



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:33 am BST

PDB ID : 2PLR  
Title : Crystal structure of dTMP kinase (st1543) from Sulfolobus Tokodaii Strain7  
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Deposited on : 2007-04-20  
Resolution : 1.60 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.

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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	:	1.8.5 (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

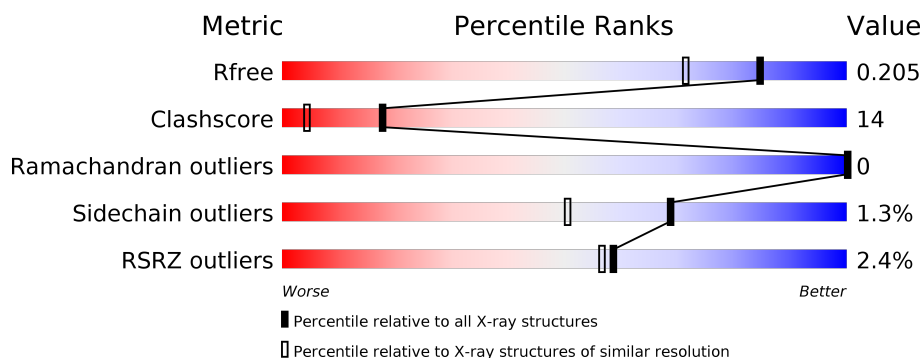
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	213	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>21%</div> </div> </div>
1	B	213	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	DTT	A	1701	-	-	X	-
9	PEG	A	1206	-	-	X	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4170 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.

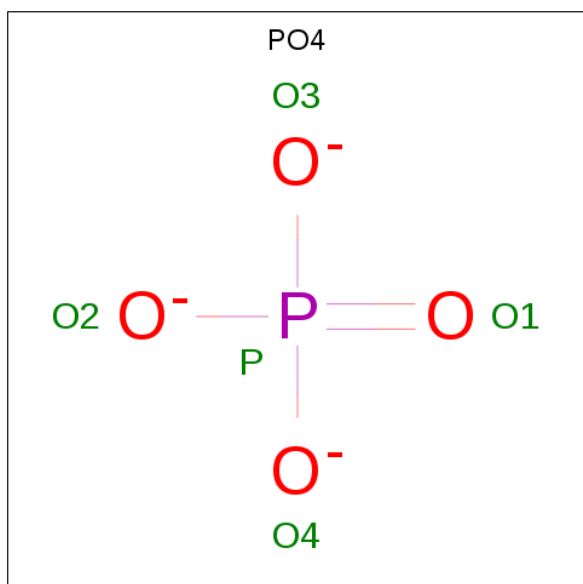
- Molecule 1 is a protein called Probable thymidylate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	Se	0	0	0
			1732	1130	282	319	1			
1	B	208	Total	C	N	O	Se	0	0	0
			1695	1106	275	313	1			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

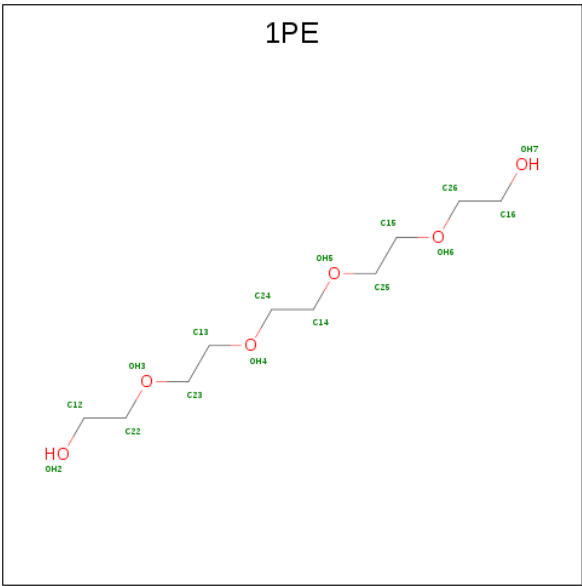
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



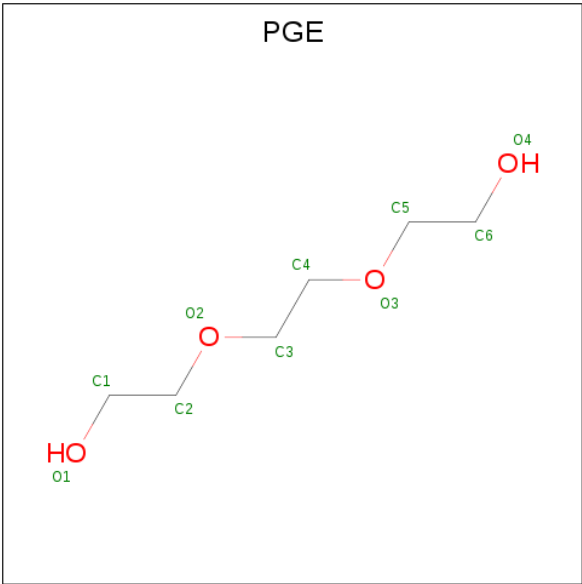
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



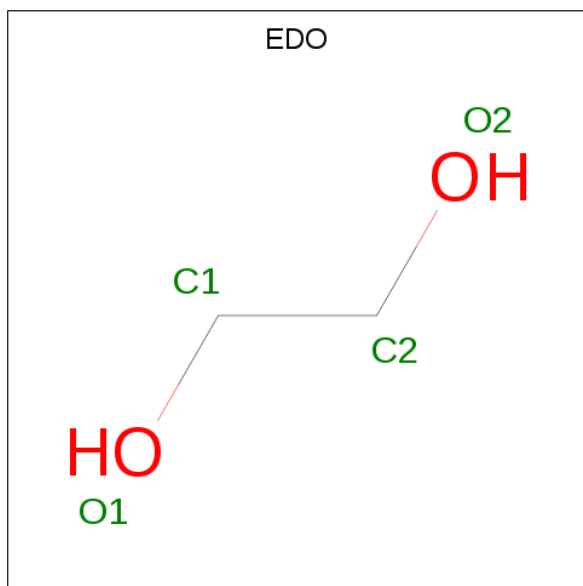
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



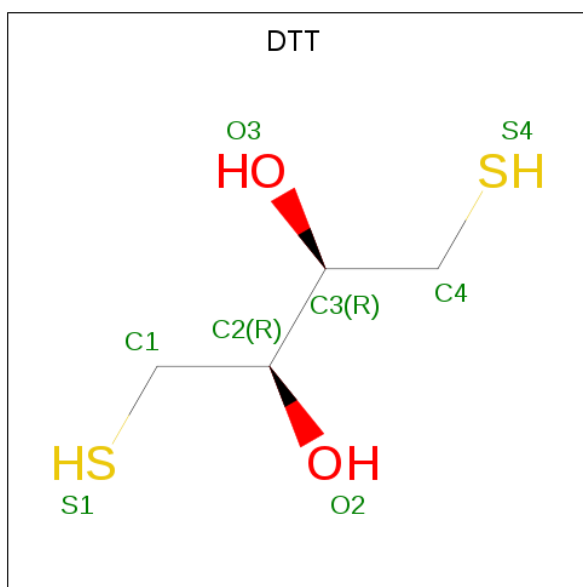
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



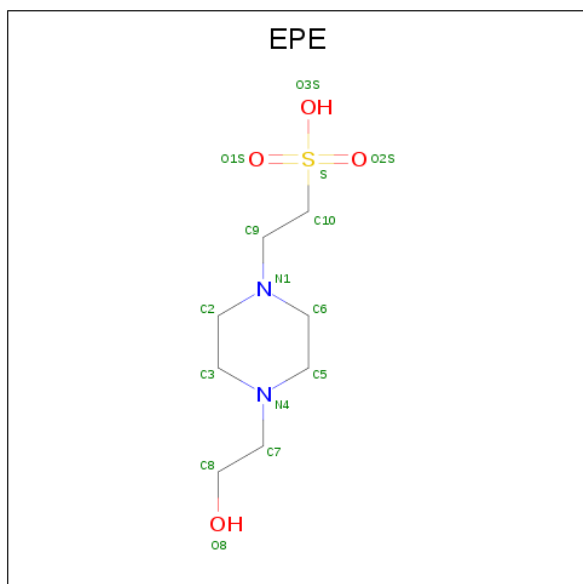
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



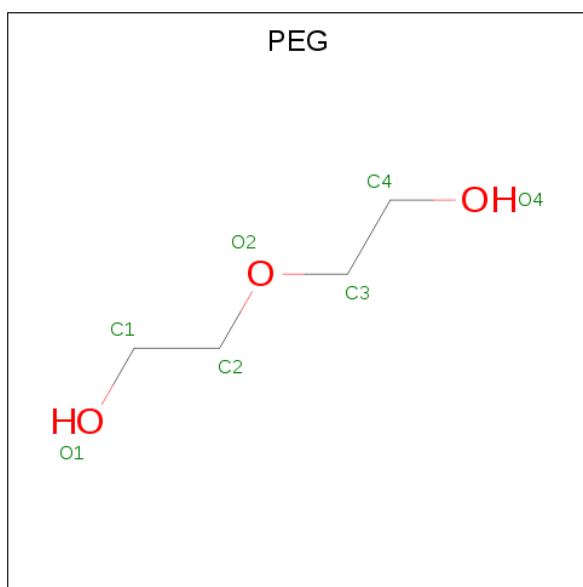
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



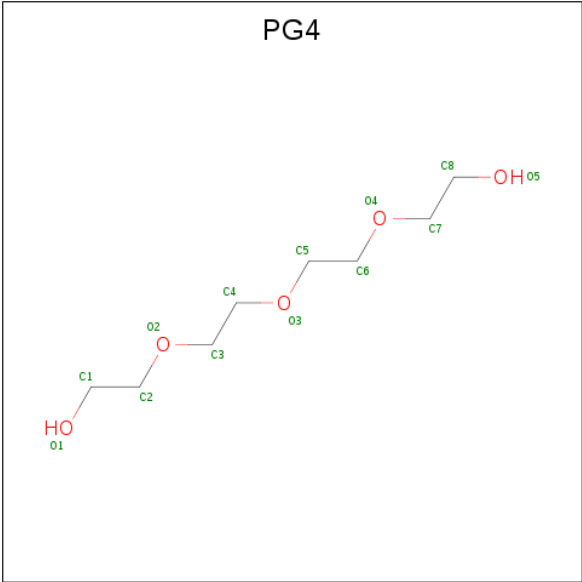
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			13	8	5		

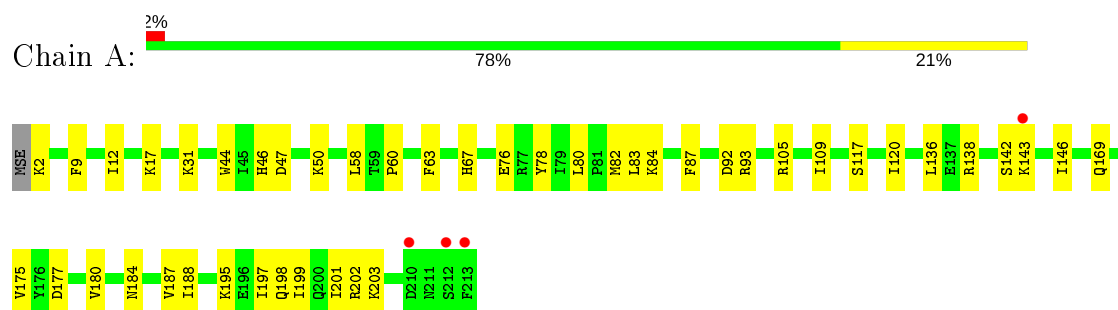
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	306	Total	O	0	0
			306	306		
11	B	215	Total	O	0	0
			215	215		

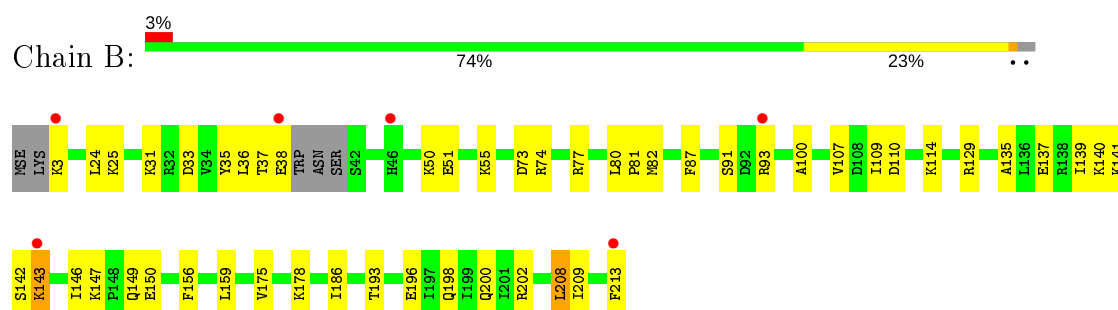
### 3 Residue-property plots [i](#)

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: Probable thymidylate kinase



- Molecule 1: Probable thymidylate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.52Å 62.87Å 137.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.59 – 1.60 46.59 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (46.59-1.60) 97.6 (46.59-1.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.185 , 0.209 0.181 , 0.205	Depositor DCC
$R_{free}$ test set	5805 reflections (10.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 63.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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: PGE, CL, PO4, EDO, 1PE, PG4, PEG, EPE, DTT

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	0/1769	0.56	0/2384
1	B	0.29	0/1729	0.57	1/2328 (0.0%)
All	All	0.29	0/3498	0.56	1/4712 (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	B	142	SER	N-CA-C	-5.67	95.70	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1732	0	1775	43	0
1	B	1695	0	1740	51	0
2	A	2	0	0	1	0
3	A	5	0	0	0	0
4	A	16	0	22	3	0
4	B	32	0	44	7	0
5	A	30	0	39	6	0
6	A	12	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	12	0	15	1	0
7	A	8	0	10	9	0
8	A	15	0	17	0	0
9	A	49	0	63	8	0
9	B	28	0	36	2	0
10	B	13	0	18	3	0
11	A	306	0	0	5	0
11	B	215	0	0	6	0
All	All	4170	0	3794	101	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 14.

All (101) 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:198:GLN:HE21	1:A:202:ARG:HE	1.10	0.91
1:B:198:GLN:HE21	1:B:202:ARG:HE	1.13	0.90
1:A:31:LYS:HD2	6:A:1505:EDO:H21	1.60	0.84
7:A:1701:DTT:S4	7:A:1701:DTT:O2	2.30	0.84
1:A:105:ARG:HD2	7:A:1701:DTT:H3	1.62	0.80
7:A:1701:DTT:HS2	7:A:1701:DTT:HO2	1.29	0.78
1:A:76:GLU:HG3	11:B:1621:HOH:O	1.87	0.75
1:B:25:LYS:HG3	1:B:36:LEU:HB2	1.70	0.74
1:A:203:LYS:HD3	5:A:1404:PGE:H42	1.71	0.72
1:B:114:LYS:HZ3	4:B:1303:1PE:H161	1.55	0.71
1:B:35:TYR:HB2	1:B:82:MSE:HE3	1.73	0.70
1:A:78:TYR:O	1:A:82:MSE:HG3	1.93	0.69
1:A:60:PRO:HA	7:A:1701:DTT:H12	1.74	0.69
1:B:198:GLN:HE21	1:B:202:ARG:NE	1.91	0.66
1:A:50:LYS:NZ	1:A:67:HIS:HE1	1.93	0.66
1:B:143:LYS:N	1:B:143:LYS:HD2	2.12	0.65
1:B:208:LEU:O	1:B:208:LEU:HD22	1.96	0.64
1:A:63:PHE:CD2	7:A:1701:DTT:H11	2.32	0.64
1:A:50:LYS:HZ1	1:A:67:HIS:HE1	1.43	0.63
1:B:143:LYS:H	1:B:143:LYS:HD2	1.67	0.58
1:B:137:GLU:OE1	1:B:141:LYS:HD3	2.03	0.58
1:B:80:LEU:HB3	1:B:81:PRO:HD3	1.86	0.57
1:B:50:LYS:HG3	11:B:1696:HOH:O	2.03	0.57
1:B:129:ARG:NH1	10:B:1601:PG4:H21	2.20	0.57
1:B:107:VAL:HG13	9:B:1203:PEG:H42	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1909:HOH:O	1:B:77:ARG:HG2	2.04	0.56
9:A:1206:PEG:H32	11:A:1913:HOH:O	2.06	0.55
1:A:63:PHE:CB	7:A:1701:DTT:H11	2.35	0.55
1:A:184:ASN:HD21	9:A:1208:PEG:H22	1.72	0.55
1:B:129:ARG:HH11	10:B:1601:PG4:H21	1.71	0.55
1:A:188:ILE:HG21	1:A:197:ILE:HG23	1.88	0.55
1:B:114:LYS:NZ	4:B:1303:1PE:H161	2.22	0.54
1:B:110:ASP:HB3	4:B:1303:1PE:H142	1.89	0.54
1:B:82:MSE:O	1:B:87:PHE:HB2	2.08	0.54
1:A:63:PHE:CG	7:A:1701:DTT:H11	2.43	0.54
5:A:1402:PGE:H2	9:A:1206:PEG:H11	1.90	0.53
9:A:1207:PEG:H12	11:A:2131:HOH:O	2.06	0.53
1:A:63:PHE:HB2	7:A:1701:DTT:H11	1.90	0.53
1:B:208:LEU:HD13	1:B:209:ILE:HG23	1.90	0.53
1:B:149:GLN:HG3	1:B:150:GLU:N	2.24	0.53
1:B:77:ARG:HB3	1:B:77:ARG:HH21	1.75	0.52
1:B:193:THR:OG1	1:B:196:GLU:HG3	2.09	0.51
1:A:142:SER:C	1:A:143:LYS:HD2	2.31	0.51
1:A:82:MSE:O	1:A:87:PHE:HB2	2.11	0.51
1:B:139:ILE:HG21	1:B:146:ILE:HD13	1.92	0.51
1:A:138:ARG:HD3	9:A:1204:PEG:H11	1.92	0.50
1:A:198:GLN:HE21	1:A:202:ARG:NE	1.93	0.50
4:A:1302:1PE:H121	11:A:2023:HOH:O	2.11	0.50
4:A:1302:1PE:H241	4:B:1303:1PE:H142	1.93	0.50
1:A:80:LEU:HG	1:A:84:LYS:HE3	1.95	0.49
1:A:46:HIS:HD2	1:A:47:ASP:OD1	1.95	0.49
1:B:110:ASP:HB3	4:B:1303:1PE:C14	2.43	0.49
1:B:139:ILE:HG21	1:B:146:ILE:CD1	2.42	0.49
1:B:156:PHE:HB3	1:B:159:LEU:HD12	1.93	0.49
1:B:135:ALA:O	1:B:139:ILE:HG13	2.13	0.48
1:B:137:GLU:O	1:B:141:LYS:HB2	2.13	0.48
1:B:74:ARG:HG2	1:B:74:ARG:HH11	1.78	0.48
1:B:186:ILE:HD13	11:B:1631:HOH:O	2.14	0.48
1:B:74:ARG:NH1	1:B:74:ARG:HG2	2.29	0.47
1:B:200:GLN:HG2	11:B:1768:HOH:O	2.14	0.47
1:B:38:GLU:O	1:B:93:ARG:NH2	2.49	0.46
1:A:109:ILE:HG21	5:A:1401:PGE:H62	1.98	0.46
1:A:180:VAL:HG21	9:A:1206:PEG:H21	1.98	0.46
1:B:129:ARG:CD	10:B:1601:PG4:H42	2.45	0.45
1:B:74:ARG:HD3	11:B:1731:HOH:O	2.15	0.45
1:A:50:LYS:HZ1	1:A:67:HIS:CE1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ASP:CG	4:B:1303:IPE:H141	2.36	0.45
1:A:105:ARG:CD	7:A:1701:DTT:H2	2.47	0.45
1:B:213:PHE:O	1:B:213:PHE:CG	2.69	0.45
1:A:67:HIS:HD2	11:A:1912:HOH:O	1.98	0.45
1:A:2:LYS:HB2	1:A:2:LYS:NZ	2.32	0.45
1:B:33:ASP:HB3	1:B:87:PHE:CE1	2.52	0.45
1:B:140:LYS:HE2	11:B:1641:HOH:O	2.16	0.44
2:A:214:CL:CL	2:A:215:CL:CL	3.10	0.44
1:B:208:LEU:HD13	1:B:209:ILE:CG2	2.47	0.44
1:B:37:THR:OG1	1:B:91:SER:HA	2.17	0.44
1:A:44:TRP:CG	1:B:55:LYS:HE3	2.52	0.44
1:A:195:LYS:O	1:A:199:ILE:HG13	2.18	0.44
1:A:83:LEU:HD13	1:A:120:ILE:HD11	2.01	0.43
1:A:184:ASN:OD1	9:A:1208:PEG:H32	2.19	0.43
1:B:73:ASP:O	1:B:77:ARG:HG3	2.17	0.43
1:B:24:LEU:HA	1:B:198:GLN:HE22	1.83	0.43
1:A:142:SER:O	1:A:143:LYS:HB2	2.19	0.43
1:B:140:LYS:NZ	9:B:1211:PEG:H31	2.34	0.43
1:B:109:ILE:HG21	4:B:1301:IPE:H252	2.00	0.42
1:B:55:LYS:HG2	6:B:1503:EDO:H22	2.02	0.42
1:A:187:VAL:HG11	9:A:1206:PEG:H31	2.01	0.42
1:B:175:VAL:O	1:B:178:LYS:HG2	2.19	0.42
1:A:136:LEU:HD11	1:A:146:ILE:HD11	2.01	0.42
1:A:175:VAL:CG2	5:A:1401:PGE:H22	2.49	0.42
1:A:12:ILE:HB	1:A:169:GLN:NE2	2.35	0.42
1:B:147:LYS:HG2	1:B:150:GLU:OE1	2.20	0.42
1:A:117:SER:HB2	4:A:1302:IPE:H122	2.00	0.42
1:A:177:ASP:HB3	5:A:1402:PGE:H4	2.02	0.41
1:A:46:HIS:CE1	1:A:50:LYS:NZ	2.88	0.41
1:A:58:LEU:HB2	1:A:63:PHE:CE2	2.55	0.41
1:B:100:ALA:HA	1:B:175:VAL:HG11	2.01	0.41
1:B:51:GLU:HG3	1:B:55:LYS:HE2	2.03	0.41
1:A:92:ASP:O	1:A:93:ARG:HB2	2.19	0.41
1:A:203:LYS:HG2	5:A:1404:PGE:H5	2.03	0.41
1:A:9:PHE:HE1	1:A:201:ILE:HD13	1.85	0.41

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	210/213 (99%)	206 (98%)	4 (2%)	0	100	100
1	B	204/213 (96%)	198 (97%)	6 (3%)	0	100	100
All	All	414/426 (97%)	404 (98%)	10 (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	190/189 (100%)	189 (100%)	1 (0%)	88	80
1	B	186/189 (98%)	182 (98%)	4 (2%)	52	27
All	All	376/378 (100%)	371 (99%)	5 (1%)	69	50

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	B	3	LYS
1	B	31	LYS
1	B	143	LYS
1	B	208	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	67	HIS
1	A	198	GLN
1	B	149	GLN
1	B	198	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	1PE	B	1303	-	15,15,15	0.69	0	14,14,14	0.89	0
9	PEG	A	1201	-	6,6,6	1.60	1 (16%)	5,5,5	0.74	0
9	PEG	A	1208	-	6,6,6	1.62	1 (16%)	5,5,5	0.71	0
9	PEG	A	1202	-	6,6,6	1.59	1 (16%)	5,5,5	0.67	0
6	EDO	B	1503	-	3,3,3	2.24	1 (33%)	2,2,2	0.35	0
9	PEG	B	1203	-	6,6,6	1.63	1 (16%)	5,5,5	0.69	0
4	1PE	B	1301	-	15,15,15	0.53	0	14,14,14	0.86	0
9	PEG	A	1207	-	6,6,6	1.66	1 (16%)	5,5,5	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	PEG	A	1205	-	6,6,6	1.62	1 (16%)	5,5,5	0.73	0
6	EDO	B	1502	-	3,3,3	2.23	1 (33%)	2,2,2	0.35	0
4	1PE	A	1302	-	15,15,15	0.49	0	14,14,14	0.81	0
9	PEG	A	1206	-	6,6,6	1.62	1 (16%)	5,5,5	0.72	0
6	EDO	B	1506	-	3,3,3	2.23	1 (33%)	2,2,2	0.35	0
5	PGE	A	1404	-	9,9,9	1.35	1 (11%)	8,8,8	0.83	0
3	PO4	A	1901	-	4,4,4	1.17	0	6,6,6	0.59	0
9	PEG	B	1210	-	6,6,6	1.63	1 (16%)	5,5,5	0.70	0
9	PEG	B	1211	-	6,6,6	1.61	1 (16%)	5,5,5	0.66	0
6	EDO	A	1501	-	3,3,3	2.23	1 (33%)	2,2,2	0.34	0
6	EDO	A	1505	-	3,3,3	2.25	1 (33%)	2,2,2	0.36	0
10	PG4	B	1601	-	12,12,12	0.43	0	11,11,11	0.93	0
5	PGE	A	1402	-	9,9,9	1.37	1 (11%)	8,8,8	0.80	0
6	EDO	A	1504	-	3,3,3	2.24	1 (33%)	2,2,2	0.35	0
9	PEG	B	1209	-	6,6,6	1.63	1 (16%)	5,5,5	0.69	0
9	PEG	A	1204	-	6,6,6	1.61	1 (16%)	5,5,5	0.72	0
8	EPE	A	1801	-	15,15,15	0.83	1 (6%)	18,20,20	1.83	5 (27%)
7	DTT	A	1701	-	7,7,7	0.66	0	4,8,8	0.93	0
5	PGE	A	1401	-	9,9,9	1.37	1 (11%)	8,8,8	0.76	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	1PE	B	1303	-	-	4/13/13/13	-
9	PEG	A	1201	-	-	2/4/4/4	-
9	PEG	A	1208	-	-	2/4/4/4	-
9	PEG	A	1202	-	-	1/4/4/4	-
6	EDO	B	1503	-	-	1/1/1/1	-
9	PEG	B	1203	-	-	1/4/4/4	-
4	1PE	B	1301	-	-	2/13/13/13	-
9	PEG	A	1207	-	-	2/4/4/4	-
9	PEG	A	1205	-	-	2/4/4/4	-
6	EDO	B	1502	-	-	1/1/1/1	-
4	1PE	A	1302	-	-	3/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PEG	A	1206	-	-	2/4/4/4	-
9	PEG	B	1210	-	-	3/4/4/4	-
5	PGE	A	1404	-	-	3/7/7/7	-
6	EDO	B	1506	-	-	1/1/1/1	-
9	PEG	B	1211	-	-	2/4/4/4	-
6	EDO	A	1501	-	-	0/1/1/1	-
6	EDO	A	1505	-	-	1/1/1/1	-
10	PG4	B	1601	-	-	3/10/10/10	-
5	PGE	A	1402	-	-	3/7/7/7	-
6	EDO	A	1504	-	-	1/1/1/1	-
9	PEG	B	1209	-	-	2/4/4/4	-
9	PEG	A	1204	-	-	3/4/4/4	-
8	EPE	A	1801	-	-	1/9/19/19	0/1/1/1
7	DTT	A	1701	-	-	7/8/8/8	-
5	PGE	A	1401	-	-	4/7/7/7	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1207	PEG	O1-C1	-3.87	1.22	1.42
6	A	1505	EDO	O1-C1	-3.83	1.22	1.42
9	B	1203	PEG	O1-C1	-3.83	1.22	1.42
5	A	1404	PGE	O1-C1	-3.81	1.22	1.42
5	A	1401	PGE	O1-C1	-3.81	1.22	1.42
9	A	1205	PEG	O1-C1	-3.80	1.22	1.42
9	B	1209	PEG	O1-C1	-3.80	1.22	1.42
6	A	1504	EDO	O1-C1	-3.80	1.22	1.42
9	B	1210	PEG	O1-C1	-3.80	1.22	1.42
9	A	1208	PEG	O1-C1	-3.79	1.22	1.42
6	B	1502	EDO	O1-C1	-3.79	1.22	1.42
6	B	1503	EDO	O1-C1	-3.79	1.22	1.42
6	B	1506	EDO	O1-C1	-3.79	1.22	1.42
9	A	1206	PEG	O1-C1	-3.79	1.22	1.42
9	A	1204	PEG	O1-C1	-3.78	1.22	1.42
6	A	1501	EDO	O1-C1	-3.78	1.22	1.42
5	A	1402	PGE	O1-C1	-3.77	1.22	1.42
9	A	1201	PEG	O1-C1	-3.75	1.22	1.42
9	B	1211	PEG	O1-C1	-3.74	1.22	1.42
9	A	1202	PEG	O1-C1	-3.72	1.22	1.42
8	A	1801	EPE	C10-S	2.85	1.81	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1801	EPE	C5-N4-C3	4.10	118.05	108.83
8	A	1801	EPE	O1S-S-C10	3.58	111.23	106.92
8	A	1801	EPE	C7-N4-C5	2.84	118.49	111.23
8	A	1801	EPE	C7-N4-C3	2.78	118.35	111.23
8	A	1801	EPE	O2S-S-C10	2.14	109.49	106.92

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1801	EPE	C8-C7-N4-C5
7	A	1701	DTT	S1-C1-C2-O2
7	A	1701	DTT	S1-C1-C2-C3
7	A	1701	DTT	C1-C2-C3-O3
7	A	1701	DTT	O2-C2-C3-O3
7	A	1701	DTT	O2-C2-C3-C4
7	A	1701	DTT	C2-C3-C4-S4
7	A	1701	DTT	O3-C3-C4-S4
5	A	1401	PGE	O2-C3-C4-O3
4	B	1303	1PE	OH7-C16-C26-OH6
9	A	1207	PEG	O2-C3-C4-O4
5	A	1404	PGE	O3-C5-C6-O4
5	A	1402	PGE	O1-C1-C2-O2
9	A	1204	PEG	O1-C1-C2-O2
9	A	1201	PEG	O2-C3-C4-O4
9	A	1206	PEG	O1-C1-C2-O2
10	B	1601	PG4	O1-C1-C2-O2
9	A	1207	PEG	O1-C1-C2-O2
9	B	1210	PEG	O2-C3-C4-O4
5	A	1401	PGE	O1-C1-C2-O2
6	B	1503	EDO	O1-C1-C2-O2
6	A	1505	EDO	O1-C1-C2-O2
6	A	1504	EDO	O1-C1-C2-O2
4	B	1303	1PE	OH4-C13-C23-OH3
9	A	1204	PEG	O2-C3-C4-O4
4	B	1303	1PE	OH5-C14-C24-OH4
9	A	1206	PEG	O2-C3-C4-O4
9	B	1210	PEG	O1-C1-C2-O2
5	A	1404	PGE	O1-C1-C2-O2
4	A	1302	1PE	OH4-C13-C23-OH3
5	A	1402	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
4	B	1301	1PE	OH6-C15-C25-OH5
4	A	1302	1PE	OH2-C12-C22-OH3
5	A	1402	PGE	C4-C3-O2-C2
4	B	1301	1PE	OH7-C16-C26-OH6
4	A	1302	1PE	OH7-C16-C26-OH6
5	A	1404	PGE	C4-C3-O2-C2
5	A	1401	PGE	C4-C3-O2-C2
10	B	1601	PG4	C4-C3-O2-C2
9	B	1210	PEG	C1-C2-O2-C3
9	A	1204	PEG	C1-C2-O2-C3
9	A	1201	PEG	C4-C3-O2-C2
4	B	1303	1PE	OH2-C12-C22-OH3
9	A	1208	PEG	O2-C3-C4-O4
9	B	1211	PEG	O2-C3-C4-O4
5	A	1401	PGE	O3-C5-C6-O4
6	B	1502	EDO	O1-C1-C2-O2
6	B	1506	EDO	O1-C1-C2-O2
9	A	1208	PEG	C4-C3-O2-C2
9	B	1211	PEG	C1-C2-O2-C3
9	B	1209	PEG	C4-C3-O2-C2
9	A	1205	PEG	C1-C2-O2-C3
9	B	1203	PEG	C1-C2-O2-C3
9	B	1209	PEG	O2-C3-C4-O4
9	A	1202	PEG	C1-C2-O2-C3
10	B	1601	PG4	O2-C3-C4-O3
9	A	1205	PEG	O1-C1-C2-O2

There are no ring outliers.

16 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1303	1PE	6	0
9	A	1208	PEG	2	0
6	B	1503	EDO	1	0
9	B	1203	PEG	1	0
4	B	1301	1PE	1	0
9	A	1207	PEG	1	0
4	A	1302	1PE	3	0
9	A	1206	PEG	4	0
5	A	1404	PGE	2	0
9	B	1211	PEG	1	0
6	A	1505	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1601	PG4	3	0
5	A	1402	PGE	2	0
9	A	1204	PEG	1	0
7	A	1701	DTT	9	0
5	A	1401	PGE	2	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	211/213 (99%)	-0.28	4 (1%) 66 65	9, 16, 34, 53	0
1	B	207/213 (97%)	0.02	6 (2%) 51 49	10, 20, 47, 80	0
All	All	418/426 (98%)	-0.13	10 (2%) 59 56	9, 18, 41, 80	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	PHE	7.7
1	A	213	PHE	4.7
1	B	38	GLU	3.0
1	B	143	LYS	2.9
1	A	143	LYS	2.8
1	A	210	ASP	2.5
1	A	212	SER	2.3
1	B	93	ARG	2.3
1	B	46	HIS	2.3
1	B	3	LYS	2.1

### 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 carbohydrates 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
5	PGE	A	1404	10/10	0.43	0.26	73,74,75,75	0
6	EDO	B	1506	4/4	0.47	0.18	55,57,58,58	0
4	1PE	B	1303	16/16	0.49	0.27	73,75,75,75	0
7	DTT	A	1701	8/8	0.60	0.22	40,47,52,57	0
9	PEG	A	1207	7/7	0.65	0.22	50,52,54,55	0
5	PGE	A	1402	10/10	0.69	0.19	48,51,55,55	0
9	PEG	A	1208	7/7	0.70	0.23	53,57,60,62	0
9	PEG	A	1204	7/7	0.71	0.14	48,51,56,56	0
9	PEG	B	1211	7/7	0.71	0.20	52,54,57,57	0
6	EDO	B	1503	4/4	0.72	0.11	58,58,58,59	0
10	PG4	B	1601	13/13	0.75	0.20	33,38,45,46	0
9	PEG	B	1210	7/7	0.75	0.15	34,38,41,46	0
6	EDO	A	1501	4/4	0.79	0.15	55,55,55,56	0
5	PGE	A	1401	10/10	0.79	0.15	46,46,48,49	0
9	PEG	A	1205	7/7	0.80	0.12	46,47,48,48	0
6	EDO	A	1504	4/4	0.80	0.11	54,55,55,55	0
9	PEG	B	1209	7/7	0.80	0.17	48,49,52,55	0
9	PEG	B	1203	7/7	0.84	0.15	26,29,33,39	0
9	PEG	A	1206	7/7	0.85	0.15	46,48,52,55	0
8	EPE	A	1801	15/15	0.86	0.24	32,35,41,46	0
6	EDO	A	1505	4/4	0.86	0.18	30,33,37,40	0
6	EDO	B	1502	4/4	0.86	0.19	57,57,58,59	0
4	1PE	B	1301	16/16	0.89	0.17	17,23,39,41	0
9	PEG	A	1202	7/7	0.90	0.14	19,25,37,38	0
4	1PE	A	1302	16/16	0.91	0.12	22,34,38,40	0
9	PEG	A	1201	7/7	0.91	0.09	18,24,32,35	0
3	PO4	A	1901	5/5	0.91	0.21	29,32,38,38	0
2	CL	A	215	1/1	0.98	0.09	30,30,30,30	0
2	CL	A	214	1/1	0.99	0.09	28,28,28,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.