Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:15 PM GMT

PDB ID	:	5CGM
Title	:	Structure of Mycobacterium thermoresistibile GlgE in complex with maltose at 1.95A resolution
Authors	:	Mendes, V.; Blaszczyk, M.; Maranha, A.; Empadinhas, N.; Blundell, T.L.
Deposited on	:	2015-07-09
Resolution	:	1.95 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
A user guide is available at
http://wwpdb.org/validation/2016/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:

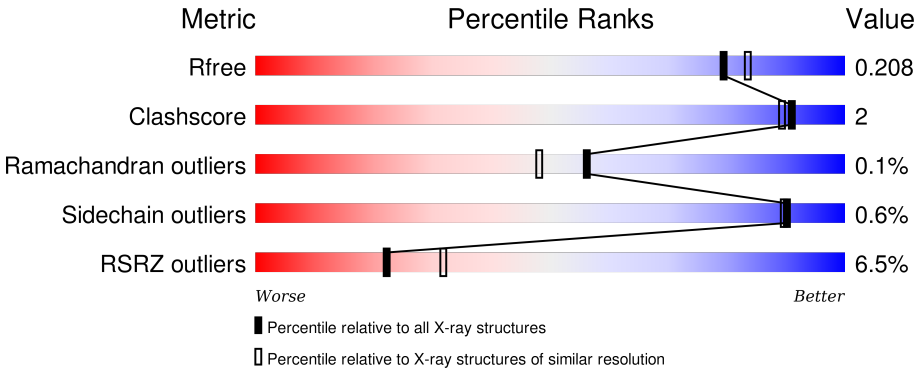
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 1.95 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	698	3% 91% 5%
1	B	698	9% 91%

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
10	EDO	A	725	-	-	-	X
10	EDO	A	727	-	-	-	X
10	EDO	A	729	-	-	-	X
10	EDO	A	731	-	-	-	X
10	EDO	B	717	-	-	-	X
10	EDO	B	718	-	-	-	X
4	NA	A	704	-	-	-	X
4	NA	A	710	-	-	-	X
4	NA	B	708	-	-	-	X
5	CL	A	715	-	-	-	X
5	CL	B	712	-	-	X	X
6	1PE	B	714	-	-	-	X
7	PGE	A	717	-	-	-	X
7	PGE	B	713	-	-	-	X
8	PG4	A	718	-	-	-	X
8	PG4	A	719	-	-	-	X
8	PG4	A	720	-	-	-	X
9	PEG	A	721	-	-	-	X
9	PEG	A	722	-	-	-	X
9	PEG	B	715	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 11643 atoms, of which 44 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.

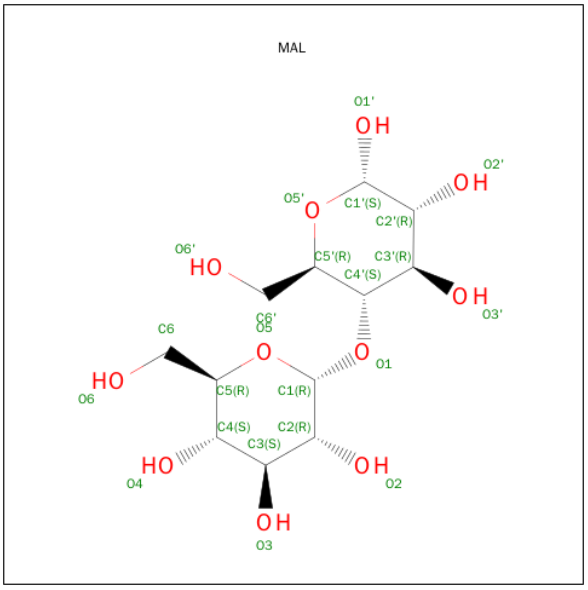
- Molecule 1 is a protein called Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	669	Total	C	N	O	S	0	6	0
			5232	3358	917	947	10			
1	B	667	Total	C	N	O	S	0	7	0
			5183	3337	898	939	9			

There are 6 discrepancies between the modelled and reference sequences:

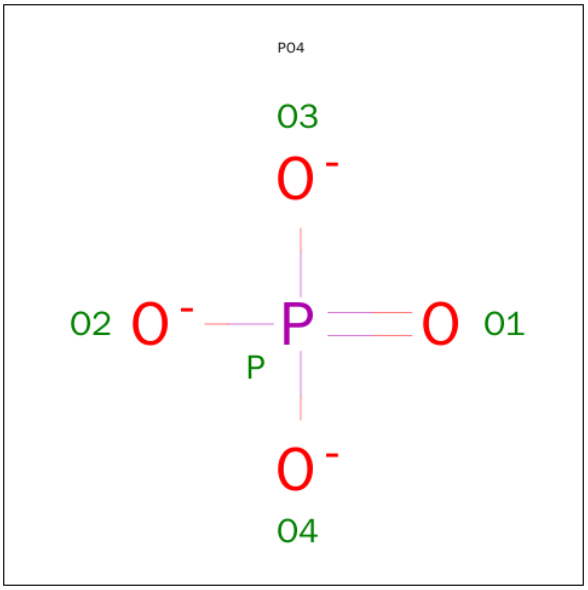
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP G7CL00
A	0	SER	-	expression tag	UNP G7CL00
A	1	VAL	-	cloning artifact	UNP G7CL00
B	-1	GLY	-	expression tag	UNP G7CL00
B	0	SER	-	expression tag	UNP G7CL00
B	1	VAL	-	cloning artifact	UNP G7CL00

- Molecule 2 is MALTOSE (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 45 12 22 11	0	0
2	B	1	Total C H O 45 12 22 11	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

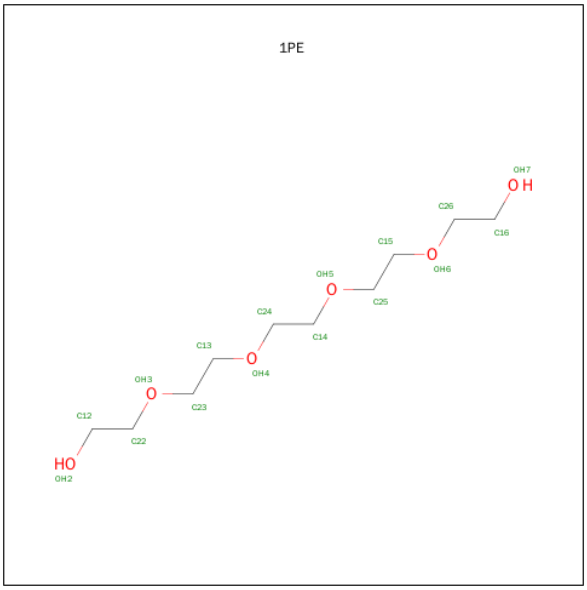
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	8	Total Na 8 8	0	0
4	A	11	Total Na 11 11	0	0

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

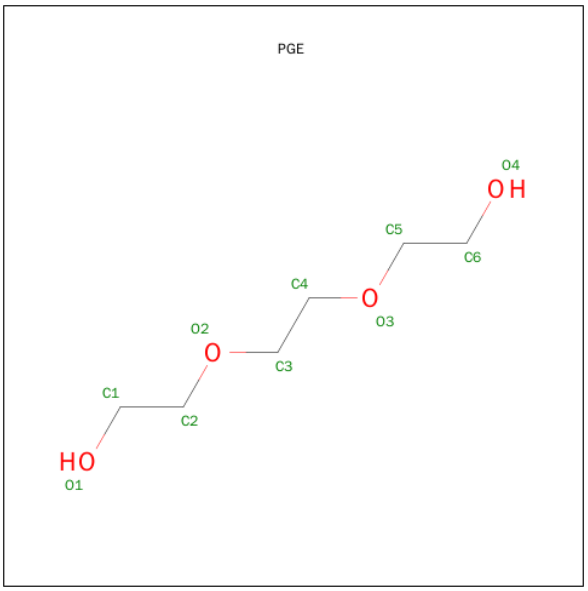
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



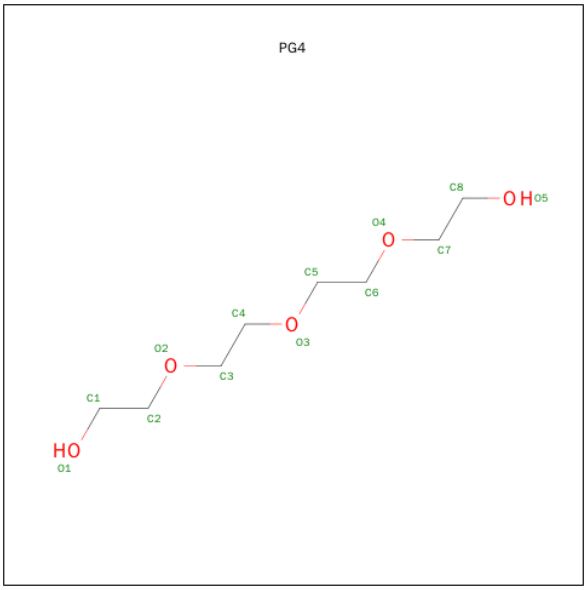
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 16 10 6	0	0
6	B	1	Total C O 16 10 6	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

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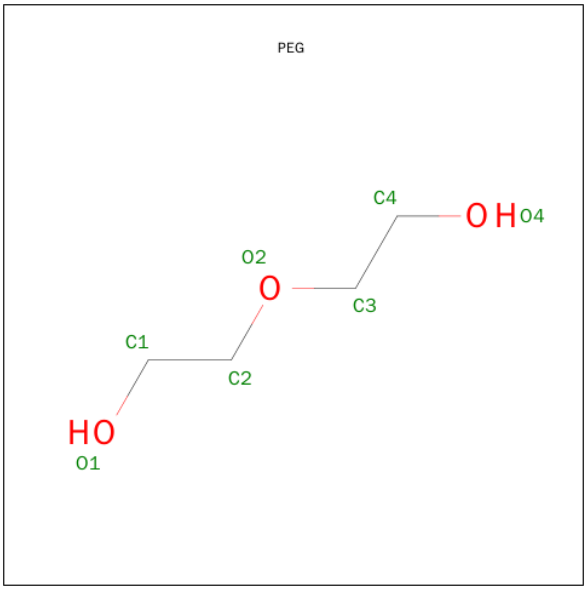
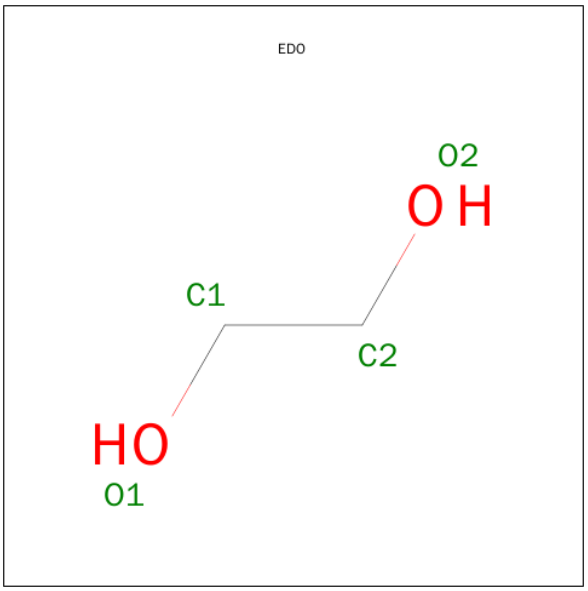
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 13 8 5	0	0

- 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 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	497	Total O 497 497	0	0

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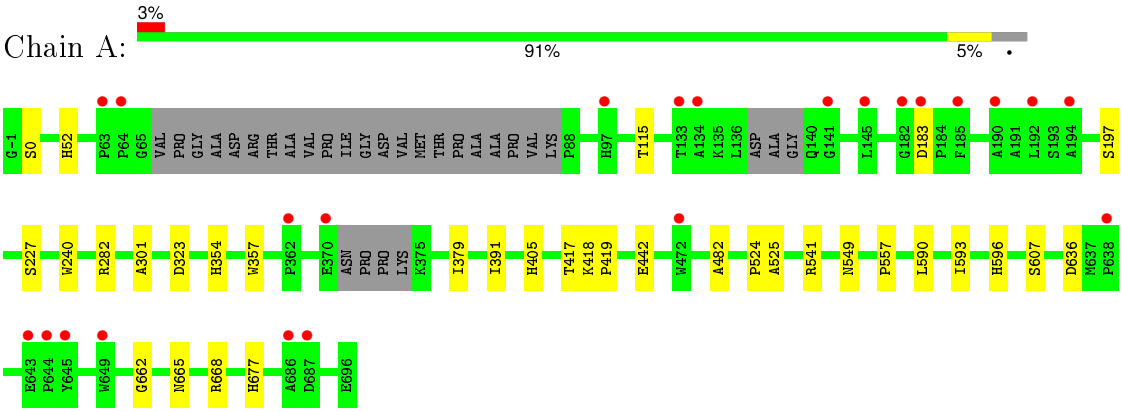
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	437	Total	O	0	0
			437	437		

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 errors 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.

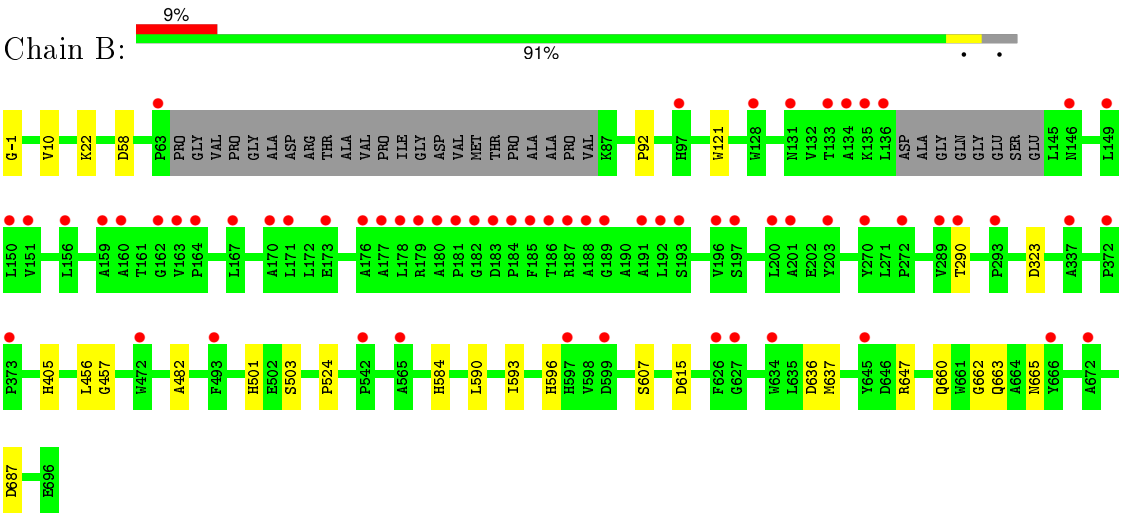
- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase

Chain A:



- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.33Å 113.90Å 220.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.66 – 1.95 37.74 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.66-1.95) 99.9 (37.74-1.95)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.175 , 0.203 0.179 , 0.208	Depositor DCC
R_{free} test set	7386 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 68.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 147570 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11643	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, CL, NA, PO4, EDO, 1PE, PG4, PEG, MAL

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	0.53	0/5408	0.62	0/7396
1	B	0.50	0/5364	0.62	0/7349
All	All	0.52	0/10772	0.62	0/14745

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5232	0	5020	23	0
1	B	5183	0	4947	20	0
2	A	23	22	21	1	0
2	B	23	22	21	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	11	0	0	0	0
4	B	8	0	0	0	0
5	A	1	0	0	1	0
5	B	1	0	0	2	0
6	A	16	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	16	0	22	0	0
7	A	10	0	14	2	0
7	B	10	0	14	0	0
8	A	39	0	54	3	0
9	A	21	0	30	0	0
9	B	7	0	10	0	0
10	A	32	0	48	4	0
10	B	12	0	18	6	0
11	A	497	0	0	3	0
11	B	437	0	0	1	0
All	All	11599	44	10240	46	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 2.

All (46) 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:662:GLY:H	1:A:665:ASN:HD21	1.18	0.91
1:B:662:GLY:H	1:B:665:ASN:HD21	1.19	0.87
1:B:22:LYS:O	10:B:717:EDO:H21	1.88	0.73
1:B:596:HIS:HD2	1:B:636:ASP:H	1.38	0.70
1:B:647:ARG:HE	1:B:660:GLN:HE21	1.38	0.70
1:A:596:HIS:HD2	1:A:636:ASP:H	1.38	0.68
1:B:456:LEU:O	5:B:712:CL:CL	2.49	0.68
1:A:323:ASP:OD1	1:A:405:HIS:HD2	1.85	0.59
1:A:282:ARG:HH12	8:A:720:PG4:H31	1.67	0.59
1:B:662:GLY:H	1:B:665:ASN:ND2	1.96	0.58
1:B:482:ALA:HB2	1:B:593[A]:ILE:HG22	1.86	0.58
1:A:596:HIS:CD2	1:A:636:ASP:H	2.19	0.57
1:A:482:ALA:HB2	1:A:593:ILE:HG22	1.89	0.55
1:B:596:HIS:CD2	1:B:636:ASP:H	2.22	0.54
1:B:92:PRO:HA	10:B:718:EDO:H21	1.89	0.54
1:A:549:ASN:HD22	8:A:719:PG4:H41	1.73	0.54
1:B:323:ASP:OD1	1:B:405:HIS:HD2	1.92	0.53
5:A:715:CL:CL	11:A:832:HOH:O	2.56	0.52
1:B:457:GLY:HA3	5:B:712:CL:CL	2.49	0.50
1:A:52:HIS:HE1	1:A:115:THR:OG1	1.97	0.47
1:A:677:HIS:HD2	11:A:822:HOH:O	1.95	0.47
1:A:662:GLY:H	1:A:665:ASN:ND2	2.00	0.46
1:B:-1:GLY:H2	1:B:10:VAL:H	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:HH22	8:A:720:PG4:H21	1.81	0.45
7:A:717:PGE:H22	11:A:1200:HOH:O	2.15	0.45
1:B:121:TRP:HZ2	10:B:718:EDO:H11	1.81	0.45
1:B:92:PRO:HA	10:B:718:EDO:C2	2.46	0.45
1:B:524:PRO:HG2	1:B:590:LEU:HG	1.98	0.44
1:B:596:HIS:HE1	1:B:607:SER:OG	2.01	0.43
1:A:442:GLU:OE1	2:A:701:MAL:O1'	2.36	0.43
1:B:637:MET:HG3	1:B:663:GLN:HG3	2.01	0.43
1:B:501:HIS:CD2	1:B:503:SER:H	2.36	0.43
1:A:301:ALA:HA	1:A:379:ILE:CG2	2.49	0.43
10:B:717:EDO:H12	11:B:878:HOH:O	2.19	0.43
1:A:417:THR:O	10:A:729:EDO:H12	2.18	0.43
1:B:584:HIS:HD2	1:B:615:ASP:OD1	2.01	0.43
1:A:596:HIS:HE1	1:A:607:SER:OG	2.03	0.42
1:A:418:LYS:HA	10:A:729:EDO:H21	2.00	0.42
1:A:354:HIS:CE1	10:A:728:EDO:H21	2.55	0.42
1:A:524:PRO:HG2	1:A:590:LEU:HG	2.01	0.42
1:A:419:PRO:HD3	10:A:729:EDO:H21	2.02	0.42
1:B:22:LYS:O	10:B:717:EDO:C2	2.62	0.41
1:A:240:TRP:CE2	1:A:557:PRO:HG2	2.56	0.41
1:A:668:ARG:H	7:A:717:PGE:H5	1.85	0.41
1:A:357:TRP:HB3	1:A:391:ILE:HD12	2.03	0.41
1:A:227:SER:O	1:A:525:ALA:HA	2.21	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	667/698 (96%)	654 (98%)	12 (2%)	1 (0%)	56 48
1	B	668/698 (96%)	655 (98%)	13 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1335/1396 (96%)	1309 (98%)	25 (2%)	1 (0%)	56 48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	SER

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	526/566 (93%)	523 (99%)	3 (1%)	90 89
1	B	517/566 (91%)	514 (99%)	3 (1%)	90 89
All	All	1043/1132 (92%)	1037 (99%)	6 (1%)	90 89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	ASP
1	A	197	SER
1	A	541	ARG
1	B	58	ASP
1	B	290	THR
1	B	687	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	147	ASN
1	A	405	HIS
1	A	578	ASN
1	A	596	HIS
1	A	665	ASN

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Mol	Chain	Res	Type
1	A	677	HIS
1	B	52	HIS
1	B	405	HIS
1	B	501	HIS
1	B	584	HIS
1	B	596	HIS
1	B	660	GLN
1	B	665	ASN
1	B	677	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 49 ligands modelled in this entry, 21 are monoatomic - leaving 28 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	MAL	A	701	4	24,24,24	1.31	3 (12%)	35,35,35	1.43	4 (11%)
3	PO4	A	702	-	4,4,4	0.97	0	6,6,6	0.24	0
3	PO4	A	703	-	4,4,4	0.72	0	6,6,6	0.23	0
6	1PE	A	716	4	15,15,15	0.52	0	14,14,14	0.39	0
7	PGE	A	717	-	9,9,9	0.54	0	8,8,8	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	PG4	A	718	-	12,12,12	0.53	0	11,11,11	0.39	0
8	PG4	A	719	-	12,12,12	0.56	0	11,11,11	0.41	0
8	PG4	A	720	-	12,12,12	0.54	0	11,11,11	0.33	0
9	PEG	A	721	-	6,6,6	0.53	0	5,5,5	0.36	0
9	PEG	A	722	-	6,6,6	0.48	0	5,5,5	0.53	0
9	PEG	A	723	-	6,6,6	0.51	0	5,5,5	0.53	0
10	EDO	A	724	-	3,3,3	0.45	0	2,2,2	0.45	0
10	EDO	A	725	-	3,3,3	0.44	0	2,2,2	0.39	0
10	EDO	A	726	-	3,3,3	0.43	0	2,2,2	0.46	0
10	EDO	A	727	-	3,3,3	0.45	0	2,2,2	0.60	0
10	EDO	A	728	-	3,3,3	0.46	0	2,2,2	0.36	0
10	EDO	A	729	-	3,3,3	0.43	0	2,2,2	0.61	0
10	EDO	A	730	-	3,3,3	0.45	0	2,2,2	0.52	0
10	EDO	A	731	-	3,3,3	0.45	0	2,2,2	0.57	0
2	MAL	B	701	-	24,24,24	1.34	3 (12%)	35,35,35	1.30	3 (8%)
3	PO4	B	702	-	4,4,4	1.22	0	6,6,6	0.25	0
3	PO4	B	703	-	4,4,4	0.98	0	6,6,6	0.23	0
7	PGE	B	713	-	9,9,9	0.51	0	8,8,8	0.81	0
6	1PE	B	714	-	15,15,15	0.55	0	14,14,14	0.36	0
9	PEG	B	715	-	6,6,6	0.51	0	5,5,5	0.40	0
10	EDO	B	716	-	3,3,3	0.42	0	2,2,2	0.48	0
10	EDO	B	717	-	3,3,3	0.40	0	2,2,2	0.37	0
10	EDO	B	718	-	3,3,3	0.45	0	2,2,2	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAL	A	701	4	-	0/8/48/48	0/2/2/2
3	PO4	A	702	-	-	0/0/0/0	0/0/0/0
3	PO4	A	703	-	-	0/0/0/0	0/0/0/0
6	1PE	A	716	4	-	0/13/13/13	0/0/0/0
7	PGE	A	717	-	-	0/7/7/7	0/0/0/0
8	PG4	A	718	-	-	0/10/10/10	0/0/0/0
8	PG4	A	719	-	-	0/10/10/10	0/0/0/0
8	PG4	A	720	-	-	0/10/10/10	0/0/0/0
9	PEG	A	721	-	-	0/4/4/4	0/0/0/0
9	PEG	A	722	-	-	0/4/4/4	0/0/0/0
9	PEG	A	723	-	-	0/4/4/4	0/0/0/0
10	EDO	A	724	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EDO	A	725	-	-	0/1/1/1	0/0/0/0
10	EDO	A	726	-	-	0/1/1/1	0/0/0/0
10	EDO	A	727	-	-	0/1/1/1	0/0/0/0
10	EDO	A	728	-	-	0/1/1/1	0/0/0/0
10	EDO	A	729	-	-	0/1/1/1	0/0/0/0
10	EDO	A	730	-	-	0/1/1/1	0/0/0/0
10	EDO	A	731	-	-	0/1/1/1	0/0/0/0
2	MAL	B	701	-	-	0/8/48/48	0/2/2/2
3	PO4	B	702	-	-	0/0/0/0	0/0/0/0
3	PO4	B	703	-	-	0/0/0/0	0/0/0/0
7	PGE	B	713	-	-	0/7/7/7	0/0/0/0
6	1PE	B	714	-	-	0/13/13/13	0/0/0/0
9	PEG	B	715	-	-	0/4/4/4	0/0/0/0
10	EDO	B	716	-	-	0/1/1/1	0/0/0/0
10	EDO	B	717	-	-	0/1/1/1	0/0/0/0
10	EDO	B	718	-	-	0/1/1/1	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	MAL	O5-C5	2.01	1.49	1.44
2	A	701	MAL	O5-C5	2.27	1.50	1.44
2	A	701	MAL	O5-C1	2.29	1.47	1.41
2	B	701	MAL	O5-C1	2.55	1.48	1.41
2	A	701	MAL	O5'-C1'	4.11	1.51	1.43
2	B	701	MAL	O5'-C1'	4.44	1.51	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	MAL	O5'-C5'-C4'	2.04	114.12	109.78
2	B	701	MAL	C1'-C2'-C3'	2.14	114.19	110.68
2	A	701	MAL	C1'-C2'-C3'	2.41	114.64	110.68
2	A	701	MAL	C1'-O5'-C5'	2.85	119.00	113.54
2	B	701	MAL	C1'-O5'-C5'	3.30	119.85	113.54
2	B	701	MAL	O5'-C1'-C2'	5.01	118.78	110.00
2	A	701	MAL	O5'-C1'-C2'	5.29	119.27	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	MAL	1	0
7	A	717	PGE	2	0
8	A	719	PG4	1	0
8	A	720	PG4	2	0
10	A	728	EDO	1	0
10	A	729	EDO	3	0
10	B	717	EDO	3	0
10	B	718	EDO	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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^2)	Q<0.9
1	A	669/698 (95%)	0.07	23 (3%)	49	60	14, 26, 52, 88	0
1	B	667/698 (95%)	0.38	64 (9%)	10	16	18, 30, 59, 88	0
All	All	1336/1396 (95%)	0.22	87 (6%)	22	32	14, 28, 56, 88	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	LEU	7.6
1	B	180	ALA	6.7
1	B	134	ALA	6.5
1	B	185	PHE	6.4
1	A	645	TYR	6.1
1	B	188	ALA	6.0
1	B	178	LEU	5.9
1	B	200	LEU	5.4
1	B	183	ASP	5.4
1	B	184	PRO	5.3
1	B	171	LEU	5.0
1	A	194	ALA	4.9
1	B	181	PRO	4.8
1	B	150	LEU	4.8
1	B	189	GLY	4.6
1	B	170	ALA	4.5
1	B	626	PHE	4.4
1	B	634	TRP	4.4
1	B	182	GLY	4.3
1	B	472	TRP	4.3
1	B	97	HIS	4.2
1	B	160	ALA	4.2
1	B	128	TRP	4.2
1	B	191	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	203	TYR	4.1
1	A	134	ALA	4.1
1	B	136	LEU	4.0
1	B	164	PRO	3.9
1	B	186	THR	3.9
1	B	133	THR	3.9
1	B	187	ARG	3.6
1	B	63	PRO	3.5
1	B	179	ARG	3.5
1	B	167	LEU	3.4
1	B	177	ALA	3.3
1	B	159	ALA	3.3
1	B	193	SER	3.3
1	A	183	ASP	3.3
1	B	666	TYR	3.2
1	A	133	THR	3.2
1	B	149	LEU	3.1
1	B	293	PRO	3.1
1	B	289	VAL	3.1
1	B	135	LYS	3.0
1	A	649	TRP	3.0
1	B	197	SER	3.0
1	B	131	ASN	3.0
1	A	472	TRP	3.0
1	B	373	PRO	3.0
1	B	196	VAL	3.0
1	A	192	LEU	3.0
1	B	201	ALA	2.9
1	B	372	PRO	2.9
1	B	627	GLY	2.9
1	A	687	ASP	2.7
1	A	185	PHE	2.6
1	B	645	TYR	2.6
1	B	565	ALA	2.6
1	A	141	GLY	2.6
1	B	156	LEU	2.6
1	A	190	ALA	2.6
1	B	146	ASN	2.6
1	A	638	PRO	2.6
1	B	151	VAL	2.5
1	A	63	PRO	2.5
1	A	182	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	290	THR	2.4
1	A	64	PRO	2.4
1	A	97	HIS	2.4
1	B	173	GLU	2.4
1	B	542	PRO	2.3
1	B	270	TYR	2.3
1	B	162	GLY	2.3
1	A	362	PRO	2.2
1	A	644	PRO	2.2
1	B	337	ALA	2.1
1	A	686	ALA	2.1
1	A	643	GLU	2.1
1	B	597	HIS	2.1
1	B	599	ASP	2.1
1	A	145	LEU	2.1
1	B	493	PHE	2.1
1	B	176	ALA	2.1
1	A	370	GLU	2.1
1	B	672	ALA	2.1
1	B	272	PRO	2.0
1	B	163	VAL	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
7	PGE	A	717	10/10	0.52	0.30	15.43	54,62,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	EDO	A	727	4/4	0.90	0.27	12.67	59,61,62,63	0
9	PEG	B	715	7/7	0.68	0.33	11.57	51,57,59,59	0
4	NA	B	708	1/1	0.97	0.16	10.08	31,31,31,31	0
8	PG4	A	720	13/13	0.71	0.33	9.77	42,61,67,68	0
8	PG4	A	718	13/13	0.61	0.37	5.52	59,65,69,69	0
10	EDO	A	725	4/4	0.71	0.20	5.45	52,53,53,54	0
10	EDO	B	718	4/4	0.82	0.34	5.42	42,43,45,46	0
5	CL	B	712	1/1	0.98	0.17	4.69	53,53,53,53	0
10	EDO	A	729	4/4	0.92	0.23	4.20	59,59,59,59	0
7	PGE	B	713	10/10	0.91	0.15	3.95	40,42,49,53	0
4	NA	A	710	1/1	0.98	0.21	3.74	37,37,37,37	0
8	PG4	A	719	13/13	0.89	0.17	3.32	43,50,59,60	0
9	PEG	A	721	7/7	0.91	0.14	3.29	54,55,57,60	0
4	NA	A	704	1/1	0.87	0.14	2.87	40,40,40,40	0
6	1PE	B	714	16/16	0.87	0.15	2.77	43,52,58,61	0
10	EDO	A	731	4/4	0.70	0.20	2.70	53,56,58,61	0
10	EDO	B	717	4/4	0.93	0.20	2.50	56,58,59,59	0
5	CL	A	715	1/1	0.98	0.18	2.43	51,51,51,51	0
9	PEG	A	722	7/7	0.92	0.21	2.03	42,45,46,47	0
4	NA	A	712	1/1	0.93	0.12	1.95	47,47,47,47	0
4	NA	B	707	1/1	0.93	0.16	1.83	39,39,39,39	0
4	NA	A	714	1/1	0.97	0.12	1.30	50,50,50,50	0
9	PEG	A	723	7/7	0.83	0.14	1.26	59,62,65,66	0
3	PO4	A	702	5/5	0.96	0.20	1.13	45,51,51,52	0
4	NA	B	704	1/1	0.98	0.14	1.03	21,21,21,21	0
3	PO4	B	703	5/5	0.91	0.16	0.97	54,59,61,63	0
3	PO4	B	702	5/5	0.96	0.24	0.87	47,49,50,50	0
4	NA	A	705	1/1	0.99	0.14	0.86	19,19,19,19	0
10	EDO	A	730	4/4	0.92	0.10	0.80	53,54,55,57	0
4	NA	A	706	1/1	0.97	0.12	0.80	33,33,33,33	0
4	NA	B	710	1/1	0.95	0.11	0.77	45,45,45,45	0
4	NA	B	706	1/1	0.92	0.10	0.64	47,47,47,47	0
4	NA	A	709	1/1	0.95	0.16	0.59	39,39,39,39	0
6	1PE	A	716	16/16	0.96	0.10	0.30	20,27,49,54	0
4	NA	B	709	1/1	0.94	0.12	-0.25	37,37,37,37	0
4	NA	A	707	1/1	0.98	0.08	-0.32	41,41,41,41	0
4	NA	B	705	1/1	0.92	0.08	-0.56	40,40,40,40	0
2	MAL	B	701	23/23	0.95	0.09	-0.96	24,28,38,42	0
2	MAL	A	701	23/23	0.96	0.08	-1.20	20,23,37,42	0
4	NA	A	711	1/1	0.98	0.08	-1.40	38,38,38,38	0
4	NA	B	711	1/1	0.99	0.13	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	EDO	A	728	4/4	0.66	0.33	-	50,54,56,57	0
3	PO4	A	703	5/5	0.91	0.20	-	66,68,69,70	0
10	EDO	B	716	4/4	0.81	0.20	-	45,49,52,55	0
4	NA	A	713	1/1	0.98	0.05	-	22,22,22,22	0
4	NA	A	708	1/1	0.97	0.07	-	42,42,42,42	0
10	EDO	A	724	4/4	0.78	0.15	-	62,63,63,64	0
10	EDO	A	726	4/4	0.83	0.13	-	42,44,47,49	0

6.5 Other polymers

There are no such residues in this entry.