



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 04:14 PM BST

PDB ID : 4DHG  
Title : Crystal structure of enolase TBIS\_1083(TARGET EFI-502310) from *Thermobispora bispora* dsm 43833, an open loop conformation  
Authors : Patskovsky, Y.; Toro, R.; Bhosle, R.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2012-01-27  
Resolution : 1.90 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 : 2.14.4.dev1  
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) : 2.14.4.dev1

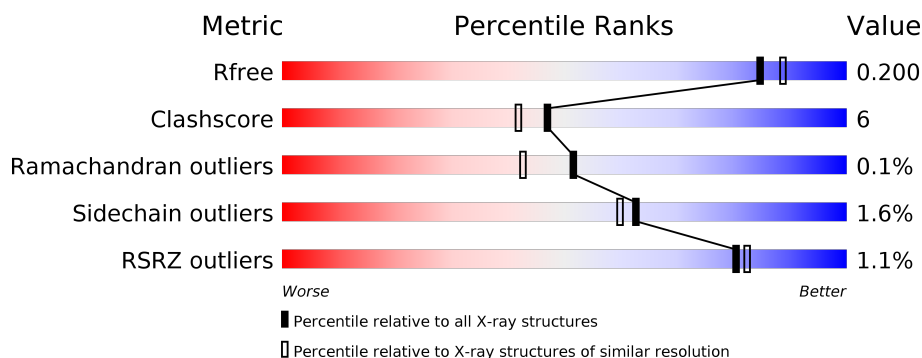
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	441	<div> <div>85%</div> <div>11% . .</div> </div>
1	B	441	<div> <div>2%</div> <div>84%</div> <div>10% . 5%</div> </div>
1	C	441	<div> <div>%</div> <div>86%</div> <div>10% .</div> </div>
1	D	441	<div> <div>85%</div> <div>10% . .</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	B	505	-	-	X	-
3	IOD	D	503	-	-	X	-
3	IOD	D	508	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14103 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 Mandelate racemase/muconate lactonizing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	3	0
			3290	2084	592	600	14			
1	B	420	Total	C	N	O	S	0	11	0
			3263	2066	588	595	14			
1	C	424	Total	C	N	O	S	0	1	0
			3242	2058	578	591	15			
1	D	427	Total	C	N	O	S	0	9	0
			3323	2108	598	603	14			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP D6Y7Y6
A	-20	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
A	-19	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
A	-18	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
A	-17	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
A	-16	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
A	-15	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
A	-14	SER	-	EXPRESSION TAG	UNP D6Y7Y6
A	-13	SER	-	EXPRESSION TAG	UNP D6Y7Y6
A	-12	GLY	-	EXPRESSION TAG	UNP D6Y7Y6
A	-11	VAL	-	EXPRESSION TAG	UNP D6Y7Y6
A	-10	ASP	-	EXPRESSION TAG	UNP D6Y7Y6
A	-9	LEU	-	EXPRESSION TAG	UNP D6Y7Y6
A	-8	GLY	-	EXPRESSION TAG	UNP D6Y7Y6
A	-7	THR	-	EXPRESSION TAG	UNP D6Y7Y6
A	-6	GLU	-	EXPRESSION TAG	UNP D6Y7Y6
A	-5	ASN	-	EXPRESSION TAG	UNP D6Y7Y6
A	-4	LEU	-	EXPRESSION TAG	UNP D6Y7Y6
A	-3	TYR	-	EXPRESSION TAG	UNP D6Y7Y6
A	-2	PHE	-	EXPRESSION TAG	UNP D6Y7Y6
A	-1	GLN	-	EXPRESSION TAG	UNP D6Y7Y6

*Continued on next page...*

*Continued from previous page...*

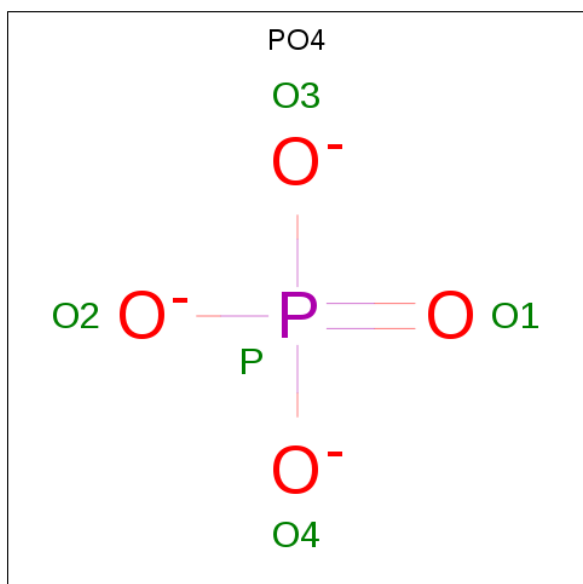
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP D6Y7Y6
B	-21	MET	-	EXPRESSION TAG	UNP D6Y7Y6
B	-20	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
B	-19	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
B	-18	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
B	-17	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
B	-16	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
B	-15	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
B	-14	SER	-	EXPRESSION TAG	UNP D6Y7Y6
B	-13	SER	-	EXPRESSION TAG	UNP D6Y7Y6
B	-12	GLY	-	EXPRESSION TAG	UNP D6Y7Y6
B	-11	VAL	-	EXPRESSION TAG	UNP D6Y7Y6
B	-10	ASP	-	EXPRESSION TAG	UNP D6Y7Y6
B	-9	LEU	-	EXPRESSION TAG	UNP D6Y7Y6
B	-8	GLY	-	EXPRESSION TAG	UNP D6Y7Y6
B	-7	THR	-	EXPRESSION TAG	UNP D6Y7Y6
B	-6	GLU	-	EXPRESSION TAG	UNP D6Y7Y6
B	-5	ASN	-	EXPRESSION TAG	UNP D6Y7Y6
B	-4	LEU	-	EXPRESSION TAG	UNP D6Y7Y6
B	-3	TYR	-	EXPRESSION TAG	UNP D6Y7Y6
B	-2	PHE	-	EXPRESSION TAG	UNP D6Y7Y6
B	-1	GLN	-	EXPRESSION TAG	UNP D6Y7Y6
B	0	SER	-	EXPRESSION TAG	UNP D6Y7Y6
C	-21	MET	-	EXPRESSION TAG	UNP D6Y7Y6
C	-20	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
C	-19	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
C	-18	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
C	-17	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
C	-16	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
C	-15	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
C	-14	SER	-	EXPRESSION TAG	UNP D6Y7Y6
C	-13	SER	-	EXPRESSION TAG	UNP D6Y7Y6
C	-12	GLY	-	EXPRESSION TAG	UNP D6Y7Y6
C	-11	VAL	-	EXPRESSION TAG	UNP D6Y7Y6
C	-10	ASP	-	EXPRESSION TAG	UNP D6Y7Y6
C	-9	LEU	-	EXPRESSION TAG	UNP D6Y7Y6
C	-8	GLY	-	EXPRESSION TAG	UNP D6Y7Y6
C	-7	THR	-	EXPRESSION TAG	UNP D6Y7Y6
C	-6	GLU	-	EXPRESSION TAG	UNP D6Y7Y6
C	-5	ASN	-	EXPRESSION TAG	UNP D6Y7Y6
C	-4	LEU	-	EXPRESSION TAG	UNP D6Y7Y6
C	-3	TYR	-	EXPRESSION TAG	UNP D6Y7Y6

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	EXPRESSION TAG	UNP D6Y7Y6
C	-1	GLN	-	EXPRESSION TAG	UNP D6Y7Y6
C	0	SER	-	EXPRESSION TAG	UNP D6Y7Y6
D	-21	MET	-	EXPRESSION TAG	UNP D6Y7Y6
D	-20	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
D	-19	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
D	-18	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
D	-17	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
D	-16	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
D	-15	HIS	-	EXPRESSION TAG	UNP D6Y7Y6
D	-14	SER	-	EXPRESSION TAG	UNP D6Y7Y6
D	-13	SER	-	EXPRESSION TAG	UNP D6Y7Y6
D	-12	GLY	-	EXPRESSION TAG	UNP D6Y7Y6
D	-11	VAL	-	EXPRESSION TAG	UNP D6Y7Y6
D	-10	ASP	-	EXPRESSION TAG	UNP D6Y7Y6
D	-9	LEU	-	EXPRESSION TAG	UNP D6Y7Y6
D	-8	GLY	-	EXPRESSION TAG	UNP D6Y7Y6
D	-7	THR	-	EXPRESSION TAG	UNP D6Y7Y6
D	-6	GLU	-	EXPRESSION TAG	UNP D6Y7Y6
D	-5	ASN	-	EXPRESSION TAG	UNP D6Y7Y6
D	-4	LEU	-	EXPRESSION TAG	UNP D6Y7Y6
D	-3	TYR	-	EXPRESSION TAG	UNP D6Y7Y6
D	-2	PHE	-	EXPRESSION TAG	UNP D6Y7Y6
D	-1	GLN	-	EXPRESSION TAG	UNP D6Y7Y6
D	0	SER	-	EXPRESSION TAG	UNP D6Y7Y6

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

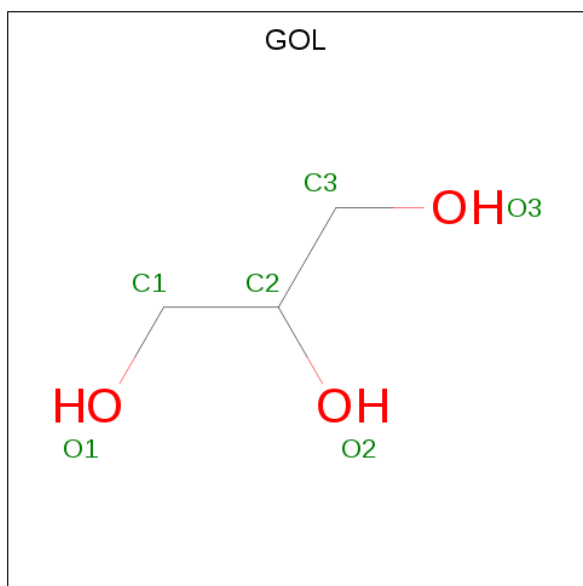


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total I 2 2	0	0
3	A	2	Total I 2 2	0	0
3	D	7	Total I 7 7	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

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

- Molecule 6 is water.

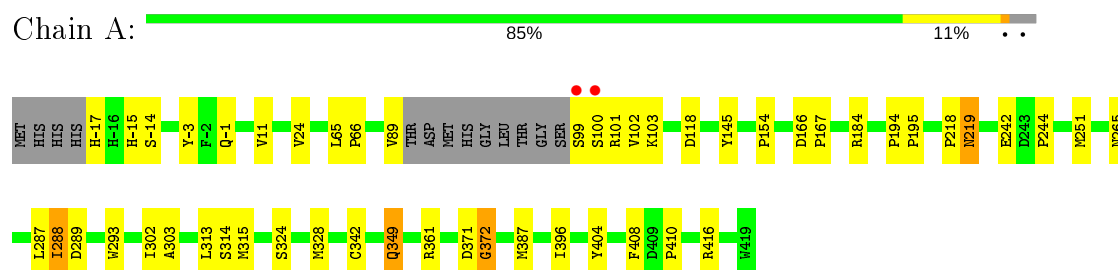
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	246	Total	O	0	0
			246	246		
6	B	219	Total	O	0	0
			219	219		
6	C	211	Total	O	0	0
			211	211		
6	D	256	Total	O	0	0
			256	256		



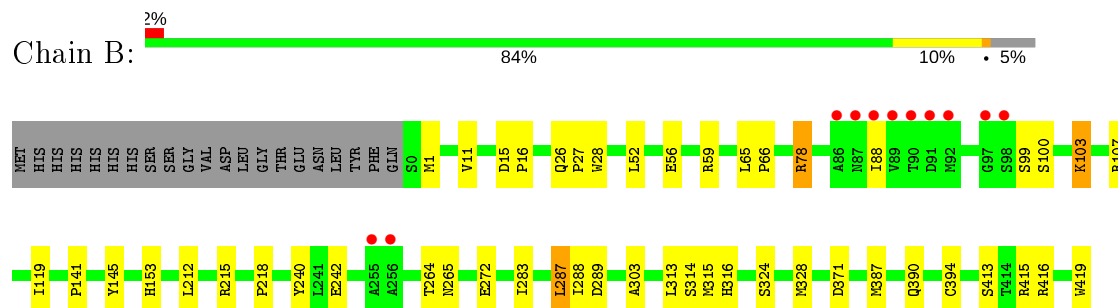
### 3 Residue-property plots [i](#)

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.

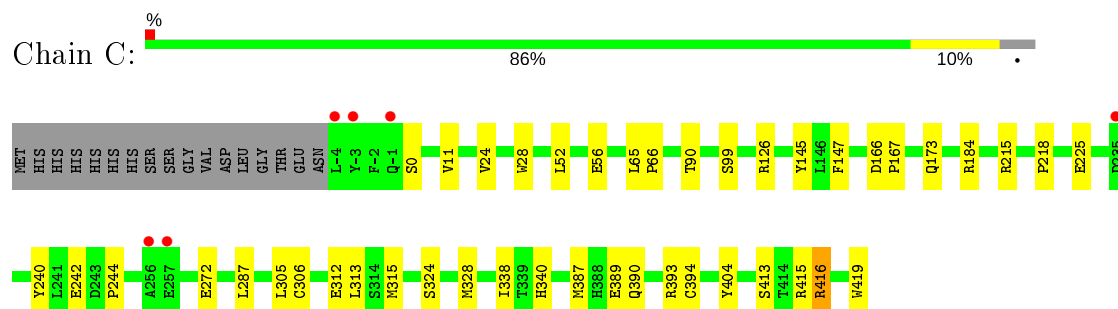
- Molecule 1: Mandelate racemase/muconate lactonizing protein



- Molecule 1: Mandelate racemase/muconate lactonizing protein

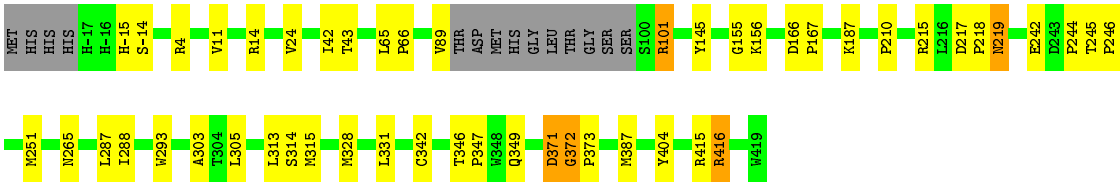


- Molecule 1: Mandelate racemase/muconate lactonizing protein



- Molecule 1: Mandelate racemase/muconate lactonizing protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.03Å 84.82Å 94.12Å 89.26° 84.07° 72.72°	Depositor
Resolution (Å)	50.00 – 1.90 40.49 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-1.90) 96.2 (40.49-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.161 , 0.200 0.163 , 0.200	Depositor DCC
$R_{free}$ test set	5483 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14103	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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, PO4, IOD, UNL

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	0.58	0/3376	0.67	1/4602 (0.0%)
1	B	0.59	2/3367 (0.1%)	0.68	2/4588 (0.0%)
1	C	0.57	2/3327 (0.1%)	0.65	2/4537 (0.0%)
1	D	0.61	1/3425 (0.0%)	0.67	0/4667
All	All	0.59	5/13495 (0.0%)	0.67	5/18394 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	TRP	CD2-CE2	5.62	1.48	1.41
1	D	293	TRP	CD2-CE2	5.43	1.47	1.41
1	C	419	TRP	CD2-CE2	5.33	1.47	1.41
1	B	419	TRP	CD2-CE2	5.16	1.47	1.41
1	C	28	TRP	CD2-CE2	5.04	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	126	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	C	126	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	371[A]	ASP	CB-CA-C	-5.11	100.19	110.40
1	B	371[B]	ASP	CB-CA-C	-5.11	100.19	110.40

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	3290	0	3245	43	0
1	B	3263	0	3251	43	0
1	C	3242	0	3211	28	0
1	D	3323	0	3295	53	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	2	0	0	1	0
3	B	2	0	0	3	0
3	D	7	0	0	6	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
5	B	4	0	0	0	0
6	A	246	0	0	4	0
6	B	219	0	0	11	0
6	C	211	0	0	1	0
6	D	256	0	0	3	0
All	All	14103	0	13026	163	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 6.

All (163) 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:C:272:GLU:HG3	6:C:673:HOH:O	1.43	1.19
1:B:78[B]:ARG:NE	3:B:505:IOD:I	2.47	1.16
1:A:315:MET:HG2	1:A:342:CYS:SG	1.97	1.05
1:D:101:ARG:HH11	1:D:101:ARG:CG	1.71	1.04
3:D:508:IOD:I	6:D:815:HOH:O	2.45	1.03
1:D:242:GLU:OE2	1:D:265:ASN:ND2	1.93	1.01
1:A:242:GLU:OE2	1:A:265:ASN:ND2	1.94	1.00
1:D:101:ARG:HH11	1:D:101:ARG:HG2	1.25	0.97

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78[B]:ARG:CD	3:B:505:IOD:I	2.88	0.92
1:B:78[A]:ARG:HG3	1:B:78[A]:ARG:HH11	1.39	0.87
1:D:101:ARG:NH1	3:D:502:IOD:I	2.77	0.86
1:B:303:ALA:HA	1:B:313:LEU:HD11	1.58	0.86
1:D:101:ARG:HH11	1:D:101:ARG:CB	1.89	0.85
1:A:315:MET:CG	1:A:342:CYS:SG	2.68	0.82
1:B:99[A]:SER:HB3	6:B:759:HOH:O	1.78	0.82
1:D:315:MET:SD	1:D:328[B]:MET:HG3	2.21	0.81
1:A:288:ILE:HD13	1:A:289:ASP:N	1.97	0.80
1:B:78[B]:ARG:HD3	3:B:505:IOD:I	2.53	0.79
1:D:101:ARG:HB3	1:D:101:ARG:NH1	1.99	0.76
1:A:324:SER:O	1:A:328:MET:HG3	1.85	0.76
1:D:218:PRO:C	1:D:219[A]:ASN:HD22	1.88	0.76
1:A:99:SER:CB	1:D:4:ARG:HH12	1.98	0.76
1:D:101:ARG:CB	1:D:101:ARG:NH1	2.49	0.76
1:A:99:SER:HB2	1:D:4:ARG:NH1	2.00	0.75
1:C:147:PHE:H	1:C:173:GLN:HE22	1.34	0.75
1:B:287:LEU:HD22	1:B:314:SER:HB3	1.68	0.75
1:D:155:GLY:O	1:D:156:LYS:HG2	1.88	0.72
1:B:315:MET:HE1	1:B:328:MET:HB3	1.72	0.71
1:B:103:LYS:HG3	6:B:683:HOH:O	1.91	0.71
1:B:99[B]:SER:HB2	6:B:759:HOH:O	1.91	0.70
1:A:99:SER:HB3	1:D:4:ARG:HH12	1.57	0.70
1:B:215:ARG:HD2	1:B:240:TYR:CZ	2.26	0.70
1:A:166:ASP:HB2	1:A:167:PRO:CD	2.22	0.69
1:D:287:LEU:HD23	1:D:314:SER:HB3	1.73	0.69
1:A:219:ASN:HB2	6:A:738:HOH:O	1.92	0.69
1:A:100:SER:OG	1:A:102:VAL:HG23	1.94	0.67
1:D:101:ARG:NH1	1:D:101:ARG:HG2	2.01	0.67
1:A:99:SER:CB	1:D:4:ARG:NH1	2.57	0.67
1:B:272:GLU:HG3	6:B:715:HOH:O	1.95	0.66
1:C:312:GLU:C	1:C:313:LEU:HD22	2.15	0.66
1:A:303:ALA:HA	1:A:313:LEU:HD11	1.77	0.65
1:B:1:MET:HE1	1:B:119:ILE:HG22	1.77	0.65
1:D:287:LEU:CD2	1:D:314:SER:HB3	2.27	0.65
1:C:215:ARG:HD3	1:C:240:TYR:CZ	2.33	0.64
1:D:218:PRO:C	1:D:219[A]:ASN:ND2	2.51	0.64
1:B:324:SER:O	1:B:328:MET:HG3	1.97	0.63
1:B:78[A]:ARG:HG3	1:B:78[A]:ARG:NH1	2.09	0.63
1:D:187[B]:LYS:CE	1:D:242:GLU:OE1	2.48	0.62
1:D:187[A]:LYS:HE3	1:D:217:ASP:HB2	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:O	1:B:56[B]:GLU:HG2	2.01	0.60
1:C:218:PRO:HD2	1:C:242:GLU:O	2.01	0.60
1:D:288:ILE:C	1:D:288:ILE:HD12	2.22	0.60
1:D:11:VAL:HB	1:D:387:MET:HB3	1.84	0.60
1:A:166:ASP:HB2	1:A:167:PRO:HD2	1.84	0.60
1:C:324:SER:O	1:C:328:MET:HG3	2.01	0.59
1:D:303:ALA:HA	1:D:313:LEU:HD11	1.84	0.58
1:D:371[B]:ASP:O	1:D:372[B]:GLY:O	2.21	0.58
1:D:14:ARG:HD3	6:D:829:HOH:O	2.04	0.58
1:C:218:PRO:HG2	1:C:244:PRO:HA	1.85	0.58
1:A:416[B]:ARG:HD3	3:D:508:IOD:I	2.74	0.57
1:A:265:ASN:HD22	1:A:287:LEU:HD12	1.70	0.57
1:A:287:LEU:CD2	1:A:314:SER:HB3	2.36	0.56
1:B:242:GLU:OE2	1:B:265:ASN:ND2	2.38	0.56
1:C:166:ASP:HB2	1:C:167:PRO:HD2	1.88	0.56
1:D:42:ILE:HA	3:D:503:IOD:I	2.76	0.56
1:D:166:ASP:HB2	1:D:167:PRO:CD	2.36	0.55
1:B:218:PRO:HD2	1:B:242:GLU:O	2.07	0.55
1:C:166:ASP:HB2	1:C:167:PRO:CD	2.37	0.54
1:C:389:GLU:OE2	1:C:393:ARG:NH1	2.41	0.53
1:A:416[A]:ARG:NH2	6:A:638:HOH:O	2.35	0.52
1:D:43:THR:N	3:D:503:IOD:I	3.02	0.52
1:D:210:PRO:HD2	3:D:505:IOD:I	2.79	0.52
1:B:15:ASP:OD1	1:B:16:PRO:HD2	2.11	0.51
1:C:306:CYS:CB	1:C:313:LEU:HD21	2.41	0.51
1:B:107:ARG:NH2	6:B:759:HOH:O	2.44	0.51
1:D:166:ASP:HB2	1:D:167:PRO:HD2	1.92	0.51
1:D:65:LEU:N	1:D:66:PRO:CD	2.74	0.51
1:C:184:ARG:HG2	1:C:184:ARG:HH11	1.76	0.50
1:B:78[A]:ARG:CG	1:B:78[A]:ARG:NH1	2.73	0.50
1:C:24:VAL:HG13	1:C:404:TYR:CD2	2.46	0.50
1:C:90:THR:HG22	1:C:99:SER:CB	2.42	0.50
1:D:187[B]:LYS:HE2	1:D:242:GLU:OE1	2.11	0.49
1:A:11:VAL:HB	1:A:387:MET:HB3	1.95	0.49
1:D:288:ILE:O	1:D:288:ILE:HD12	2.12	0.49
1:A:103:LYS:NZ	1:A:103:LYS:HB2	2.27	0.49
1:C:52:LEU:O	1:C:56:GLU:HG2	2.13	0.49
1:B:99[A]:SER:CB	6:B:759:HOH:O	2.50	0.48
1:B:1:MET:HE1	1:B:119:ILE:CG2	2.44	0.47
1:C:413:SER:O	1:C:415:ARG:HD3	2.15	0.47
1:A:315:MET:HG2	1:A:342:CYS:HG	1.74	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:N	1:A:66:PRO:CD	2.78	0.47
1:B:288:ILE:CG2	1:B:315:MET:HG2	2.45	0.47
1:B:153:HIS:HB3	6:B:786:HOH:O	2.14	0.47
1:A:303:ALA:HA	1:A:313:LEU:CD1	2.44	0.46
1:A:349:GLN:NE2	1:A:349:GLN:HA	2.29	0.46
1:B:65:LEU:N	1:B:66:PRO:CD	2.78	0.46
1:C:312:GLU:OE1	1:C:340:HIS:NE2	2.43	0.46
1:D:-15:HIS:O	1:D:-14:SER:HB2	2.16	0.46
1:D:218:PRO:HD2	1:D:242:GLU:O	2.16	0.46
1:A:410:PRO:HB2	1:D:89:VAL:HG11	1.98	0.46
1:B:212:LEU:HD12	1:B:212:LEU:N	2.30	0.46
1:C:305:LEU:C	1:C:305:LEU:HD23	2.36	0.46
1:C:11:VAL:HB	1:C:387:MET:HB3	1.98	0.46
1:A:154:PRO:HG2	1:A:408:PHE:CE1	2.51	0.45
1:D:349[B]:GLN:CA	1:D:349[B]:GLN:HE21	2.29	0.45
1:A:315:MET:HG3	1:A:342:CYS:HB3	1.98	0.45
1:A:-15:HIS:O	1:A:-14:SER:HB2	2.17	0.45
1:A:287:LEU:HD22	1:A:314:SER:HB3	1.97	0.45
1:C:287:LEU:N	1:C:287:LEU:HD12	2.30	0.45
1:D:187[B]:LYS:HG3	1:D:215:ARG:HB2	1.97	0.45
1:B:88:ILE:HG23	1:B:100:SER:O	2.16	0.45
1:D:101:ARG:HB3	1:D:101:ARG:CZ	2.46	0.45
1:B:264:THR:HG22	1:B:283:ILE:HD13	1.99	0.45
1:A:-17:HIS:HB3	6:A:776:HOH:O	2.16	0.45
1:A:103:LYS:HG3	6:A:747:HOH:O	2.17	0.45
1:B:288:ILE:HG23	1:B:315:MET:HG2	1.98	0.45
1:B:59[A]:ARG:HD3	6:B:818:HOH:O	2.17	0.44
1:D:24:VAL:HG13	1:D:404:TYR:CD2	2.52	0.44
1:A:24:VAL:HG13	1:A:404:TYR:CD2	2.52	0.44
1:A:101:ARG:HA	3:A:502:IOD:I	2.87	0.44
1:C:65:LEU:N	1:C:66:PRO:CD	2.80	0.44
1:C:90:THR:HG22	1:C:99:SER:HB2	1.99	0.44
1:D:315:MET:HB2	1:D:342:CYS:SG	2.58	0.44
1:A:371:ASP:O	1:A:372:GLY:O	2.36	0.43
1:B:78[B]:ARG:HD2	6:B:792:HOH:O	2.18	0.43
1:C:390:GLN:O	1:C:394:CYS:HB3	2.18	0.43
1:B:315:MET:HB3	1:B:315:MET:HE3	1.70	0.43
1:B:315:MET:CE	1:B:328:MET:HB3	2.47	0.43
1:A:396:ILE:HD13	6:B:749:HOH:O	2.18	0.43
1:D:65:LEU:N	1:D:66:PRO:HD2	2.34	0.43
1:D:244:PRO:HD2	1:D:251:MET:SD	2.59	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:SER:OG	1:B:103:LYS:HB2	2.19	0.42
1:B:416:ARG:NH2	6:B:697:HOH:O	2.44	0.42
1:A:244:PRO:HD2	1:A:251:MET:SD	2.59	0.42
1:A:288:ILE:HD13	1:A:288:ILE:C	2.39	0.42
1:B:215:ARG:HD2	1:B:240:TYR:CE1	2.54	0.42
1:D:305:LEU:C	1:D:305:LEU:HD23	2.40	0.42
1:C:184:ARG:HG2	1:C:184:ARG:NH1	2.33	0.42
1:A:194:PRO:HA	1:A:195:PRO:HD3	1.91	0.42
1:C:416:ARG:HD3	1:C:416:ARG:HA	1.81	0.42
1:B:289:ASP:HB2	1:B:316:HIS:HB3	2.01	0.42
1:B:303:ALA:CA	1:B:313:LEU:HD11	2.39	0.42
1:D:346:THR:N	1:D:347:PRO:CD	2.83	0.42
1:A:293:TRP:CE3	1:A:302:ILE:HG13	2.54	0.42
1:B:413:SER:O	1:B:415:ARG:HD3	2.19	0.42
1:A:103:LYS:CB	1:A:103:LYS:NZ	2.83	0.41
1:B:11:VAL:HB	1:B:387:MET:HB3	2.03	0.41
1:B:26:GLN:HB3	1:B:27:PRO:HD2	2.03	0.41
1:D:187[A]:LYS:NZ	6:D:817:HOH:O	2.52	0.41
1:A:218:PRO:HD2	1:A:242:GLU:O	2.20	0.41
1:D:245:THR:OG1	1:D:246:PRO:HD2	2.21	0.41
1:D:416[A]:ARG:HB2	1:D:416[A]:ARG:HE	1.60	0.41
1:D:315:MET:CE	1:D:331:LEU:HD23	2.51	0.41
1:D:372[A]:GLY:HA2	1:D:373[A]:PRO:HD3	1.90	0.41
1:A:361:ARG:CZ	1:A:361:ARG:HB2	2.50	0.41
1:A:-3:TYR:O	1:A:-1:GLN:HG2	2.21	0.40
1:C:306:CYS:HB2	1:C:313:LEU:HD21	2.03	0.40
1:C:313:LEU:N	1:C:313:LEU:HD22	2.34	0.40
1:B:390:GLN:O	1:B:394:CYS:HB3	2.20	0.40
1:C:315[B]:MET:CE	1:C:338:ILE:HD13	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	427/441 (97%)	419 (98%)	7 (2%)	1 (0%)	47	38
1	B	429/441 (97%)	425 (99%)	4 (1%)	0	100	100
1	C	423/441 (96%)	416 (98%)	7 (2%)	0	100	100
1	D	432/441 (98%)	421 (98%)	9 (2%)	2 (0%)	29	18
All	All	1711/1764 (97%)	1681 (98%)	27 (2%)	3 (0%)	51	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	372[A]	GLY
1	D	372[B]	GLY
1	A	372	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/347 (97%)	332 (98%)	6 (2%)	59	55
1	B	338/347 (97%)	332 (98%)	6 (2%)	59	55
1	C	333/347 (96%)	329 (99%)	4 (1%)	71	70
1	D	343/347 (99%)	334 (97%)	9 (3%)	46	39
All	All	1352/1388 (97%)	1327 (98%)	25 (2%)	62	55

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	VAL
1	A	145	TYR
1	A	184	ARG
1	A	219	ASN
1	A	288	ILE
1	A	349	GLN
1	B	78[A]	ARG
1	B	78[B]	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	103	LYS
1	B	141	PRO
1	B	145	TYR
1	B	287	LEU
1	C	0	SER
1	C	145	TYR
1	C	225	GLU
1	C	416	ARG
1	D	101	ARG
1	D	145	TYR
1	D	219[A]	ASN
1	D	219[B]	ASN
1	D	371[A]	ASP
1	D	371[B]	ASP
1	D	415	ARG
1	D	416[A]	ARG
1	D	416[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	A	349	GLN
1	B	265	ASN
1	C	173	GLN
1	C	203	GLN
1	C	265	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 19 ligands modelled in this entry, 1 is unknown and 11 are monoatomic - leaving 7 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	PO4	A	501	-	4,4,4	0.81	0	6,6,6	0.53	0
4	GOL	B	504	-	5,5,5	0.31	0	5,5,5	0.18	0
4	GOL	A	503	-	5,5,5	0.29	0	5,5,5	0.36	0
2	PO4	C	501	-	4,4,4	1.17	0	6,6,6	0.85	0
2	PO4	D	501	-	4,4,4	0.75	0	6,6,6	0.78	0
2	PO4	B	501	-	4,4,4	0.99	0	6,6,6	0.58	0
4	GOL	C	502	-	5,5,5	0.21	0	5,5,5	0.49	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	A	503	-	-	2/4/4/4	-
4	GOL	C	502	-	-	0/4/4/4	-
4	GOL	B	504	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	504	GOL	C1-C2-C3-O3
4	B	504	GOL	O1-C1-C2-C3
4	A	503	GOL	C1-C2-C3-O3
4	B	504	GOL	O2-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	A	503	GOL	O2-C2-C3-O3
4	B	504	GOL	O1-C1-C2-O2

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	428/441 (97%)	-0.59	2 (0%) 91 92	22, 33, 59, 100	0
1	B	420/441 (95%)	-0.28	11 (2%) 56 58	20, 35, 67, 135	0
1	C	424/441 (96%)	-0.39	6 (1%) 75 77	20, 35, 59, 96	0
1	D	427/441 (96%)	-0.51	0 100 100	20, 32, 57, 89	0
All	All	1699/1764 (96%)	-0.44	19 (1%) 80 82	20, 34, 61, 135	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	THR	4.8
1	B	89	VAL	4.4
1	C	-4	LEU	4.2
1	B	86	ALA	4.1
1	A	99	SER	3.9
1	C	-3	TYR	3.6
1	B	91	ASP	3.2
1	B	88	ILE	3.1
1	B	98	SER	3.0
1	B	97	GLY	2.9
1	B	256	ALA	2.5
1	B	92	MET	2.5
1	B	255	ALA	2.4
1	B	87	ASN	2.3
1	C	-1	GLN	2.2
1	C	256	ALA	2.2
1	C	235	ASP	2.1
1	C	257	GLU	2.0
1	A	100	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	504	6/6	0.85	0.18	63,78,94,100	0
5	UNL	B	503	4/-	0.89	0.20	46,59,71,105	0
4	GOL	C	502	6/6	0.94	0.12	34,53,68,72	0
3	IOD	D	506	1/1	0.94	0.10	61,61,61,61	1
3	IOD	D	505	1/1	0.95	0.09	66,66,66,66	1
4	GOL	A	503	6/6	0.95	0.22	44,46,50,70	0
3	IOD	A	504	1/1	0.96	0.06	59,59,59,59	1
3	IOD	D	508	1/1	0.97	0.05	61,61,61,61	1
2	PO4	C	501	5/5	0.98	0.11	41,46,73,83	0
2	PO4	D	501	5/5	0.98	0.07	36,40,64,74	0
3	IOD	D	504	1/1	0.98	0.07	46,46,46,46	1
3	IOD	D	503	1/1	0.98	0.21	79,79,79,79	1
2	PO4	B	501	5/5	0.98	0.12	40,53,75,87	0
3	IOD	D	507	1/1	0.98	0.07	46,46,46,46	1
3	IOD	A	502	1/1	0.99	0.05	36,36,36,36	1
3	IOD	D	502	1/1	0.99	0.05	35,35,35,35	1
3	IOD	B	502	1/1	0.99	0.11	63,63,63,63	1
3	IOD	B	505	1/1	0.99	0.04	55,55,55,55	0
2	PO4	A	501	5/5	0.99	0.08	40,47,77,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.