1	D	145	TYR	2.9
1	I	22	ARG	2.8
1	B	23	PHE	2.8
1	G	97	SER	2.8
1	C	236	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	92	GLU	2.7
1	G	93	SER	2.7
1	B	145	TYR	2.6
1	C	5	VAL	2.6
1	G	5	VAL	2.6
1	B	229	ILE	2.6
1	F	146	GLY	2.6
1	E	325	ALA	2.5
1	G	145	TYR	2.5
1	I	96	LEU	2.5
1	H	24	HIS	2.5
1	G	147	GLU	2.5
1	I	64	ARG	2.5
1	J	91	THR	2.4
1	E	284	GLY	2.3
1	H	5	VAL	2.3
1	F	144	GLY	2.3
1	I	91	THR	2.3
1	B	93	SER	2.3
1	D	144	GLY	2.3
1	C	145	TYR	2.2
1	D	91	THR	2.2
1	D	92	GLU	2.2
1	F	95	LYS	2.2
1	G	24	HIS	2.2
1	D	25	ASN	2.2
1	A	5	VAL	2.2
1	E	143	ALA	2.2
1	G	95	LYS	2.1
1	I	145	TYR	2.1
1	J	95	LYS	2.1
1	E	94	PHE	2.1
1	E	196	ASN	2.0
1	G	25	ASN	2.0
1	C	22	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	GOL	C	403	6/6	0.80	0.28	79,95,102,103	0
4	GOL	B	403	6/6	0.84	0.24	74,89,95,98	0
2	CA	I	401	1/1	0.86	0.16	75,75,75,75	0
4	GOL	G	403	6/6	0.87	0.29	94,112,119,121	0
4	GOL	I	403	6/6	0.87	0.21	78,94,96,99	0
4	GOL	F	403	6/6	0.88	0.25	82,98,103,104	0
2	CA	A	401	1/1	0.89	0.13	59,59,59,59	0
4	GOL	H	403	6/6	0.90	0.17	80,96,98,98	0
4	GOL	D	403	6/6	0.90	0.16	53,69,77,83	0
2	CA	E	401	1/1	0.91	0.15	66,66,66,66	0
4	GOL	J	403	6/6	0.91	0.24	80,97,100,100	0
4	GOL	E	403	6/6	0.92	0.22	86,103,107,109	0
4	GOL	A	403	6/6	0.92	0.20	87,104,108,109	0
2	CA	G	401	1/1	0.92	0.10	57,57,57,57	0
2	CA	H	401	1/1	0.93	0.09	63,63,63,63	0
2	CA	F	401	1/1	0.96	0.08	61,61,61,61	0
2	CA	B	401	1/1	0.97	0.04	59,59,59,59	0
3	CL	A	402	1/1	0.98	0.04	44,44,44,44	0
3	CL	I	402	1/1	0.99	0.03	51,51,51,51	0
3	CL	J	402	1/1	0.99	0.06	39,39,39,39	0
2	CA	C	401	1/1	0.99	0.03	54,54,54,54	0
2	CA	J	401	1/1	0.99	0.02	44,44,44,44	0
2	CA	D	401	1/1	0.99	0.02	43,43,43,43	0
3	CL	B	402	1/1	0.99	0.04	46,46,46,46	0
3	CL	C	402	1/1	0.99	0.04	47,47,47,47	0
3	CL	D	402	1/1	0.99	0.03	35,35,35,35	0
3	CL	E	402	1/1	0.99	0.04	44,44,44,44	0
3	CL	F	402	1/1	0.99	0.03	41,41,41,41	0
3	CL	G	402	1/1	0.99	0.06	35,35,35,35	0
3	CL	H	402	1/1	0.99	0.04	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.