



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:08 pm BST

PDB ID : 3U41  
Title : Crystal structure of Escherichia coli DmsD in space group P212121  
Authors : Stevens, C.M.; Paetzel, M.  
Deposited on : 2011-10-06  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

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

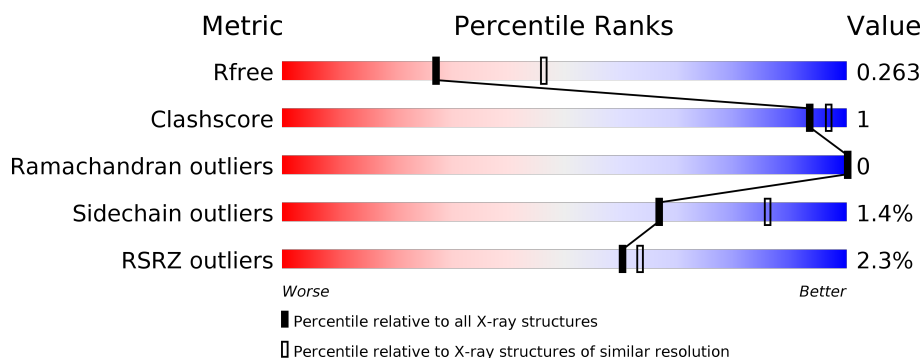
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	207	<div> <div>96%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	B	207	<div> <div>93%</div> <div>6%</div> <div></div> </div>
1	C	207	<div> <div>96%</div> <div></div> <div></div> </div>
1	D	207	<div> <div>94%</div> <div></div> <div></div> </div>
1	E	207	<div> <div>%</div> <div>96%</div> <div></div> </div>
1	F	207	<div> <div>95%</div> <div></div> <div></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	207	<div><div></div><div>3%</div><div>93%</div><div>5%</div><div></div></div>
1	H	207	<div><div></div><div>14%</div><div>88%</div><div>9%</div><div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13942 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 Twin-arginine leader-binding protein dmsD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	1	0
			1659	1082	276	295	6			
1	B	204	Total	C	N	O	S	0	1	0
			1660	1082	279	293	6			
1	C	204	Total	C	N	O	S	0	1	0
			1657	1081	273	297	6			
1	D	204	Total	C	N	O	S	0	1	0
			1658	1081	279	292	6			
1	E	204	Total	C	N	O	S	0	0	0
			1655	1078	276	295	6			
1	F	204	Total	C	N	O	S	0	0	0
			1638	1069	271	292	6			
1	G	203	Total	C	N	O	S	0	1	0
			1648	1074	275	294	5			
1	H	203	Total	C	N	O	S	0	0	0
			1627	1058	272	292	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P69853
A	-1	SER	-	EXPRESSION TAG	UNP P69853
A	0	HIS	-	EXPRESSION TAG	UNP P69853
B	-2	GLY	-	EXPRESSION TAG	UNP P69853
B	-1	SER	-	EXPRESSION TAG	UNP P69853
B	0	HIS	-	EXPRESSION TAG	UNP P69853
C	-2	GLY	-	EXPRESSION TAG	UNP P69853
C	-1	SER	-	EXPRESSION TAG	UNP P69853
C	0	HIS	-	EXPRESSION TAG	UNP P69853
D	-2	GLY	-	EXPRESSION TAG	UNP P69853
D	-1	SER	-	EXPRESSION TAG	UNP P69853
D	0	HIS	-	EXPRESSION TAG	UNP P69853
E	-2	GLY	-	EXPRESSION TAG	UNP P69853

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	EXPRESSION TAG	UNP P69853
E	0	HIS	-	EXPRESSION TAG	UNP P69853
F	-2	GLY	-	EXPRESSION TAG	UNP P69853
F	-1	SER	-	EXPRESSION TAG	UNP P69853
F	0	HIS	-	EXPRESSION TAG	UNP P69853
G	-2	GLY	-	EXPRESSION TAG	UNP P69853
G	-1	SER	-	EXPRESSION TAG	UNP P69853
G	0	HIS	-	EXPRESSION TAG	UNP P69853
H	-2	GLY	-	EXPRESSION TAG	UNP P69853
H	-1	SER	-	EXPRESSION TAG	UNP P69853
H	0	HIS	-	EXPRESSION TAG	UNP P69853

- Molecule 2 is GLYCEROL (three-letter code: 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		

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

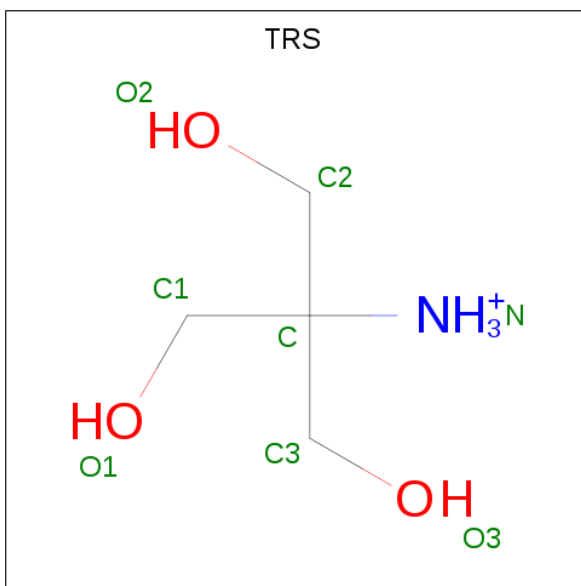
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			5	3	2		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



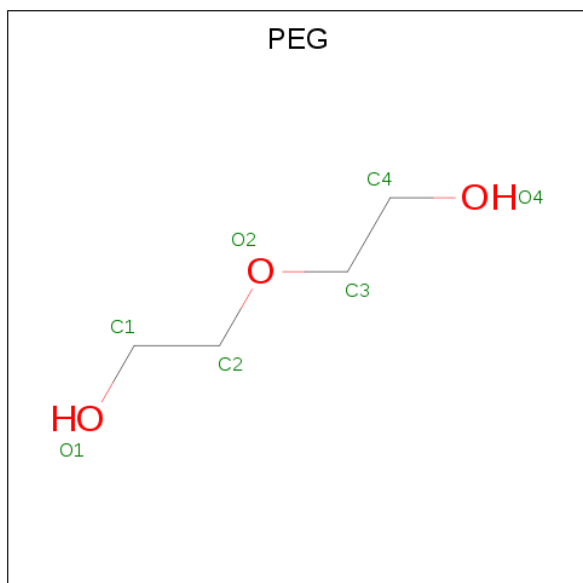
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	C	1	Total	C	N	O	0	0
			8	4	1	3		



- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cl	0	0
			1	1		
5	F	2	Total	Cl	0	0
			2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	66	Total	O	0	0
			66	66		
7	B	73	Total	O	0	0
			73	73		
7	C	87	Total	O	0	0
			87	87		
7	D	79	Total	O	0	0
			79	79		
7	E	65	Total	O	0	0
			65	65		
7	F	50	Total	O	0	0
			50	50		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	17	Total	O	0	0
			17	17		
7	H	21	Total	O	0	0
			21	21		

### 3 Residue-property plots [i](#)

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

- Molecule 1: Twin-arginine leader-binding protein dmsD

Chain A:  96% ..



- Molecule 1: Twin-arginine leader-binding protein dmsD

Chain B:  93% 6% .



- Molecule 1: Twin-arginine leader-binding protein dmsD

Chain C:  96% ..



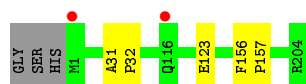
- Molecule 1: Twin-arginine leader-binding protein dmsD

Chain D:  94% ..



- Molecule 1: Twin-arginine leader-binding protein dmsD

Chain E:  96% ..

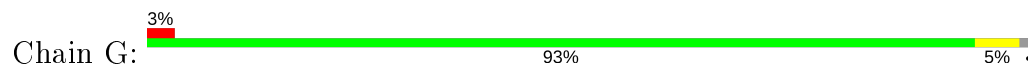


- Molecule 1: Twin-arginine leader-binding protein dmsD

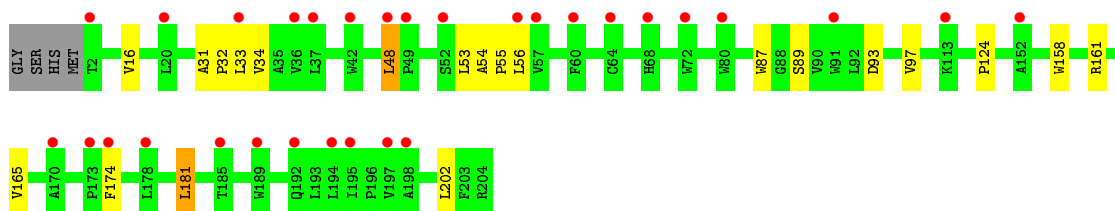
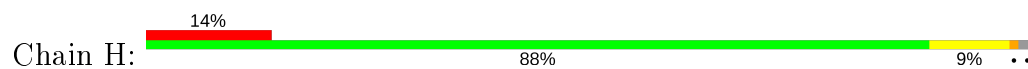
Chain F:  95% ..



- Molecule 1: Twin-arginine leader-binding protein dmsD



- Molecule 1: Twin-arginine leader-binding protein dmsD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.28Å 96.22Å 210.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 2.50 48.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.60-2.50) 94.1 (48.56-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.43 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.230 , 0.271 0.225 , 0.263	Depositor DCC
$R_{free}$ test set	3180 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 19.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.074 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13942	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.30	0/1718	0.45	0/2347
1	B	0.31	0/1719	0.48	0/2348
1	C	0.30	0/1716	0.46	0/2345
1	D	0.31	0/1717	0.49	0/2346
1	E	0.30	0/1711	0.45	0/2338
1	F	0.30	0/1694	0.45	0/2318
1	G	0.29	0/1707	0.44	0/2334
1	H	0.30	0/1682	0.45	0/2301
All	All	0.30	0/13664	0.46	0/18677

There are no bond length outliers.

There are no bond angle outliers.

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	1659	0	1602	3	0
1	B	1660	0	1607	5	0
1	C	1657	0	1595	2	0
1	D	1658	0	1602	5	0
1	E	1655	0	1596	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1638	0	1567	4	0
1	G	1648	0	1584	4	0
1	H	1627	0	1552	11	0
2	A	36	0	48	0	0
2	B	30	0	40	0	0
2	C	48	0	64	1	0
2	D	54	0	72	3	0
2	E	47	0	61	1	0
2	F	30	0	40	1	0
2	H	6	0	8	0	0
3	A	5	0	0	0	0
4	B	8	0	12	0	0
4	C	8	0	12	0	0
5	C	1	0	0	0	0
5	F	2	0	0	0	0
6	D	7	0	10	0	0
7	A	66	0	0	0	0
7	B	73	0	0	0	0
7	C	87	0	0	0	0
7	D	79	0	0	0	0
7	E	65	0	0	0	0
7	F	50	0	0	0	0
7	G	17	0	0	0	0
7	H	21	0	0	0	0
All	All	13942	0	13072	36	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 1.

All (36) 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:D:50:GLU:H	2:D:302:GOL:H11	1.65	0.61
1:D:49:PRO:HA	2:D:302:GOL:H31	1.85	0.58
1:H:34:VAL:HG23	1:H:174:PHE:CZ	2.46	0.50
1:E:123:GLU:HB3	2:E:304:GOL:H2	1.94	0.50
1:B:120:LYS:HB3	1:B:123:GLU:HG3	1.94	0.49
1:H:87:TRP:CD1	1:H:124:PRO:HG2	2.49	0.47
1:G:142:GLY:HA3	1:H:97:VAL:HG11	1.97	0.47
1:D:199:VAL:HG23	1:D:199:VAL:O	2.16	0.45
1:D:167:ILE:O	1:D:176[B]:ARG:NH1	2.50	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ALA:HB3	1:E:32:PRO:HD3	1.98	0.45
1:B:31:ALA:HB3	1:B:32:PRO:HD3	1.99	0.45
1:A:45:GLN:HG2	1:D:80:TRP:CE3	2.52	0.45
1:F:24:ALA:HB1	2:F:301:GOL:H2	1.99	0.44
1:C:54:ALA:HB3	1:C:55:PRO:HD3	2.00	0.44
1:B:150:LEU:C	1:B:150:LEU:HD23	2.39	0.43
1:H:48:LEU:CD1	1:H:53:LEU:HD11	2.49	0.42
1:A:156:PHE:N	1:A:157:PRO:CD	2.82	0.42
1:B:91:TRP:CZ3	1:B:204:ARG:HG3	2.55	0.42
1:H:54:ALA:HB3	1:H:55:PRO:HD3	2.01	0.42
1:B:14:ALA:HB3	1:B:136:ALA:HB2	2.01	0.42
1:H:161:ARG:O	1:H:165:VAL:HG12	2.19	0.42
1:A:72:TRP:CE3	1:A:76:PHE:CD2	3.08	0.41
1:H:31:ALA:HB3	1:H:32:PRO:HD3	2.02	0.41
1:H:89:SER:O	1:H:93:ASP:HB3	2.19	0.41
1:G:64:CYS:SG	1:G:65:GLU:N	2.94	0.41
1:F:148:GLU:HG3	1:F:193:LEU:HD22	2.02	0.41
1:F:156:PHE:N	1:F:157:PRO:CD	2.83	0.41
1:F:119:MET:SD	1:F:119:MET:N	2.93	0.41
1:G:151:LEU:HB3	1:G:156:PHE:CE2	2.55	0.41
1:H:53:LEU:N	1:H:53:LEU:HD12	2.36	0.41
1:C:156:PHE:N	1:C:157:PRO:CD	2.84	0.41
1:G:156:PHE:N	1:G:157:PRO:CD	2.85	0.40
1:H:16:VAL:HG12	1:H:33:LEU:HD22	2.02	0.40
1:H:56:LEU:HD21	1:H:181:LEU:HG	2.03	0.40
1:E:156:PHE:N	1:E:157:PRO:CD	2.84	0.40
2:C:301:GOL:C2	2:D:308:GOL:H2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	203/207 (98%)	199 (98%)	4 (2%)	0	100	100
1	B	203/207 (98%)	200 (98%)	3 (2%)	0	100	100
1	C	203/207 (98%)	200 (98%)	3 (2%)	0	100	100
1	D	203/207 (98%)	199 (98%)	4 (2%)	0	100	100
1	E	202/207 (98%)	199 (98%)	3 (2%)	0	100	100
1	F	202/207 (98%)	195 (96%)	7 (4%)	0	100	100
1	G	202/207 (98%)	196 (97%)	6 (3%)	0	100	100
1	H	201/207 (97%)	193 (96%)	8 (4%)	0	100	100
All	All	1619/1656 (98%)	1581 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	171/173 (99%)	170 (99%)	1 (1%)	86	95
1	B	171/173 (99%)	168 (98%)	3 (2%)	59	81
1	C	171/173 (99%)	170 (99%)	1 (1%)	86	95
1	D	170/173 (98%)	167 (98%)	3 (2%)	59	81
1	E	171/173 (99%)	171 (100%)	0	100	100
1	F	167/173 (96%)	164 (98%)	3 (2%)	59	81
1	G	170/173 (98%)	166 (98%)	4 (2%)	49	74
1	H	166/173 (96%)	162 (98%)	4 (2%)	49	74
All	All	1357/1384 (98%)	1338 (99%)	19 (1%)	67	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	LYS
1	B	63	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	119	MET
1	B	194	LEU
1	C	8	ASP
1	D	95	GLU
1	D	119	MET
1	D	169	LYS
1	F	1	MET
1	F	2	THR
1	F	119	MET
1	G	11	SER
1	G	15	ARG
1	G	184	LEU
1	G	188	GLN
1	H	48	LEU
1	H	158	TRP
1	H	181	LEU
1	H	202	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	7	GLN
1	B	63	GLN
1	B	121	GLN
1	B	144	GLN
1	G	121	GLN
1	G	188	GLN
1	H	6	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 49 ligands modelled in this entry, 3 are monoatomic - leaving 46 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	$\# Z  > 2$
2	GOL	F	305	-	5,5,5	0.41	0	5,5,5	0.13	0
2	GOL	D	301	-	5,5,5	0.28	0	5,5,5	0.10	0
2	GOL	F	301	-	5,5,5	0.39	0	5,5,5	0.33	0
2	GOL	D	308	-	5,5,5	0.46	0	5,5,5	0.40	0
2	GOL	A	302	-	5,5,5	0.38	0	5,5,5	0.27	0
2	GOL	D	304	-	5,5,5	0.41	0	5,5,5	0.25	0
2	GOL	C	306	-	5,5,5	0.37	0	5,5,5	0.06	0
2	GOL	A	306	-	5,5,5	0.32	0	5,5,5	0.16	0
4	TRS	C	309	-	7,7,7	0.43	0	9,9,9	0.22	0
2	GOL	D	303	-	5,5,5	0.45	0	5,5,5	0.35	0
2	GOL	E	304	-	5,5,5	0.37	0	5,5,5	0.49	0
2	GOL	E	303	-	5,5,5	0.33	0	5,5,5	0.40	0
2	GOL	B	302	-	5,5,5	0.28	0	5,5,5	0.19	0
2	GOL	A	304	-	5,5,5	0.33	0	5,5,5	0.21	0
2	GOL	D	306	-	5,5,5	0.36	0	5,5,5	0.16	0
2	GOL	A	301	-	5,5,5	0.33	0	5,5,5	0.19	0
2	GOL	E	306	-	5,5,5	0.35	0	5,5,5	0.23	0
3	SO4	A	307	-	4,4,4	0.33	0	6,6,6	0.09	0
2	GOL	E	302	-	5,5,5	0.31	0	5,5,5	0.49	0
2	GOL	B	304	-	5,5,5	0.53	0	5,5,5	0.41	0
2	GOL	A	303	-	5,5,5	0.33	0	5,5,5	0.11	0
2	GOL	E	308	-	5,5,5	0.51	0	5,5,5	0.29	0
2	GOL	H	301	-	5,5,5	0.32	0	5,5,5	0.16	0
2	GOL	D	309	-	5,5,5	0.40	0	5,5,5	0.28	0
2	GOL	C	304	-	5,5,5	0.35	0	5,5,5	0.10	0
2	GOL	D	305	-	5,5,5	0.35	0	5,5,5	0.18	0
4	TRS	B	306	-	7,7,7	0.40	0	9,9,9	0.60	0
2	GOL	E	305	-	3,4,5	0.29	0	1,4,5	0.21	0
2	GOL	E	301	-	5,5,5	0.39	0	5,5,5	0.36	0
6	PEG	D	310	-	6,6,6	0.56	0	5,5,5	0.22	0
2	GOL	F	304	-	5,5,5	0.35	0	5,5,5	0.23	0
2	GOL	B	303	-	5,5,5	0.37	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	D	307	-	5,5,5	0.49	0	5,5,5	0.34	0
2	GOL	C	303	-	5,5,5	0.35	0	5,5,5	0.14	0
2	GOL	E	307	-	5,5,5	0.31	0	5,5,5	0.16	0
2	GOL	C	307	-	5,5,5	0.35	0	5,5,5	0.33	0
2	GOL	F	302	-	5,5,5	0.37	0	5,5,5	0.22	0
2	GOL	D	302	-	5,5,5	0.21	0	5,5,5	0.63	0
2	GOL	B	301	-	5,5,5	0.40	0	5,5,5	0.27	0
2	GOL	C	301	-	5,5,5	0.27	0	5,5,5	0.34	0
2	GOL	B	305	-	5,5,5	0.29	0	5,5,5	0.27	0
2	GOL	A	305	-	5,5,5	0.36	0	5,5,5	0.20	0
2	GOL	C	302	-	5,5,5	0.43	0	5,5,5	0.31	0
2	GOL	C	305	-	5,5,5	0.43	0	5,5,5	0.47	0
2	GOL	C	308	-	5,5,5	0.37	0	5,5,5	0.46	0
2	GOL	F	303	-	5,5,5	0.32	0	5,5,5	0.11	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	F	305	-	-	2/4/4/4	-
2	GOL	E	308	-	-	4/4/4/4	-
2	GOL	F	301	-	-	2/4/4/4	-
2	GOL	D	308	-	-	2/4/4/4	-
2	GOL	A	302	-	-	0/4/4/4	-
2	GOL	D	304	-	-	2/4/4/4	-
2	GOL	C	306	-	-	2/4/4/4	-
2	GOL	A	306	-	-	1/4/4/4	-
4	TRS	C	309	-	-	6/9/9/9	-
2	GOL	D	303	-	-	3/4/4/4	-
2	GOL	E	304	-	-	2/4/4/4	-
2	GOL	E	303	-	-	2/4/4/4	-
2	GOL	B	302	-	-	0/4/4/4	-
2	GOL	A	304	-	-	2/4/4/4	-
2	GOL	D	306	-	-	2/4/4/4	-
2	GOL	A	301	-	-	2/4/4/4	-
2	GOL	E	306	-	-	2/4/4/4	-
2	GOL	E	302	-	-	4/4/4/4	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	304	-	-	0/4/4/4	-
2	GOL	A	303	-	-	2/4/4/4	-
2	GOL	D	301	-	-	2/4/4/4	-
2	GOL	H	301	-	-	2/4/4/4	-
2	GOL	D	309	-	-	2/4/4/4	-
2	GOL	C	304	-	-	0/4/4/4	-
2	GOL	D	305	-	-	2/4/4/4	-
4	TRS	B	306	-	-	0/9/9/9	-
2	GOL	E	305	-	-	0/2/2/4	-
2	GOL	E	301	-	-	2/4/4/4	-
6	PEG	D	310	-	-	3/4/4/4	-
2	GOL	F	304	-	-	0/4/4/4	-
2	GOL	B	303	-	-	3/4/4/4	-
2	GOL	D	307	-	-	2/4/4/4	-
2	GOL	C	303	-	-	2/4/4/4	-
2	GOL	E	307	-	-	2/4/4/4	-
2	GOL	C	307	-	-	0/4/4/4	-
2	GOL	F	302	-	-	2/4/4/4	-
2	GOL	D	302	-	-	4/4/4/4	-
2	GOL	B	301	-	-	4/4/4/4	-
2	GOL	C	301	-	-	0/4/4/4	-
2	GOL	B	305	-	-	2/4/4/4	-
2	GOL	A	305	-	-	2/4/4/4	-
2	GOL	C	302	-	-	1/4/4/4	-
2	GOL	C	305	-	-	3/4/4/4	-
2	GOL	C	308	-	-	0/4/4/4	-
2	GOL	F	303	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	GOL	O1-C1-C2-C3
2	D	308	GOL	O1-C1-C2-C3
2	D	304	GOL	C1-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	D	304	GOL	O2-C2-C3-O3
2	C	306	GOL	O1-C1-C2-C3
4	C	309	TRS	N-C-C1-O1
4	C	309	TRS	N-C-C2-O2
4	C	309	TRS	C1-C-C3-O3
4	C	309	TRS	N-C-C3-O3
2	E	303	GOL	C1-C2-C3-O3
2	D	306	GOL	O1-C1-C2-C3
2	A	301	GOL	C1-C2-C3-O3
2	E	306	GOL	C1-C2-C3-O3
2	E	306	GOL	O2-C2-C3-O3
2	E	302	GOL	O1-C1-C2-C3
2	H	301	GOL	C1-C2-C3-O3
2	D	305	GOL	C1-C2-C3-O3
2	E	301	GOL	C1-C2-C3-O3
2	B	303	GOL	O1-C1-C2-O2
2	B	303	GOL	O1-C1-C2-C3
2	D	307	GOL	C1-C2-C3-O3
2	C	303	GOL	O1-C1-C2-C3
2	D	302	GOL	O1-C1-C2-C3
2	B	301	GOL	O1-C1-C2-C3
2	B	305	GOL	C1-C2-C3-O3
2	B	305	GOL	O2-C2-C3-O3
2	A	305	GOL	O1-C1-C2-C3
2	C	305	GOL	C1-C2-C3-O3
2	F	303	GOL	O1-C1-C2-C3
2	A	301	GOL	O2-C2-C3-O3
2	E	308	GOL	O1-C1-C2-O2
2	F	302	GOL	O2-C2-C3-O3
2	A	305	GOL	O1-C1-C2-O2
6	D	310	PEG	O2-C3-C4-O4
2	F	305	GOL	O1-C1-C2-C3
2	F	301	GOL	C1-C2-C3-O3
2	A	306	GOL	C1-C2-C3-O3
2	D	303	GOL	O1-C1-C2-C3
2	A	304	GOL	C1-C2-C3-O3
2	E	302	GOL	C1-C2-C3-O3
2	A	303	GOL	O1-C1-C2-C3
2	E	308	GOL	O1-C1-C2-C3
2	E	308	GOL	C1-C2-C3-O3
2	E	307	GOL	C1-C2-C3-O3
2	F	302	GOL	C1-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	301	GOL	C1-C2-C3-O3
2	F	305	GOL	O1-C1-C2-O2
2	D	301	GOL	O1-C1-C2-O2
2	D	308	GOL	O1-C1-C2-O2
2	C	306	GOL	O1-C1-C2-O2
2	E	303	GOL	O2-C2-C3-O3
2	A	304	GOL	O2-C2-C3-O3
2	D	306	GOL	O1-C1-C2-O2
2	E	302	GOL	O2-C2-C3-O3
2	H	301	GOL	O2-C2-C3-O3
2	D	305	GOL	O2-C2-C3-O3
2	E	301	GOL	O2-C2-C3-O3
2	D	307	GOL	O2-C2-C3-O3
2	C	303	GOL	O1-C1-C2-O2
2	C	305	GOL	O2-C2-C3-O3
2	F	303	GOL	O1-C1-C2-O2
6	D	310	PEG	O1-C1-C2-O2
2	F	301	GOL	O2-C2-C3-O3
2	E	308	GOL	O2-C2-C3-O3
2	D	302	GOL	O1-C1-C2-O2
2	B	301	GOL	O1-C1-C2-O2
2	E	302	GOL	O1-C1-C2-O2
2	D	302	GOL	O2-C2-C3-O3
2	E	304	GOL	O1-C1-C2-O2
2	D	309	GOL	O1-C1-C2-O2
4	C	309	TRS	C2-C-C3-O3
2	E	304	GOL	O1-C1-C2-C3
2	B	303	GOL	C1-C2-C3-O3
2	C	302	GOL	C1-C2-C3-O3
2	D	303	GOL	O1-C1-C2-O2
2	E	307	GOL	O2-C2-C3-O3
2	B	301	GOL	O2-C2-C3-O3
2	D	309	GOL	O1-C1-C2-C3
2	D	302	GOL	C1-C2-C3-O3
2	A	303	GOL	O1-C1-C2-O2
4	C	309	TRS	C3-C-C1-O1
2	D	303	GOL	C1-C2-C3-O3
2	C	305	GOL	O1-C1-C2-C3
6	D	310	PEG	C1-C2-O2-C3

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	GOL	1	0
2	D	308	GOL	1	0
2	E	304	GOL	1	0
2	D	302	GOL	2	0
2	C	301	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<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	204/207 (98%)	-0.28	0 <span>100</span> <span>100</span>	31, 38, 52, 80	0
1	B	204/207 (98%)	-0.22	0 <span>100</span> <span>100</span>	30, 38, 51, 71	0
1	C	204/207 (98%)	-0.24	0 <span>100</span> <span>100</span>	33, 38, 50, 79	0
1	D	204/207 (98%)	-0.18	0 <span>100</span> <span>100</span>	30, 39, 58, 71	0
1	E	204/207 (98%)	-0.28	2 (0%) <span>82</span> <span>84</span>	30, 41, 62, 88	0
1	F	204/207 (98%)	-0.24	0 <span>100</span> <span>100</span>	33, 42, 61, 96	0
1	G	203/207 (98%)	0.23	6 (2%) <span>50</span> <span>53</span>	41, 66, 96, 123	0
1	H	203/207 (98%)	0.91	30 (14%) <span>2</span> <span>2</span>	45, 82, 128, 144	0
All	All	1630/1656 (98%)	-0.04	38 (2%) <span>60</span> <span>63</span>	30, 42, 93, 144	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	33	LEU	5.8
1	H	60	PHE	5.5
1	H	174	PHE	4.8
1	H	56	LEU	4.4
1	H	189	TRP	3.9
1	H	194	LEU	3.8
1	H	170	ALA	3.7
1	H	37	LEU	3.6
1	H	2	THR	3.5
1	H	91	TRP	3.3
1	H	195	ILE	3.3
1	H	20	LEU	3.0
1	H	49	PRO	3.0
1	H	173	PRO	2.8
1	H	80	TRP	2.8
1	H	52	SER	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	68	HIS	2.8
1	H	64	CYS	2.7
1	H	152	ALA	2.7
1	G	36	VAL	2.7
1	H	178	LEU	2.6
1	H	192	GLN	2.6
1	H	185	THR	2.5
1	G	41	GLY	2.5
1	H	198	ALA	2.5
1	G	51	ALA	2.5
1	H	57	VAL	2.4
1	E	1	MET	2.4
1	H	197	VAL	2.2
1	H	36	VAL	2.2
1	H	42	TRP	2.2
1	H	113	LYS	2.2
1	H	48	LEU	2.2
1	G	175	TYR	2.1
1	G	8	ASP	2.1
1	E	116	GLN	2.1
1	H	72	TRP	2.1
1	G	64	CYS	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	GOL	H	301	6/6	0.44	0.27	79,81,82,82	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	D	302	6/6	0.58	0.27	72,73,75,75	0
2	GOL	C	303	6/6	0.73	0.23	46,47,48,49	0
2	GOL	A	301	6/6	0.75	0.25	51,53,55,56	0
2	GOL	D	304	6/6	0.76	0.28	41,42,43,45	0
2	GOL	C	307	6/6	0.77	0.30	44,54,55,57	0
2	GOL	C	305	6/6	0.77	0.36	37,38,40,41	0
2	GOL	D	306	6/6	0.78	0.29	63,65,66,66	0
2	GOL	F	304	6/6	0.78	0.23	60,61,61,61	0
2	GOL	C	302	6/6	0.79	0.22	42,43,45,45	0
4	TRS	C	309	8/8	0.79	0.21	29,30,31,31	8
2	GOL	C	308	6/6	0.79	0.29	33,37,37,37	0
2	GOL	E	305	5/6	0.80	0.27	65,65,65,66	0
2	GOL	C	304	6/6	0.80	0.28	45,47,47,48	0
2	GOL	E	308	6/6	0.81	0.30	32,32,35,35	0
2	GOL	F	302	6/6	0.81	0.22	56,58,60,60	0
2	GOL	A	303	6/6	0.81	0.30	39,40,41,41	0
6	PEG	D	310	7/7	0.82	0.22	34,36,37,37	0
2	GOL	D	309	6/6	0.82	0.30	41,43,43,43	0
2	GOL	D	307	6/6	0.82	0.26	32,34,34,34	0
2	GOL	D	308	6/6	0.82	0.21	28,28,29,29	0
2	GOL	D	305	6/6	0.82	0.18	47,52,53,53	0
2	GOL	B	302	6/6	0.83	0.24	59,59,60,61	0
2	GOL	D	303	6/6	0.83	0.18	39,41,42,43	0
2	GOL	E	303	6/6	0.83	0.41	49,51,52,54	0
2	GOL	B	304	6/6	0.83	0.44	46,50,51,52	0
2	GOL	C	301	6/6	0.84	0.26	25,25,26,28	0
2	GOL	E	301	6/6	0.84	0.12	46,47,47,48	0
2	GOL	A	304	6/6	0.85	0.33	39,42,44,45	0
2	GOL	F	301	6/6	0.85	0.44	39,41,45,48	0
2	GOL	A	305	6/6	0.86	0.17	66,68,69,69	0
2	GOL	E	304	6/6	0.86	0.47	20,20,21,22	0
4	TRS	B	306	8/8	0.86	0.14	29,32,32,32	0
2	GOL	A	302	6/6	0.86	0.39	39,42,45,45	0
2	GOL	A	306	6/6	0.88	0.34	46,50,51,54	0
2	GOL	F	305	6/6	0.89	0.14	39,41,41,42	0
2	GOL	F	303	6/6	0.89	0.22	44,44,45,46	0
2	GOL	D	301	6/6	0.90	0.24	34,36,37,37	0
2	GOL	E	306	6/6	0.90	0.26	60,61,61,62	0
2	GOL	E	302	6/6	0.90	0.34	41,42,43,44	0
2	GOL	C	306	6/6	0.90	0.15	59,61,61,63	0
2	GOL	B	305	6/6	0.90	0.24	34,35,37,39	0
2	GOL	B	301	6/6	0.91	0.17	39,40,40,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	C	310	1/1	0.92	0.09	48,48,48,48	0
2	GOL	B	303	6/6	0.93	0.26	36,38,39,41	0
3	SO4	A	307	5/5	0.94	0.14	62,65,67,67	0
2	GOL	E	307	6/6	0.95	0.13	52,57,59,60	0
5	CL	F	307	1/1	0.95	0.05	61,61,61,61	0
5	CL	F	306	1/1	0.96	0.06	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.