



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 08:10 PM EDT

PDB ID : 4H1T  
Title : X-RAY Structure of the Complex VchUPh with Phosphate ion at 1.92A Resolution.  
Authors : Prokofev, I.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Sotnichenko, S.E.; Betzel, C.; Mikhailov, A.M.  
Deposited on : 2012-09-11  
Resolution : 1.92 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 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

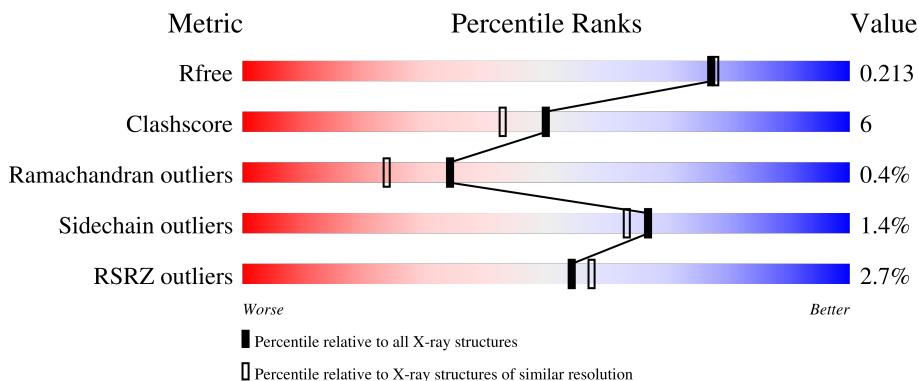
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 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	253	 3% 85% 15%
1	B	253	 7% 84% 15%
1	C	253	 % 84% 15%
1	D	253	 4% 83% 16%
1	E	253	 % 86% 13%

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Mol	Chain	Length	Quality of chain
1	F	253	 87% 11% **

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
3	EDO	C	307	-	-	X	-
5	PEG	A	321	-	-	-	X
5	PEG	C	317	-	-	-	X
5	PEG	F	316	-	-	-	X
5	PEG	F	317	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13160 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	Total 1934	C 1218	N 334	O 368	S 14	0	10	0
1	B	251	Total 1914	C 1202	N 331	O 366	S 15	0	6	0
1	C	251	Total 1924	C 1207	N 336	O 368	S 13	0	7	0
1	D	250	Total 1899	C 1191	N 329	O 364	S 15	0	5	0
1	E	251	Total 1915	C 1201	N 334	O 366	S 14	0	6	0
1	F	250	Total 1899	C 1194	N 331	O 361	S 13	0	5	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Na 1	0	0
2	E	1	Total 1	Na 1	0	0

- Molecule 3 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
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

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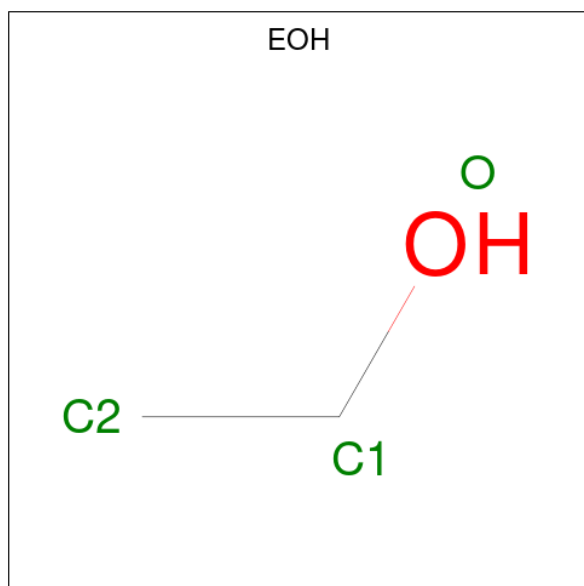
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is ETHANOL (three-letter code: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).



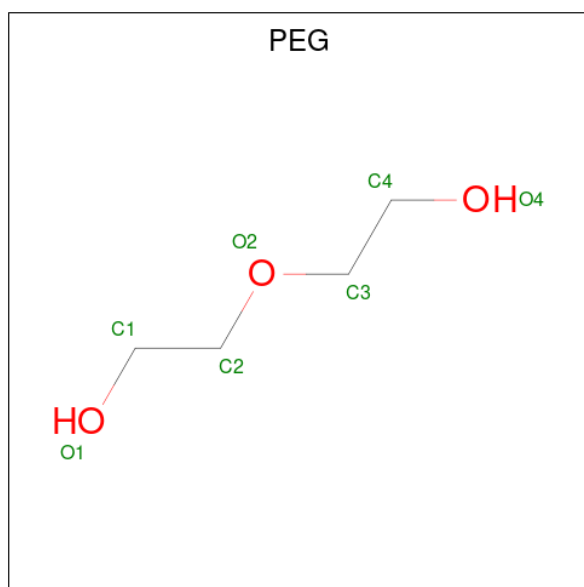
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	B	1	Total C O 3 2 1	0	0

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

- Molecule 5 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
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

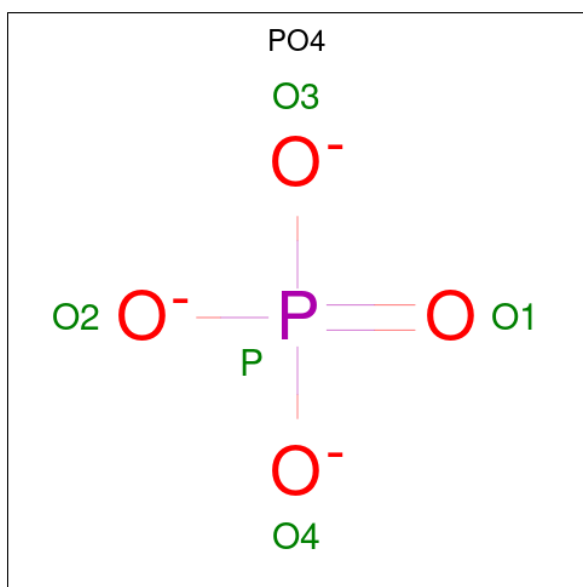
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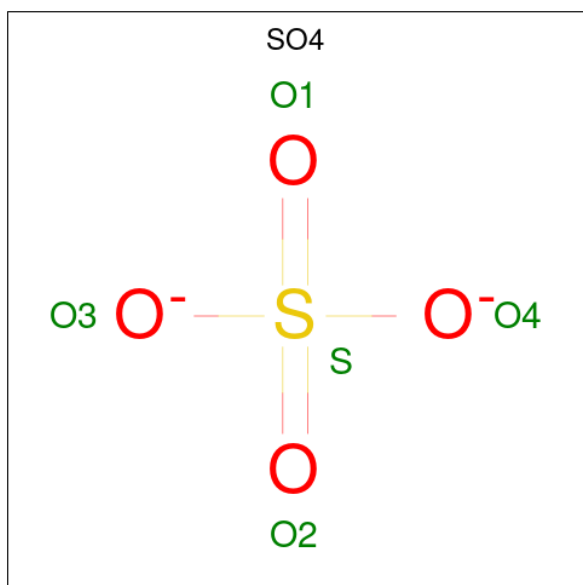
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	E	1	Total C O 7 4 3	0	0
5	E	1	Total C O 6 4 2	0	0
5	E	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total K 1 1	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	196	Total O 196 196	0	0
10	B	165	Total O 165 165	0	0
10	C	233	Total O 233 233	0	0
10	D	202	Total O 202 202	0	0
10	E	206	Total O 206 206	0	0

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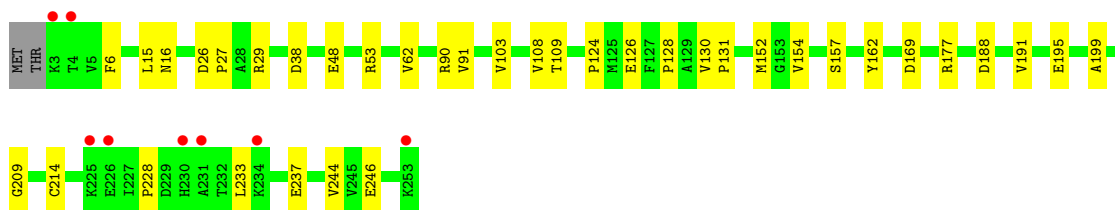
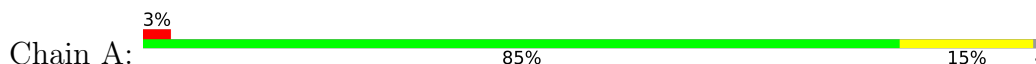
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
10	F	228	Total 228	O 228	0	0

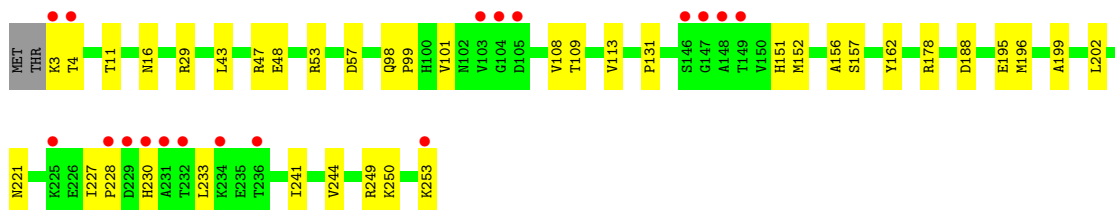
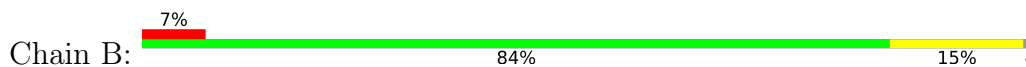
### 3 Residue-property plots [i](#)

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.

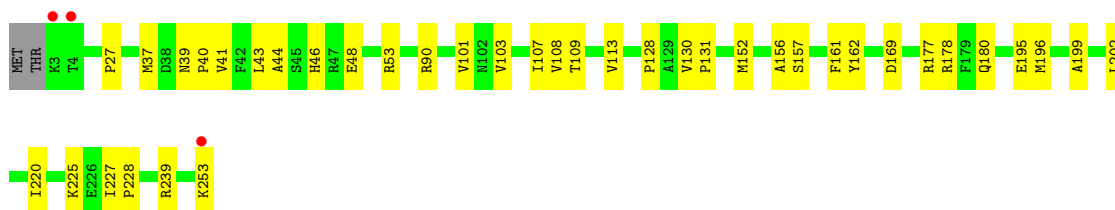
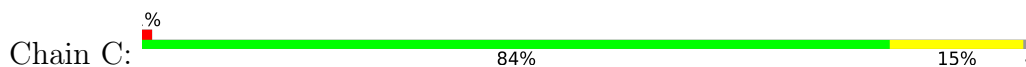
- Molecule 1: Uridine phosphorylase



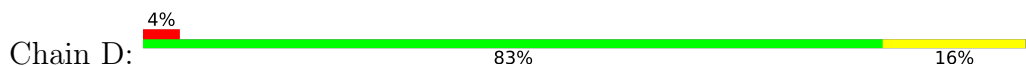
- Molecule 1: Uridine phosphorylase

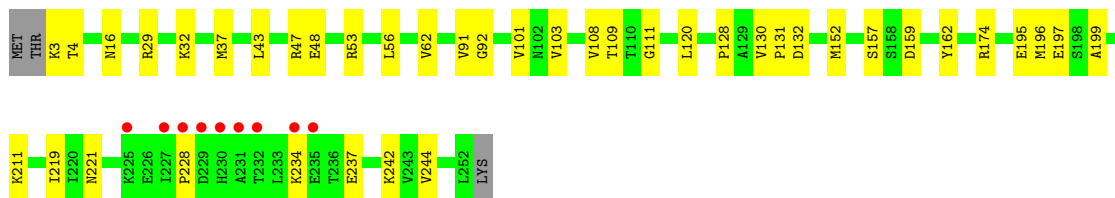


- Molecule 1: Uridine phosphorylase

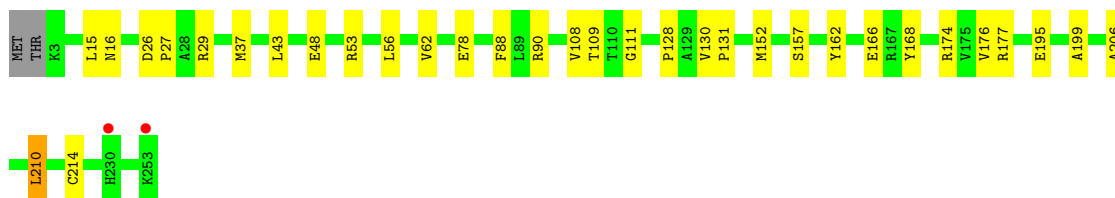
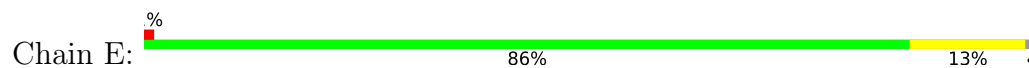


- Molecule 1: Uridine phosphorylase

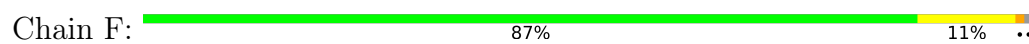




- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.69Å 71.08Å 87.94Å 69.62° 72.56° 85.74°	Depositor
Resolution (Å)	26.27 – 1.92 29.36 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.2 (26.27-1.92) 98.3 (29.36-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.80 (at 1.92Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, $R_{free}$	0.177 , 0.217 0.173 , 0.213	Depositor DCC
$R_{free}$ test set	5130 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.7	Xtrriage
Anisotropy	0.184	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: EDO, PO4, K, EOH, PEG, CL, NA, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/1992	0.44	0/2701
1	B	0.23	0/1960	0.45	0/2655
1	C	0.24	0/1970	0.46	0/2671
1	D	0.24	0/1942	0.44	0/2633
1	E	0.24	0/1961	0.45	0/2658
1	F	0.25	0/1945	0.47	1/2638 (0.0%)
All	All	0.24	0/11770	0.45	1/15956 (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	F	229	ASP	CB-CG-OD2	5.16	122.94	118.30

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	1934	0	1970	25	0
1	B	1914	0	1935	24	0
1	C	1924	0	1943	28	0
1	D	1899	0	1910	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1915	0	1935	22	0
1	F	1899	0	1925	24	0
2	A	1	0	0	0	0
2	E	1	0	0	0	0
3	A	64	0	96	4	0
3	B	20	0	30	1	0
3	C	24	0	36	7	0
3	D	16	0	24	4	0
3	E	20	0	30	0	0
3	F	28	0	42	7	0
4	A	6	0	12	0	0
4	B	3	0	6	0	0
4	C	3	0	6	1	0
4	D	3	0	6	0	0
4	F	3	0	6	0	0
5	A	49	0	70	2	0
5	B	21	0	30	3	0
5	C	42	0	60	5	0
5	D	14	0	20	0	0
5	E	20	0	27	0	0
5	F	49	0	70	3	0
6	B	10	0	0	1	0
6	C	5	0	0	0	0
6	F	5	0	0	0	0
7	B	10	0	0	0	0
7	C	5	0	0	1	0
7	D	5	0	0	0	0
7	E	10	0	0	1	0
7	F	5	0	0	0	0
8	C	1	0	0	0	0
9	C	1	0	0	0	0
9	F	1	0	0	0	0
10	A	196	0	0	0	0
10	B	165	0	0	0	0
10	C	233	0	0	2	0
10	D	202	0	0	0	0
10	E	206	0	0	0	0
10	F	228	0	0	2	0
All	All	13160	0	12189	139	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 (139) 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:92:GLY:HA2	3:D:304:EDO:H12	1.69	0.75
1:F:196:MET:HG3	3:F:304:EDO:H12	1.69	0.75
1:F:188:ASP:HA	5:F:318:PEG:H42	1.70	0.74
1:C:227:ILE:HG12	3:C:310:EDO:H22	1.70	0.74
1:F:230:HIS:HB2	3:F:307:EDO:H21	1.68	0.73
1:B:250:LYS:HA	1:B:253:LYS:HD3	1.69	0.73
1:A:126[A]:GLU:OE2	1:F:178[A]:ARG:NH2	2.25	0.69
1:F:178[A]:ARG:NH1	10:F:525:HOH:O	2.21	0.68
1:C:177[A]:ARG:NH2	1:E:177:ARG:O	2.28	0.68
1:E:128:PRO:HB2	1:E:130[B]:VAL:HG13	1.75	0.67
1:C:196:MET:HG3	3:C:307:EDO:H11	1.76	0.66
1:A:177:ARG:O	1:E:177:ARG:NH2	2.28	0.66
1:F:165:GLN:HE22	3:F:304:EDO:H21	1.62	0.64
1:F:230:HIS:HB2	3:F:307:EDO:C2	2.27	0.64
1:C:169:ASP:HB2	3:C:310:EDO:H21	1.80	0.64
1:A:6:PHE:HA	5:A:323:PEG:H32	1.80	0.63
1:E:16:ASN:HB2	1:E:53:ARG:HD2	1.79	0.63
1:C:48:GLU:HB3	1:D:48:GLU:HB3	1.81	0.62
1:B:230:HIS:HA	1:B:233:LEU:HD12	1.81	0.62
1:F:37:MET:HG2	1:F:56:LEU:HD13	1.81	0.62
1:D:16:ASN:HB2	1:D:53:ARG:HD2	1.83	0.61
1:B:29:ARG:NH2	6:B:301:PO4:O2	2.36	0.58
1:E:48:GLU:HB3	1:F:48:GLU:HB3	1.85	0.58
1:F:185:GLU:HB2	3:F:310:EDO:H21	1.85	0.58
1:D:196:MET:HG3	3:D:305:EDO:H12	1.85	0.58
1:A:29[B]:ARG:NH1	1:A:237:GLU:OE1	2.37	0.57
1:F:230:HIS:HB2	3:F:307:EDO:C1	2.33	0.57
1:D:128:PRO:HB2	1:D:130[B]:VAL:HG13	1.85	0.57
1:A:48:GLU:HB3	1:B:48:GLU:HB3	1.88	0.56
3:A:308:EDO:H11	1:B:47:ARG:HH22	1.71	0.56
1:C:178:ARG:NH2	10:C:625:HOH:O	2.36	0.56
1:B:16:ASN:HB2	1:B:53:ARG:HD2	1.88	0.56
1:F:157:SER:HB3	1:F:199:ALA:HB2	1.88	0.55
1:A:154[A]:VAL:HG23	1:A:191:VAL:HA	1.88	0.55
1:C:195:GLU:HA	3:C:307:EDO:H22	1.89	0.54
1:A:103:VAL:HG21	1:A:228:PRO:HG3	1.90	0.54
5:C:316:PEG:H31	1:D:120:LEU:HD13	1.90	0.54
1:E:37:MET:HG2	1:E:56:LEU:HD13	1.89	0.54
1:A:16:ASN:HB2	1:A:53:ARG:HD2	1.90	0.54
1:C:157:SER:HB3	1:C:199:ALA:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ASP:OD1	1:B:249:ARG:NH1	2.42	0.52
1:C:239:ARG:NH1	7:C:304:SO4:O2	2.42	0.52
1:F:113:VAL:HB	1:F:156:ALA:HA	1.92	0.52
1:F:128:PRO:HB2	1:F:130[B]:VAL:HG13	1.92	0.52
1:F:124:PRO:HB2	1:F:126:GLU:OE1	2.10	0.52
1:A:157:SER:HB3	1:A:199:ALA:HB2	1.93	0.51
5:C:316:PEG:H12	1:D:120:LEU:HD22	1.93	0.51
1:B:157:SER:HB3	1:B:199:ALA:HB2	1.92	0.51
1:D:29:ARG:HG3	3:D:304:EDO:H21	1.92	0.50
1:D:157:SER:HB3	1:D:199:ALA:HB2	1.94	0.50
1:D:130[B]:VAL:HG11	1:E:111:GLY:HA3	1.93	0.50
3:D:303:EDO:H21	1:E:206:ALA:HB1	1.94	0.50
1:C:161:PHE:HD1	3:C:307:EDO:H12	1.76	0.49
1:F:249:ARG:NH1	10:F:559:HOH:O	2.44	0.49
1:E:26:ASP:HB3	1:E:29[B]:ARG:HD2	1.93	0.49
1:A:177:ARG:HE	3:A:303:EDO:H12	1.77	0.49
1:E:90:ARG:HG2	1:E:214[B]:CYS:SG	2.53	0.49
1:C:37:MET:HA	5:C:317:PEG:H42	1.95	0.49
1:B:196:MET:HG3	3:B:306:EDO:H22	1.94	0.48
1:A:188:ASP:O	1:E:174[B]:ARG:NH2	2.46	0.48
1:D:43:LEU:HD11	1:D:53:ARG:HB2	1.94	0.48
1:D:111:GLY:HA3	1:E:130[B]:VAL:HG11	1.95	0.48
1:E:157:SER:HB3	1:E:199:ALA:HB2	1.96	0.48
1:D:29:ARG:HD2	1:D:32:LYS:HD2	1.96	0.47
1:B:43:LEU:HD11	1:B:53:ARG:HB2	1.96	0.47
5:F:314:PEG:H41	5:F:314:PEG:H21	1.71	0.47
1:D:37:MET:HG2	1:D:56:LEU:HD13	1.97	0.47
1:F:90:ARG:NE	1:F:195:GLU:OE2	2.44	0.46
1:A:124:PRO:HB2	1:A:126[B]:GLU:OE2	2.16	0.46
1:A:91:VAL:HB	1:A:244:VAL:HG21	1.97	0.46
1:E:88:PHE:HE2	1:E:210:LEU:HG	1.81	0.46
1:A:128:PRO:HB2	1:A:130[A]:VAL:HG13	1.98	0.46
1:A:209:GLY:HA3	5:F:314:PEG:H32	1.98	0.46
1:B:178:ARG:NE	5:B:313:PEG:O1	2.32	0.45
1:B:4:THR:HG22	1:B:11:THR:HG22	1.98	0.45
1:E:108:VAL:HB	1:E:152:MET:SD	2.57	0.45
1:B:3:LYS:HE2	1:B:3:LYS:HB2	1.86	0.45
1:B:151:HIS:HA	5:B:311:PEG:H22	1.98	0.45
1:F:43:LEU:HD11	1:F:53:ARG:HB2	1.98	0.45
1:B:131:PRO:HD3	1:B:202:LEU:HD13	1.98	0.45
1:B:188:ASP:HB3	1:D:174:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:VAL:HG21	1:D:228:PRO:HG3	1.99	0.45
1:F:230:HIS:CG	1:F:230:HIS:O	2.69	0.45
1:C:227:ILE:CG1	3:C:310:EDO:H22	2.43	0.44
1:C:40:PRO:HD2	5:C:313:PEG:H22	1.99	0.44
1:E:109:THR:O	1:E:131:PRO:HG3	2.18	0.44
1:D:109:THR:O	1:D:131:PRO:HG3	2.17	0.44
1:E:166:GLU:HG2	1:E:168:TYR:CE2	2.52	0.44
1:B:109:THR:O	1:B:131:PRO:HG3	2.18	0.44
1:B:113:VAL:HB	1:B:156:ALA:HA	2.00	0.43
1:C:108:VAL:HB	1:C:152:MET:SD	2.58	0.43
1:C:44:ALA:HB1	1:C:46:HIS:CE1	2.53	0.43
1:E:15:LEU:HG	1:E:62:VAL:HG21	2.00	0.43
1:C:220:ILE:HD11	1:C:225:LYS:HG3	2.01	0.43
1:E:26:ASP:HA	1:E:27:PRO:HD2	1.85	0.43
1:F:211:LYS:HG2	3:F:306:EDO:H22	2.00	0.43
1:A:109:THR:O	1:A:131:PRO:HG3	2.19	0.43
1:D:101:VAL:O	1:D:221:ASN:ND2	2.51	0.43
1:F:23:ILE:HG13	1:F:90:ARG:HA	2.01	0.43
1:D:130[B]:VAL:HG12	1:E:130[B]:VAL:HG12	2.00	0.43
1:A:90:ARG:HB3	1:A:214[A]:CYS:HA	2.01	0.42
1:A:233:LEU:HB3	3:A:318:EDO:H21	2.01	0.42
1:B:178:ARG:HG2	5:B:313:PEG:H21	2.00	0.42
1:D:108:VAL:HB	1:D:152:MET:SD	2.60	0.42
1:A:26:ASP:HA	1:A:27:PRO:HD2	1.90	0.42
1:A:90:ARG:HB3	1:A:214[B]:CYS:HA	2.01	0.42
1:C:101:VAL:HG11	1:C:107:ILE:HD11	2.02	0.42
1:C:161:PHE:CD1	3:C:307:EDO:H12	2.54	0.42
1:C:180:GLN:NE2	10:C:558:HOH:O	2.44	0.42
1:C:103:VAL:HG21	4:C:311:EOH:H12	2.01	0.42
1:C:113:VAL:HB	1:C:156:ALA:HA	2.01	0.42
1:A:108:VAL:HB	1:A:152:MET:SD	2.60	0.42
1:B:241:ILE:HA	1:B:244:VAL:HG12	2.02	0.41
1:E:43:LEU:HD11	1:E:53:ARG:HB2	2.00	0.41
1:D:91:VAL:HB	1:D:244:VAL:HG21	2.01	0.41
1:D:234:LYS:HE2	1:D:234:LYS:HB3	1.90	0.41
1:B:101:VAL:O	1:B:221:ASN:ND2	2.52	0.41
1:D:103:VAL:HG13	1:D:219:ILE:HA	2.02	0.41
1:C:227:ILE:HA	1:C:228:PRO:HD3	1.92	0.41
1:C:90:ARG:HH21	1:C:195:GLU:CG	2.34	0.41
1:E:78:GLU:HG2	1:F:162:TYR:CD2	2.55	0.41
1:B:98:GLN:HA	1:B:99:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:GLU:CD	1:D:197:GLU:H	2.22	0.41
1:A:169:ASP:N	1:A:169:ASP:OD1	2.44	0.41
1:B:108:VAL:HB	1:B:152:MET:SD	2.61	0.41
1:D:132:ASP:OD1	1:D:211:LYS:HG3	2.21	0.41
1:C:39[A]:ASN:HA	5:C:313:PEG:H32	2.04	0.41
1:F:48:GLU:HG3	1:F:67:GLY:HA3	2.03	0.41
1:A:38:ASP:OD2	5:A:320:PEG:H11	2.22	0.40
1:B:227:ILE:HA	1:B:228:PRO:HD3	1.91	0.40
1:C:27:PRO:HD2	1:D:47:ARG:HA	2.03	0.40
1:A:15:LEU:HG	1:A:62:VAL:CG2	2.52	0.40
3:A:303:EDO:H22	7:E:303:SO4:O1	2.20	0.40
1:C:128:PRO:HB2	1:C:130[A]:VAL:HG13	2.02	0.40
1:C:41:VAL:HG11	1:C:53:ARG:NH2	2.37	0.40
1:C:109:THR:O	1:C:131:PRO:HG3	2.22	0.40
1:D:132:ASP:CG	1:D:211:LYS:HG3	2.42	0.40
1:F:66:THR:HB	1:F:73:THR:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	259/253 (102%)	251 (97%)	7 (3%)	1 (0%)	34 24
1	B	255/253 (101%)	249 (98%)	5 (2%)	1 (0%)	34 24
1	C	256/253 (101%)	249 (97%)	6 (2%)	1 (0%)	34 24
1	D	253/253 (100%)	249 (98%)	3 (1%)	1 (0%)	34 24
1	E	255/253 (101%)	247 (97%)	7 (3%)	1 (0%)	34 24
1	F	253/253 (100%)	250 (99%)	2 (1%)	1 (0%)	34 24
All	All	1531/1518 (101%)	1495 (98%)	30 (2%)	6 (0%)	34 24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	TYR
1	F	162	TYR
1	B	162	TYR
1	C	162	TYR
1	D	162	TYR
1	E	162	TYR

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	211/203 (104%)	208 (99%)	3 (1%)	67 63
1	B	207/203 (102%)	206 (100%)	1 (0%)	88 89
1	C	208/203 (102%)	205 (99%)	3 (1%)	67 63
1	D	205/203 (101%)	199 (97%)	6 (3%)	42 33
1	E	207/203 (102%)	204 (99%)	3 (1%)	67 63
1	F	205/203 (101%)	201 (98%)	4 (2%)	55 49
All	All	1243/1218 (102%)	1223 (98%)	20 (2%)	67 58

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	246[A]	GLU
1	A	246[B]	GLU
1	B	195	GLU
1	C	43	LEU
1	C	202	LEU
1	C	253	LYS
1	D	3	LYS
1	D	4	THR
1	D	62	VAL
1	D	159	ASP

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Mol	Chain	Res	Type
1	D	237	GLU
1	D	242	LYS
1	E	176	VAL
1	E	195	GLU
1	E	210	LEU
1	F	77[A]	VAL
1	F	77[B]	VAL
1	F	178[A]	ARG
1	F	178[B]	ARG

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

Mol	Chain	Res	Type
1	B	144	GLN
1	D	144	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 monosaccharides in this entry.

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

Of 93 ligands modelled in this entry, 5 are monoatomic - leaving 88 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
6	PO4	B	302	-	4,4,4	0.92	0	6,6,6	0.44	0
4	EOH	D	306	-	2,2,2	0.45	0	1,1,1	0.19	0
5	PEG	D	308	-	6,6,6	0.64	0	5,5,5	0.70	0
3	EDO	B	309	-	3,3,3	0.47	0	2,2,2	0.32	0
3	EDO	F	304	-	3,3,3	0.43	0	2,2,2	0.32	0
5	PEG	C	315	-	6,6,6	0.70	0	5,5,5	0.75	0
7	SO4	E	303	-	4,4,4	0.15	0	6,6,6	0.16	0
5	PEG	C	312	-	6,6,6	0.63	0	5,5,5	0.67	0
4	EOH	A	312	-	2,2,2	0.45	0	1,1,1	0.14	0
5	PEG	F	313	-	6,6,6	0.64	0	5,5,5	0.68	0
5	PEG	C	316	-	6,6,6	0.65	0	5,5,5	0.71	0
5	PEG	B	312	-	6,6,6	0.63	0	5,5,5	0.67	0
3	EDO	C	305	-	3,3,3	0.36	0	2,2,2	0.35	0
5	PEG	A	320	-	6,6,6	0.63	0	5,5,5	0.65	0
4	EOH	B	308	-	2,2,2	0.45	0	1,1,1	0.16	0
5	PEG	A	321	-	6,6,6	0.63	0	5,5,5	0.70	0
5	PEG	C	314	-	6,6,6	0.62	0	5,5,5	0.76	0
3	EDO	A	308	-	3,3,3	0.45	0	2,2,2	0.35	0
5	PEG	F	316	-	6,6,6	0.63	0	5,5,5	0.69	0
3	EDO	E	306	-	3,3,3	0.46	0	2,2,2	0.41	0
3	EDO	A	310	-	3,3,3	0.47	0	2,2,2	0.25	0
5	PEG	A	324	-	6,6,6	0.63	0	5,5,5	0.71	0
3	EDO	D	302	-	3,3,3	0.45	0	2,2,2	0.34	0
5	PEG	F	317	-	6,6,6	0.64	0	5,5,5	0.69	0
3	EDO	C	310	-	3,3,3	0.50	0	2,2,2	0.19	0
3	EDO	A	307	-	3,3,3	0.44	0	2,2,2	0.34	0
5	PEG	F	312	-	6,6,6	0.64	0	5,5,5	0.64	0
3	EDO	F	306	-	3,3,3	0.43	0	2,2,2	0.33	0
3	EDO	A	303	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	A	317	-	3,3,3	0.47	0	2,2,2	0.34	0
3	EDO	A	313	-	3,3,3	0.46	0	2,2,2	0.33	0
7	SO4	C	304	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	C	306	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	A	314	-	3,3,3	0.46	0	2,2,2	0.34	0
7	SO4	E	302	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	A	311	-	3,3,3	0.48	0	2,2,2	0.28	0
3	EDO	E	307	-	3,3,3	0.46	0	2,2,2	0.26	0
7	SO4	F	303	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	F	305	-	3,3,3	0.45	0	2,2,2	0.34	0
5	PEG	E	309	-	6,6,6	0.64	0	5,5,5	0.71	0
3	EDO	B	306	-	3,3,3	0.45	0	2,2,2	0.34	0
5	PEG	F	314	-	6,6,6	0.60	0	5,5,5	1.30	1 (20%)
5	PEG	C	313	-	6,6,6	0.64	0	5,5,5	0.65	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	B	305	-	3,3,3	0.46	0	2,2,2	0.36	0
7	SO4	B	304	-	4,4,4	0.14	0	6,6,6	0.06	0
5	PEG	B	311	-	6,6,6	0.64	0	5,5,5	0.68	0
3	EDO	B	307	-	3,3,3	0.46	0	2,2,2	0.34	0
3	EDO	E	304	-	3,3,3	0.45	0	2,2,2	0.36	0
4	EOH	C	311	-	2,2,2	0.45	0	1,1,1	0.12	0
3	EDO	A	306	-	3,3,3	0.44	0	2,2,2	0.37	0
3	EDO	A	309	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	B	310	-	3,3,3	0.45	0	2,2,2	0.33	0
5	PEG	A	325	-	6,6,6	0.64	0	5,5,5	0.71	0
3	EDO	A	318	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	F	309	-	3,3,3	0.48	0	2,2,2	0.31	0
5	PEG	F	318	-	6,6,6	0.57	0	5,5,5	0.83	0
3	EDO	A	316	-	3,3,3	0.46	0	2,2,2	0.33	0
6	PO4	C	301	-	4,4,4	0.94	0	6,6,6	0.48	0
3	EDO	D	305	-	3,3,3	0.47	0	2,2,2	0.32	0
3	EDO	E	305	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	F	310	-	3,3,3	0.46	0	2,2,2	0.31	0
3	EDO	A	315	-	3,3,3	0.46	0	2,2,2	0.32	0
6	PO4	F	301	-	4,4,4	0.95	0	6,6,6	0.49	0
7	SO4	D	301	-	4,4,4	0.13	0	6,6,6	0.06	0
5	PEG	B	313	-	6,6,6	0.63	0	5,5,5	0.71	0
4	EOH	A	319	-	2,2,2	0.45	0	1,1,1	0.17	0
3	EDO	A	304	-	3,3,3	0.48	0	2,2,2	0.25	0
3	EDO	E	308	-	3,3,3	0.47	0	2,2,2	0.30	0
5	PEG	C	317	-	6,6,6	0.64	0	5,5,5	0.68	0
6	PO4	B	301	-	4,4,4	0.88	0	6,6,6	0.44	0
3	EDO	C	308	-	3,3,3	0.43	0	2,2,2	0.36	0
5	PEG	A	323	-	6,6,6	0.62	0	5,5,5	0.68	0
3	EDO	A	305	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	A	302	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	F	308	-	3,3,3	0.52	0	2,2,2	0.15	0
5	PEG	F	315	-	6,6,6	0.62	0	5,5,5	0.69	0
4	EOH	F	311	-	2,2,2	0.45	0	1,1,1	0.19	0
3	EDO	D	304	-	3,3,3	0.47	0	2,2,2	0.28	0
5	PEG	D	307	-	6,6,6	0.63	0	5,5,5	0.75	0
5	PEG	A	322	-	6,6,6	0.60	0	5,5,5	0.68	0
3	EDO	D	303	-	3,3,3	0.44	0	2,2,2	0.31	0
3	EDO	C	307	-	3,3,3	0.44	0	2,2,2	0.32	0
5	PEG	E	310	-	5,5,6	0.57	0	4,4,5	0.90	0
7	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	C	309	-	3,3,3	0.46	0	2,2,2	0.32	0
5	PEG	E	311	-	6,6,6	0.65	0	5,5,5	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	A	326	-	6,6,6	0.63	0	5,5,5	0.73	0
3	EDO	F	307	-	3,3,3	0.45	0	2,2,2	0.30	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	E	308	-	-	0/1/1/1	-
5	PEG	B	311	-	-	2/4/4/4	-
3	EDO	A	307	-	-	1/1/1/1	-
5	PEG	F	312	-	-	1/4/4/4	-
5	PEG	C	317	-	-	4/4/4/4	-
3	EDO	F	306	-	-	1/1/1/1	-
3	EDO	A	303	-	-	0/1/1/1	-
3	EDO	B	307	-	-	0/1/1/1	-
3	EDO	A	317	-	-	0/1/1/1	-
3	EDO	B	309	-	-	0/1/1/1	-
3	EDO	F	304	-	-	1/1/1/1	-
5	PEG	C	315	-	-	4/4/4/4	-
5	PEG	D	308	-	-	2/4/4/4	-
3	EDO	E	304	-	-	1/1/1/1	-
3	EDO	C	308	-	-	0/1/1/1	-
3	EDO	A	306	-	-	0/1/1/1	-
3	EDO	A	309	-	-	0/1/1/1	-
5	PEG	A	323	-	-	2/4/4/4	-
3	EDO	A	313	-	-	0/1/1/1	-
5	PEG	C	312	-	-	1/4/4/4	-
3	EDO	A	305	-	-	0/1/1/1	-
3	EDO	B	310	-	-	0/1/1/1	-
5	PEG	A	325	-	-	2/4/4/4	-
3	EDO	C	306	-	-	0/1/1/1	-
3	EDO	A	314	-	-	0/1/1/1	-
3	EDO	A	318	-	-	0/1/1/1	-
3	EDO	F	309	-	-	1/1/1/1	-
5	PEG	B	312	-	-	4/4/4/4	-
3	EDO	C	305	-	-	0/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	F	308	-	-	0/1/1/1	-
5	PEG	C	316	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	F	313	-	-	1/4/4/4	-
5	PEG	F	315	-	-	2/4/4/4	-
3	EDO	A	316	-	-	0/1/1/1	-
5	PEG	A	320	-	-	0/4/4/4	-
3	EDO	D	304	-	-	0/1/1/1	-
5	PEG	A	321	-	-	2/4/4/4	-
5	PEG	D	307	-	-	2/4/4/4	-
5	PEG	A	322	-	-	0/4/4/4	-
3	EDO	D	303	-	-	0/1/1/1	-
3	EDO	D	305	-	-	0/1/1/1	-
5	PEG	C	314	-	-	2/4/4/4	-
3	EDO	A	308	-	-	1/1/1/1	-
3	EDO	A	311	-	-	0/1/1/1	-
3	EDO	E	305	-	-	1/1/1/1	-
3	EDO	E	306	-	-	0/1/1/1	-
3	EDO	A	310	-	-	0/1/1/1	-
3	EDO	A	304	-	-	0/1/1/1	-
3	EDO	E	307	-	-	0/1/1/1	-
3	EDO	C	307	-	-	0/1/1/1	-
3	EDO	F	310	-	-	1/1/1/1	-
5	PEG	A	324	-	-	2/4/4/4	-
5	PEG	E	310	-	-	1/3/3/4	-
5	PEG	F	316	-	-	0/4/4/4	-
3	EDO	F	305	-	-	0/1/1/1	-
5	PEG	F	318	-	-	3/4/4/4	-
3	EDO	A	315	-	-	0/1/1/1	-
5	PEG	E	309	-	-	3/4/4/4	-
3	EDO	B	306	-	-	0/1/1/1	-
5	PEG	B	313	-	-	3/4/4/4	-
3	EDO	C	309	-	-	0/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
5	PEG	E	311	-	-	0/4/4/4	-
5	PEG	A	326	-	-	1/4/4/4	-
5	PEG	C	313	-	-	2/4/4/4	-
5	PEG	F	314	-	-	4/4/4/4	-
5	PEG	F	317	-	-	2/4/4/4	-
3	EDO	F	307	-	-	0/1/1/1	-
3	EDO	B	305	-	-	0/1/1/1	-
3	EDO	C	310	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	314	PEG	C3-O2-C2	2.42	123.77	113.29

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	314	PEG	C4-C3-O2-C2
5	A	321	PEG	O1-C1-C2-O2
5	F	318	PEG	O1-C1-C2-O2
5	A	324	PEG	O2-C3-C4-O4
5	B	312	PEG	O1-C1-C2-O2
5	B	313	PEG	O1-C1-C2-O2
5	C	314	PEG	O1-C1-C2-O2
5	C	315	PEG	O1-C1-C2-O2
5	C	317	PEG	O2-C3-C4-O4
5	C	315	PEG	C4-C3-O2-C2
5	A	324	PEG	O1-C1-C2-O2
5	C	312	PEG	O2-C3-C4-O4
5	C	313	PEG	O2-C3-C4-O4
5	E	309	PEG	O1-C1-C2-O2
5	F	314	PEG	O1-C1-C2-O2
5	F	318	PEG	O2-C3-C4-O4
5	C	316	PEG	O1-C1-C2-O2
5	F	318	PEG	C1-C2-O2-C3
5	F	313	PEG	O2-C3-C4-O4
3	E	305	EDO	O1-C1-C2-O2
3	F	309	EDO	O1-C1-C2-O2
5	A	326	PEG	C1-C2-O2-C3
5	B	311	PEG	O2-C3-C4-O4
5	D	307	PEG	O2-C3-C4-O4
5	F	314	PEG	O2-C3-C4-O4
5	B	312	PEG	O2-C3-C4-O4
3	A	307	EDO	O1-C1-C2-O2
5	E	310	PEG	C1-C2-O2-C3
5	C	314	PEG	O2-C3-C4-O4
3	A	308	EDO	O1-C1-C2-O2
5	F	315	PEG	O2-C3-C4-O4
5	F	314	PEG	C1-C2-O2-C3
5	B	312	PEG	C4-C3-O2-C2
5	C	317	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
5	F	317	PEG	C4-C3-O2-C2
5	B	313	PEG	C4-C3-O2-C2
5	E	309	PEG	C4-C3-O2-C2
5	A	325	PEG	C1-C2-O2-C3
5	F	315	PEG	C4-C3-O2-C2
5	B	312	PEG	C1-C2-O2-C3
5	F	312	PEG	C1-C2-O2-C3
5	C	315	PEG	O2-C3-C4-O4
3	F	304	EDO	O1-C1-C2-O2
5	C	317	PEG	C1-C2-O2-C3
5	A	325	PEG	C4-C3-O2-C2
5	C	313	PEG	C1-C2-O2-C3
5	D	308	PEG	C1-C2-O2-C3
5	A	323	PEG	C1-C2-O2-C3
5	F	317	PEG	C1-C2-O2-C3
5	B	311	PEG	O1-C1-C2-O2
3	E	304	EDO	O1-C1-C2-O2
5	E	309	PEG	C1-C2-O2-C3
5	B	313	PEG	O2-C3-C4-O4
5	C	315	PEG	C1-C2-O2-C3
3	F	306	EDO	O1-C1-C2-O2
5	C	316	PEG	C4-C3-O2-C2
5	A	323	PEG	C4-C3-O2-C2
5	C	317	PEG	O1-C1-C2-O2
3	F	310	EDO	O1-C1-C2-O2
5	D	307	PEG	C4-C3-O2-C2
5	A	321	PEG	C1-C2-O2-C3
5	D	308	PEG	C4-C3-O2-C2

There are no ring outliers.

26 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	304	EDO	2	0
7	E	303	SO4	1	0
5	C	316	PEG	2	0
5	A	320	PEG	1	0
3	A	308	EDO	1	0
3	C	310	EDO	3	0
3	F	306	EDO	1	0
3	A	303	EDO	2	0
7	C	304	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	306	EDO	1	0
5	F	314	PEG	2	0
5	C	313	PEG	2	0
5	B	311	PEG	1	0
4	C	311	EOH	1	0
3	A	318	EDO	1	0
5	F	318	PEG	1	0
3	D	305	EDO	1	0
3	F	310	EDO	1	0
5	B	313	PEG	2	0
5	C	317	PEG	1	0
6	B	301	PO4	1	0
5	A	323	PEG	1	0
3	D	304	EDO	2	0
3	D	303	EDO	1	0
3	C	307	EDO	4	0
3	F	307	EDO	3	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	251/253 (99%)	-0.10	8 (3%) 47 50	4, 10, 27, 56	0
1	B	251/253 (99%)	0.13	18 (7%) 15 17	4, 11, 34, 59	0
1	C	251/253 (99%)	-0.28	3 (1%) 79 81	4, 8, 20, 54	0
1	D	250/253 (98%)	-0.10	9 (3%) 42 46	4, 9, 27, 53	0
1	E	251/253 (99%)	-0.31	2 (0%) 86 87	4, 9, 22, 57	0
1	F	250/253 (98%)	-0.29	1 (0%) 92 93	4, 7, 21, 40	0
All	All	1504/1518 (99%)	-0.16	41 (2%) 54 57	4, 9, 26, 59	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	THR	5.6
1	B	149	THR	5.4
1	E	253	LYS	5.4
1	B	147	GLY	5.2
1	B	231	ALA	4.9
1	C	253	LYS	4.7
1	D	230	HIS	4.7
1	A	253	LYS	4.3
1	D	231	ALA	4.1
1	B	229	ASP	4.1
1	B	230	HIS	4.0
1	B	148	ALA	3.7
1	D	229	ASP	3.7
1	B	234	LYS	3.7
1	B	236	THR	3.6
1	A	3	LYS	3.6
1	B	104	GLY	3.5
1	D	225	LYS	3.4
1	A	231	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	230	HIS	3.1
1	B	103	VAL	3.0
1	A	230	HIS	3.0
1	C	3	LYS	2.8
1	A	226	GLU	2.7
1	C	4	THR	2.7
1	B	4	THR	2.7
1	B	3	LYS	2.6
1	A	225	LYS	2.6
1	A	234	LYS	2.6
1	B	228	PRO	2.6
1	E	230	HIS	2.5
1	B	225	LYS	2.4
1	D	228	PRO	2.4
1	D	232	THR	2.4
1	D	234	LYS	2.4
1	B	253	LYS	2.2
1	B	146	SER	2.1
1	A	4	THR	2.1
1	D	227	ILE	2.1
1	D	235	GLU	2.0
1	B	105	ASP	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(Å <sup>2</sup> )	Q<0.9
5	PEG	C	317	7/7	0.24	0.49	46,55,61,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PEG	F	316	7/7	0.40	0.45	42,45,53,63	0
3	EDO	B	310	4/4	0.56	0.29	42,50,51,55	0
3	EDO	A	310	4/4	0.57	0.39	16,26,26,38	4
5	PEG	A	323	7/7	0.61	0.39	47,53,58,59	0
5	PEG	F	317	7/7	0.63	0.54	28,39,50,67	0
3	EDO	A	308	4/4	0.65	0.25	30,33,40,45	0
5	PEG	D	308	7/7	0.65	0.32	28,33,42,49	0
3	EDO	F	308	4/4	0.70	0.24	24,39,39,40	4
5	PEG	F	314	7/7	0.72	0.26	13,20,39,44	7
5	PEG	B	313	7/7	0.73	0.28	21,32,39,43	0
3	EDO	E	307	4/4	0.74	0.39	13,17,24,26	4
5	PEG	A	325	7/7	0.74	0.31	33,48,64,69	0
3	EDO	C	309	4/4	0.74	0.19	33,43,44,53	0
5	PEG	A	322	7/7	0.74	0.38	15,32,55,58	0
5	PEG	F	318	7/7	0.75	0.37	13,20,25,26	7
3	EDO	F	309	4/4	0.76	0.37	31,33,52,52	0
5	PEG	F	313	7/7	0.76	0.32	28,53,62,63	0
5	PEG	A	321	7/7	0.77	0.47	34,40,65,65	0
3	EDO	B	309	4/4	0.77	0.35	27,36,40,44	0
5	PEG	A	320	7/7	0.77	0.36	17,41,48,48	0
3	EDO	A	315	4/4	0.79	0.37	10,24,34,38	4
3	EDO	E	306	4/4	0.79	0.30	15,16,20,22	4
5	PEG	B	311	7/7	0.80	0.26	21,33,49,52	0
3	EDO	E	308	4/4	0.80	0.23	21,33,39,60	0
3	EDO	A	304	4/4	0.80	0.28	13,15,16,28	4
5	PEG	E	309	7/7	0.81	0.39	21,26,44,48	0
3	EDO	A	311	4/4	0.81	0.23	26,31,37,44	0
5	PEG	C	316	7/7	0.81	0.33	15,30,52,58	0
5	PEG	B	312	7/7	0.82	0.41	18,29,51,55	0
3	EDO	A	302	4/4	0.82	0.22	11,16,24,28	4
5	PEG	C	312	7/7	0.82	0.21	11,18,31,36	7
3	EDO	A	309	4/4	0.82	0.35	22,26,27,37	4
5	PEG	A	326	7/7	0.82	0.29	18,26,56,61	0
3	EDO	A	314	4/4	0.82	0.33	33,37,40,47	0
7	SO4	C	304	5/5	0.82	0.36	65,69,85,88	0
3	EDO	A	305	4/4	0.83	0.25	18,29,37,44	0
3	EDO	A	307	4/4	0.83	0.22	17,17,25,30	4
3	EDO	B	305	4/4	0.83	0.28	35,36,41,43	0
3	EDO	B	306	4/4	0.83	0.27	9,17,24,25	4
3	EDO	A	317	4/4	0.84	0.30	32,36,41,52	0
3	EDO	B	307	4/4	0.84	0.39	29,33,37,37	4
5	PEG	F	315	7/7	0.85	0.27	23,40,51,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PEG	E	310	6/7	0.85	0.17	15,28,34,36	0
5	PEG	E	311	7/7	0.85	0.51	17,50,70,73	0
3	EDO	A	318	4/4	0.85	0.24	34,36,38,48	0
3	EDO	C	307	4/4	0.85	0.23	9,25,27,31	4
5	PEG	F	312	7/7	0.86	0.28	21,28,46,48	0
5	PEG	C	314	7/7	0.86	0.28	15,31,37,42	0
3	EDO	C	310	4/4	0.87	0.37	23,26,33,38	0
3	EDO	E	304	4/4	0.87	0.21	8,11,15,17	4
5	PEG	D	307	7/7	0.87	0.20	25,31,44,45	0
3	EDO	F	305	4/4	0.87	0.19	2,10,25,26	0
3	EDO	C	308	4/4	0.87	0.21	10,10,11,16	4
4	EOH	A	319	3/3	0.88	0.24	26,26,36,44	0
4	EOH	D	306	3/3	0.88	0.20	23,23,26,30	0
3	EDO	F	304	4/4	0.88	0.20	11,24,24,31	0
3	EDO	F	306	4/4	0.88	0.22	13,13,17,18	4
7	SO4	E	303	5/5	0.88	0.42	42,44,66,85	0
4	EOH	A	312	3/3	0.89	0.29	21,21,24,35	0
7	SO4	B	304	5/5	0.89	0.30	41,48,77,79	0
3	EDO	C	306	4/4	0.89	0.22	10,15,22,27	4
3	EDO	A	303	4/4	0.89	0.13	20,21,24,24	0
5	PEG	C	315	7/7	0.90	0.21	15,24,37,37	7
3	EDO	D	302	4/4	0.90	0.16	26,28,35,53	0
5	PEG	A	324	7/7	0.91	0.26	25,37,48,50	0
5	PEG	C	313	7/7	0.91	0.23	22,22,33,44	0
4	EOH	F	311	3/3	0.91	0.41	34,34,36,42	0
3	EDO	D	303	4/4	0.91	0.21	8,10,12,33	4
6	PO4	B	302	5/5	0.91	0.33	42,43,63,68	0
3	EDO	D	304	4/4	0.91	0.19	17,18,32,41	0
4	EOH	B	308	3/3	0.91	0.24	19,19,22,30	0
3	EDO	D	305	4/4	0.91	0.16	7,23,32,34	0
3	EDO	E	305	4/4	0.92	0.18	3,9,12,38	4
4	EOH	C	311	3/3	0.92	0.17	16,16,25,36	0
3	EDO	F	307	4/4	0.92	0.19	21,22,26,43	0
3	EDO	A	316	4/4	0.92	0.25	23,23,37,44	0
3	EDO	A	306	4/4	0.93	0.21	13,16,18,19	4
7	SO4	E	302	5/5	0.93	0.19	38,46,58,58	0
3	EDO	A	313	4/4	0.93	0.22	14,19,21,23	4
3	EDO	C	305	4/4	0.94	0.25	4,5,6,8	4
7	SO4	D	301	5/5	0.94	0.19	22,23,43,47	0
7	SO4	F	303	5/5	0.94	0.21	20,24,32,33	0
3	EDO	F	310	4/4	0.95	0.20	17,25,28,29	0
6	PO4	B	301	5/5	0.96	0.10	14,17,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SO4	B	303	5/5	0.96	0.10	23,25,36,40	0
9	CL	F	302	1/1	0.98	0.07	15,15,15,15	0
6	PO4	F	301	5/5	0.99	0.07	5,5,8,8	0
2	NA	A	301	1/1	0.99	0.07	3,3,3,3	0
8	K	C	302	1/1	0.99	0.04	14,14,14,14	0
9	CL	C	303	1/1	0.99	0.05	13,13,13,13	0
6	PO4	C	301	5/5	0.99	0.07	4,4,6,7	0
2	NA	E	301	1/1	1.00	0.10	3,3,3,3	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.