Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 10:49 PM EDT

PDB ID	:	4LHC
Title	:	Crystal structure of Synechocystis sp. PCC 6803 glycine decarboxylase (P-protein), holo form with pyridoxal-5'-phosphate and glycine
Authors	:	Hasse, D.; Andersson, E.; Carlsson, G.; Masloboy, A.; Hagemann, M.; Bauwe, H.; Andersson, I.
Deposited on	:	2013-07-01
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

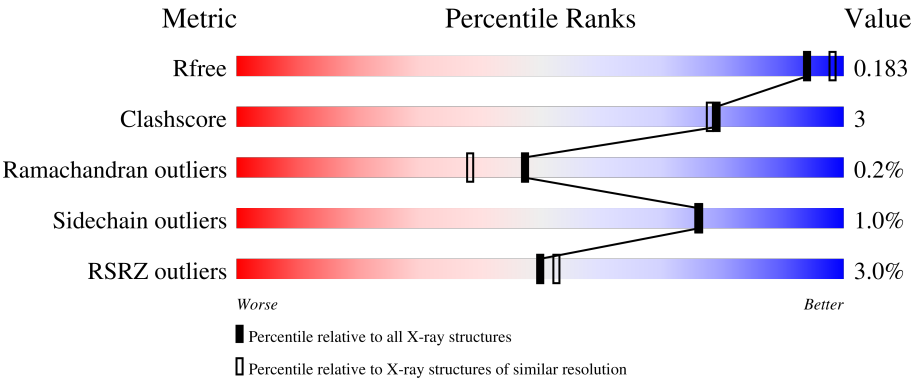
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	983	2% 90% 5% .
1	B	983	4% 89% 7% .

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
2	GLY	A	1002	-	X	-	-
2	GLY	A	1003	-	X	-	-
2	GLY	A	1004	-	X	-	-
2	GLY	B	1001	-	X	-	-
6	BCN	A	1017	-	-	X	-

2 Entry composition

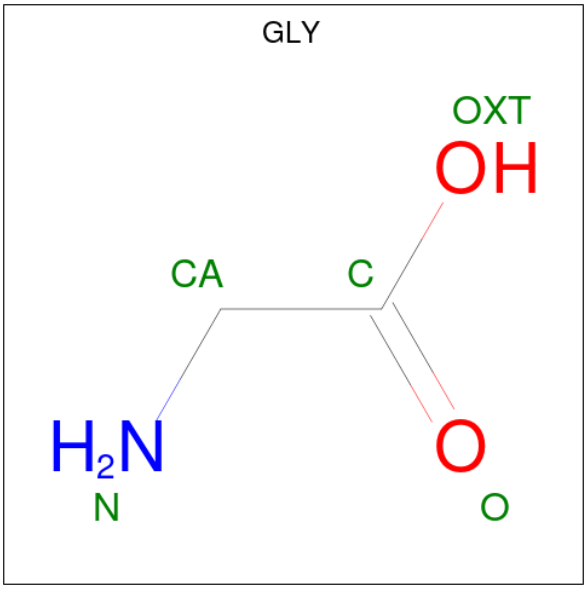
There are 7 unique types of molecules in this entry. The entry contains 16238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycine dehydrogenase [decarboxylating].

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	942	Total	C	N	O	P	S	0	18	0
			7355	4676	1243	1390	1	45			
1	B	942	Total	C	N	O	P	S	0	17	0
			7347	4672	1238	1392	1	44			

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		

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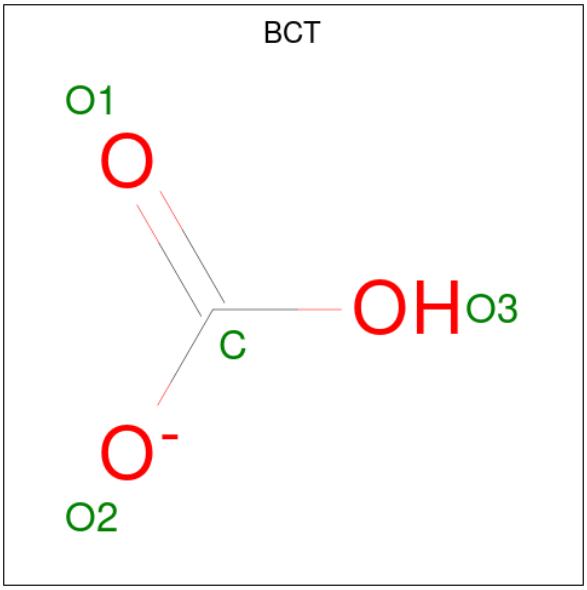
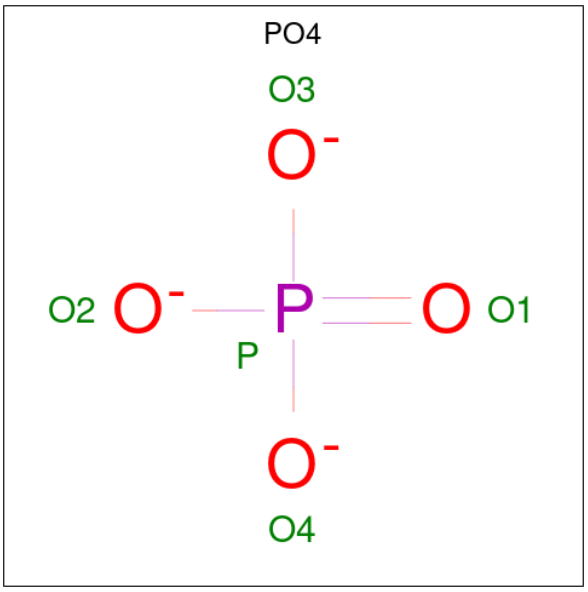
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 5 2 1 2	0	0

- Molecule 3 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



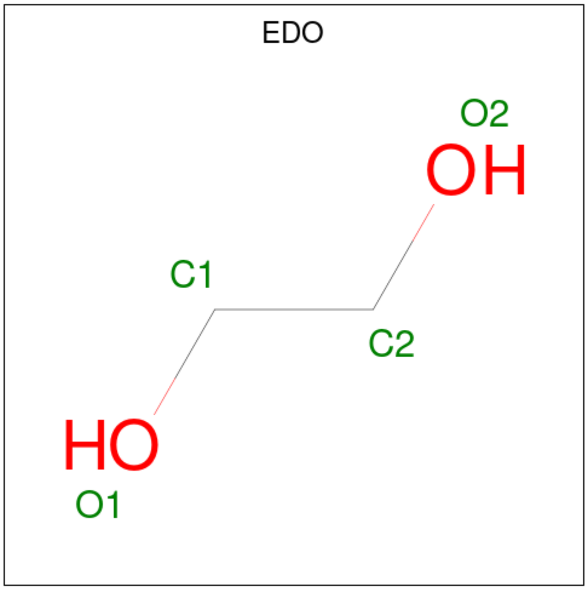
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 1 3	0	0
3	A	1	Total C O 4 1 3	0	0
3	B	1	Total C O 4 1 3	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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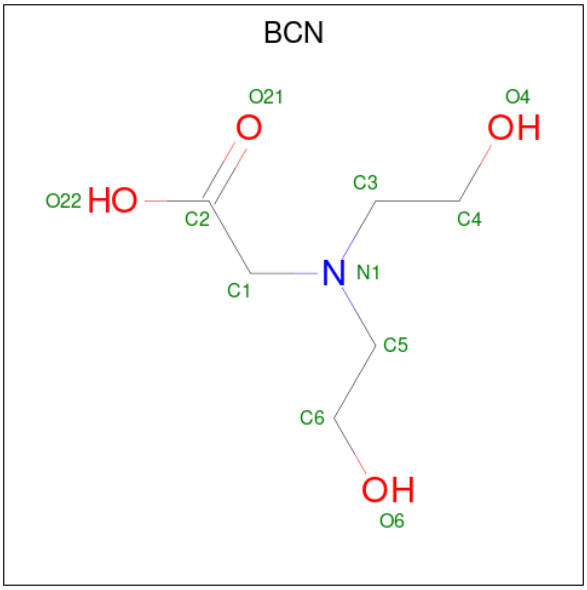
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is BICINE (three-letter code: BCN) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 11 6 1 4	0	0

- Molecule 7 is water.

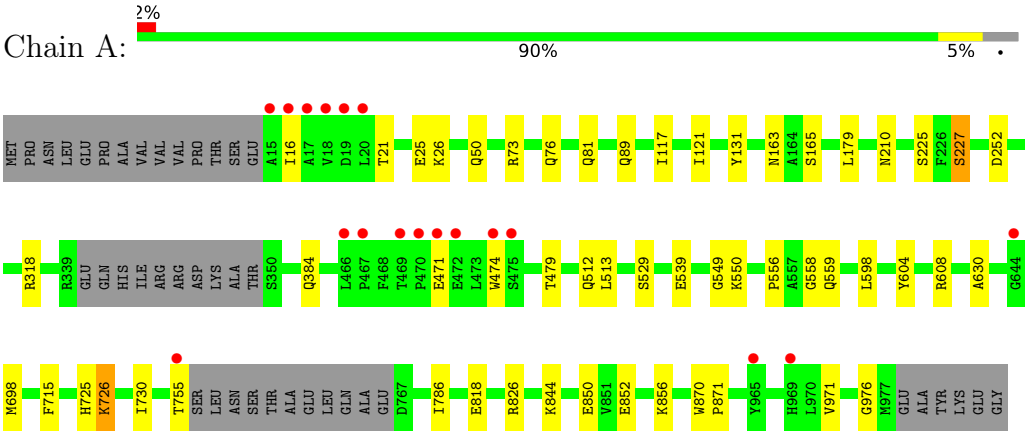
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	705	Total O 705 705	0	0
7	B	689	Total O 689 689	0	0

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.

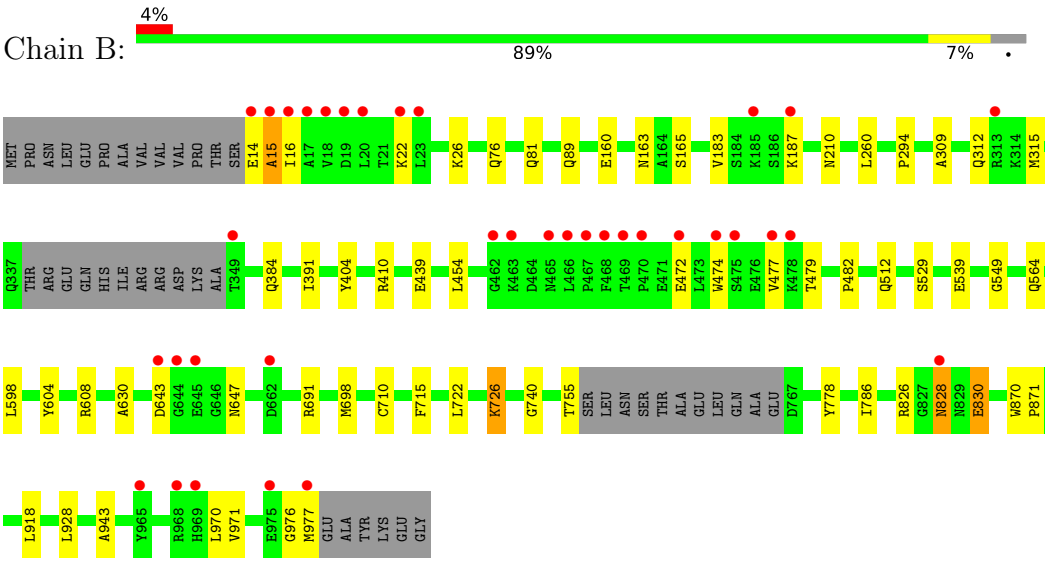
• Molecule 1: Glycine dehydrogenase [decarboxylating]

Chain A:



• Molecule 1: Glycine dehydrogenase [decarboxylating]

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	160.05Å 160.05Å 159.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.78 – 1.90 49.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.78-1.90) 99.9 (49.78-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.13 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.155 , 0.186 0.153 , 0.183	Depositor DCC
R_{free} test set	9313 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16238	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: BCT, PO4, EDO, LLP, BCN

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	0.34	0/7533	0.51	0/10245
1	B	0.35	0/7526	0.51	0/10236
All	All	0.35	0/15059	0.51	0/20481

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	7355	0	7220	39	0
1	B	7347	0	7211	43	0
2	A	20	0	8	1	0
2	B	5	0	2	1	0
3	A	8	0	0	0	0
3	B	4	0	0	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	28	0	42	5	0
5	B	36	0	54	7	0
6	A	11	0	12	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	705	0	0	5	0
7	B	689	0	0	6	0
All	All	16238	0	14549	83	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 3.

All (83) 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:559:GLN:HE21	6:A:1017:BCN:H41	1.42	0.83
1:A:210[B]:ASN:ND2	7:A:1637:HOH:O	2.24	0.71
1:A:384:GLN:HG2	1:A:479:THR:HG21	1.77	0.66
1:B:210[B]:ASN:ND2	7:B:1634:HOH:O	2.31	0.63
1:A:16:ILE:HD11	1:B:454:LEU:HD21	1.81	0.63
1:A:818:GLU:OE2	1:A:826:ARG:NH2	2.32	0.62
1:A:549:GLY:HA3	5:A:1011:EDO:H21	1.82	0.61
1:A:604:TYR:CZ	1:A:608[A]:ARG:HD2	2.34	0.61
1:B:971:VAL:HG11	1:B:976:GLY:HA3	1.83	0.61
2:A:1004:GLY:N	7:A:1576:HOH:O	2.34	0.59
1:B:698[B]:MET:HE1	1:B:715:PHE:CZ	2.37	0.59
1:A:73:ARG:HH22	5:A:1013:EDO:H11	1.66	0.59
1:B:755:THR:H	5:B:1011:EDO:H21	1.68	0.59
1:B:14:GLU:HA	1:B:16:ILE:N	2.19	0.57
1:A:252:ASP:OD1	5:A:1014:EDO:H11	2.05	0.57
1:A:471:GLU:HG3	1:B:22:LYS:HB2	1.88	0.56
1:A:550:LYS:HG2	5:A:1011:EDO:H11	1.87	0.56
1:A:870:TRP:CD1	1:A:871:PRO:HA	2.43	0.53
1:B:726:LLP:O3	1:B:726:LLP:NZ	2.41	0.53
1:A:558:GLY:HA3	6:A:1017:BCN:H51	1.91	0.53
1:A:726:LLP:NZ	1:A:726:LLP:O3	2.41	0.53
1:B:81:GLN:NE2	1:B:89:GLN:OE1	2.29	0.51
1:B:294:PRO:HB3	5:B:1006:EDO:H21	1.92	0.51
1:A:294:PRO:HB3	5:A:1011:EDO:H22	1.92	0.51
1:B:512[A]:GLN:HG3	7:B:1367:HOH:O	2.10	0.51
1:B:604:TYR:CZ	1:B:608:ARG:HD2	2.46	0.51
1:B:474:TRP:O	1:B:477:VAL:HG22	2.11	0.50
2:B:1001:GLY:N	7:B:1513:HOH:O	2.45	0.50
1:A:698[B]:MET:HE1	1:A:715:PHE:CZ	2.47	0.50
1:A:179:LEU:HD22	1:A:283:ILE:HD11	1.94	0.49
1:B:870:TRP:CG	1:B:871:PRO:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:870:TRP:CD1	1:B:871:PRO:HA	2.48	0.49
1:A:26:LYS:HB3	1:B:474:TRP:CE2	2.48	0.49
1:B:163:ASN:HB3	1:B:315:MET:HE3	1.95	0.48
1:A:852[B]:GLU:O	1:A:856:LYS:HG2	2.13	0.48
1:A:556:PRO:HB3	6:A:1017:BCN:H62	1.96	0.48
1:A:844:LYS:NZ	1:A:850:GLU:OE2	2.45	0.47
1:A:512[A]:GLN:HG3	7:A:1494:HOH:O	2.14	0.47
1:B:549:GLY:HA3	5:B:1006:EDO:H11	1.96	0.47
1:A:598:LEU:HD13	1:A:630:ALA:HA	1.97	0.47
1:B:571:GLU:OE2	5:B:1013:EDO:H21	2.15	0.47
1:A:315:MET:HE2	1:A:315:MET:HB3	1.88	0.46
5:B:1011:EDO:H22	7:B:1678:HOH:O	2.16	0.46
1:A:512[B]:GLN:HG3	1:A:513:LEU:N	2.30	0.46
1:A:539:GLU:HB3	1:A:786:ILE:HG23	1.97	0.46
1:A:726:LLP:H4'1	7:A:1698:HOH:O	2.15	0.45
1:B:14:GLU:N	1:B:15:ALA:HB3	2.31	0.45
1:A:21:THR:O	1:A:25:GLU:HG3	2.15	0.45
1:B:404:TYR:CE1	1:B:482:PRO:HD3	2.52	0.45
1:B:691:ARG:NH1	7:B:1557:HOH:O	2.49	0.45
1:B:722:LEU:O	1:B:740:GLY:HA2	2.16	0.45
1:A:971:VAL:HG11	1:A:976:GLY:HA3	1.99	0.44
1:B:598:LEU:HD13	1:B:630:ALA:HA	1.99	0.44
1:B:826:ARG:HD2	1:B:830:GLU:HG3	1.99	0.44
1:A:870:TRP:CG	1:A:871:PRO:HA	2.53	0.44
1:B:384:GLN:HG2	1:B:479:THR:HG21	1.99	0.44
1:A:163:ASN:HB2	1:A:318:ARG:O	2.17	0.44
1:A:559:GLN:NE2	6:A:1017:BCN:H41	2.20	0.44
1:B:643:ASP:OD2	1:B:647:ASN:N	2.51	0.44
1:B:183:VAL:HG21	1:B:260:LEU:HD11	1.99	0.43
6:A:1017:BCN:H42	6:A:1017:BCN:H12	1.67	0.43
1:B:160:GLU:OE1	1:B:309:ALA:N	2.28	0.43
1:A:81:GLN:NE2	1:A:89:GLN:OE1	2.36	0.43
1:A:725:HIS:HA	1:A:730:ILE:HB	2.02	0.42
6:A:1017:BCN:O4	7:A:1729:HOH:O	2.22	0.42
1:B:410:ARG:NH2	1:B:439:GLU:OE1	2.53	0.42
1:B:564[B]:GLN:HG2	7:B:1448:HOH:O	2.18	0.42
1:B:828:ASN:OD1	1:B:828:ASN:N	2.52	0.42
1:A:559:GLN:HE21	6:A:1017:BCN:C4	2.22	0.42
1:B:336:LEU:HD11	1:B:970:LEU:HD22	2.01	0.42
1:B:539:GLU:HB3	1:B:786:ILE:HG23	2.01	0.42
1:B:710:CYS:HA	5:B:1012:EDO:H22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:HG23	1:A:121:ILE:HD12	2.01	0.41
1:A:225:SER:OG	1:A:227:SER:HB3	2.19	0.41
1:A:474:TRP:CE2	1:B:26:LYS:HB3	2.56	0.41
1:B:187:LYS:HE2	1:B:187:LYS:HB2	1.95	0.41
1:B:899:ILE:HG23	1:B:918:LEU:HD21	2.02	0.41
1:B:391:ILE:HD12	1:B:477:VAL:HG12	2.02	0.41
1:B:928:LEU:HD11	1:B:943:ALA:HB2	2.03	0.40
1:B:163:ASN:HB3	1:B:315:MET:CE	2.51	0.40
1:B:778:TYR:OH	5:B:1013:EDO:H11	2.20	0.40
1:A:384:GLN:CG	1:A:479:THR:HG21	2.49	0.40
1:B:928:LEU:CD1	1:B:943:ALA:HB2	2.51	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	953/983 (97%)	929 (98%)	23 (2%)	1 (0%)	51	42
1	B	952/983 (97%)	926 (97%)	24 (2%)	2 (0%)	47	38
All	All	1905/1966 (97%)	1855 (97%)	47 (2%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	SER
1	B	165	SER
1	B	15	ALA

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	781/798 (98%)	774 (99%)	7 (1%)	78 79
1	B	780/798 (98%)	771 (99%)	9 (1%)	71 70
All	All	1561/1596 (98%)	1545 (99%)	16 (1%)	76 76

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	76	GLN
1	A	131	TYR
1	A	227	SER
1	A	315	MET
1	A	529	SER
1	A	755	THR
1	B	76	GLN
1	B	312	GLN
1	B	472	GLU
1	B	529	SER
1	B	570	LEU
1	B	828	ASN
1	B	830	GLU
1	B	873	LEU
1	B	977	MET

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

Mol	Chain	Res	Type
1	A	50	GLN
1	A	431	ASN
1	A	559	GLN
1	A	626	ASN
1	B	63	GLN
1	B	626	ASN

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Mol	Chain	Res	Type
1	B	904	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	LLP	B	726	1	23,24,25	1.80	5 (21%)	25,32,34	2.14	3 (12%)
1	LLP	A	726	1	23,24,25	1.74	6 (26%)	25,32,34	2.12	2 (8%)

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
1	LLP	B	726	1	-	1/16/17/19	0/1/1/1
1	LLP	A	726	1	-	1/16/17/19	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	726	LLP	O3-C3	-5.52	1.24	1.37
1	B	726	LLP	O3-C3	-5.45	1.24	1.37
1	B	726	LLP	CE-NZ	2.80	1.52	1.46
1	B	726	LLP	C2-N1	2.44	1.38	1.33
1	A	726	LLP	CE-NZ	2.31	1.51	1.46
1	A	726	LLP	C4'-NZ	2.30	1.35	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	726	LLP	C4-C4'	2.29	1.51	1.46
1	A	726	LLP	C2-N1	2.29	1.38	1.33
1	B	726	LLP	C4'-NZ	2.25	1.34	1.27
1	A	726	LLP	C4-C4'	2.14	1.50	1.46
1	A	726	LLP	C6-N1	2.05	1.38	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	726	LLP	OP4-C5'-C5	8.97	126.45	109.35
1	A	726	LLP	OP4-C5'-C5	8.68	125.88	109.35
1	A	726	LLP	C4-C4'-NZ	-3.64	107.58	124.31
1	B	726	LLP	C4-C4'-NZ	-3.41	108.65	124.31
1	B	726	LLP	C3-C4-C5	2.01	119.80	118.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	726	LLP	C4-C4'-NZ-CE
1	B	726	LLP	C4-C4'-NZ-CE

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	726	LLP	1	0
1	A	726	LLP	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

31 ligands are modelled in this entry.

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	PO4	B	1005	-	4,4,4	0.89	0	6,6,6	0.65	0
5	EDO	A	1016	-	3,3,3	0.44	0	2,2,2	0.27	0
5	EDO	B	1013	-	3,3,3	0.48	0	2,2,2	0.19	0
4	PO4	A	1007	-	4,4,4	0.95	0	6,6,6	0.55	0
5	EDO	A	1012	-	3,3,3	0.39	0	2,2,2	0.21	0
5	EDO	B	1009	-	3,3,3	0.49	0	2,2,2	0.44	0
2	GLY	A	1001	-	4,4,4	1.15	1 (25%)	3,4,4	1.56	0
4	PO4	B	1003	-	4,4,4	0.89	0	6,6,6	0.43	0
5	EDO	A	1013	-	3,3,3	0.49	0	2,2,2	0.22	0
3	BCT	A	1006	-	2,3,3	0.68	0	2,3,3	0.27	0
3	BCT	B	1002	-	2,3,3	0.63	0	2,3,3	0.41	0
4	PO4	B	1004	-	4,4,4	0.87	0	6,6,6	0.52	0
5	EDO	A	1015	-	3,3,3	0.45	0	2,2,2	0.35	0
2	GLY	A	1004	-	4,4,4	1.11	1 (25%)	3,4,4	1.73	2 (66%)
5	EDO	B	1012	-	3,3,3	0.43	0	2,2,2	0.42	0
5	EDO	B	1006	-	3,3,3	0.43	0	2,2,2	0.21	0
5	EDO	B	1014	-	3,3,3	0.45	0	2,2,2	0.25	0
5	EDO	A	1010	-	3,3,3	0.49	0	2,2,2	0.39	0
5	EDO	A	1014	-	3,3,3	0.51	0	2,2,2	0.12	0
5	EDO	B	1011	-	3,3,3	0.49	0	2,2,2	0.31	0
4	PO4	A	1008	-	4,4,4	0.87	0	6,6,6	0.48	0
5	EDO	B	1008	-	3,3,3	0.47	0	2,2,2	0.43	0
2	GLY	A	1002	-	4,4,4	1.12	1 (25%)	3,4,4	1.77	1 (33%)
3	BCT	A	1005	-	2,3,3	0.64	0	2,3,3	0.29	0
2	GLY	A	1003	-	4,4,4	1.09	1 (25%)	3,4,4	1.70	2 (66%)
6	BCN	A	1017	-	10,10,10	0.73	0	11,11,11	1.08	0
2	GLY	B	1001	-	4,4,4	1.12	1 (25%)	3,4,4	1.70	1 (33%)
5	EDO	B	1010	-	3,3,3	0.45	0	2,2,2	0.42	0
4	PO4	A	1009	-	4,4,4	0.91	0	6,6,6	0.40	0
5	EDO	A	1011	-	3,3,3	0.43	0	2,2,2	0.30	0
5	EDO	B	1007	-	3,3,3	0.34	0	2,2,2	0.73	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
5	EDO	A	1016	-	-	0/1/1/1	-
5	EDO	B	1013	-	-	1/1/1/1	-
5	EDO	A	1012	-	-	0/1/1/1	-
5	EDO	B	1009	-	-	0/1/1/1	-
2	GLY	A	1001	-	-	2/2/2/2	-
5	EDO	A	1013	-	-	0/1/1/1	-
5	EDO	A	1015	-	-	1/1/1/1	-
2	GLY	A	1004	-	-	2/2/2/2	-
5	EDO	B	1012	-	-	1/1/1/1	-
5	EDO	B	1006	-	-	0/1/1/1	-
5	EDO	B	1014	-	-	1/1/1/1	-
5	EDO	A	1010	-	-	0/1/1/1	-
5	EDO	A	1014	-	-	0/1/1/1	-
5	EDO	B	1011	-	-	1/1/1/1	-
5	EDO	B	1008	-	-	0/1/1/1	-
2	GLY	A	1002	-	-	2/2/2/2	-
2	GLY	A	1003	-	-	2/2/2/2	-
6	BCN	A	1017	-	-	1/10/10/10	-
2	GLY	B	1001	-	-	2/2/2/2	-
5	EDO	B	1010	-	-	0/1/1/1	-
5	EDO	A	1011	-	-	0/1/1/1	-
5	EDO	B	1007	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GLY	OXT-C	-2.15	1.23	1.30
2	A	1002	GLY	OXT-C	-2.13	1.23	1.30
2	B	1001	GLY	OXT-C	-2.13	1.23	1.30
2	A	1004	GLY	OXT-C	-2.10	1.23	1.30
2	A	1003	GLY	OXT-C	-2.04	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1002	GLY	OXT-C-O	-2.39	117.34	123.30
2	B	1001	GLY	OXT-C-O	-2.25	117.69	123.30
2	A	1004	GLY	OXT-C-O	-2.10	118.08	123.30
2	A	1004	GLY	OXT-C-CA	2.08	121.72	113.45
2	A	1003	GLY	OXT-C-O	-2.06	118.17	123.30
2	A	1003	GLY	OXT-C-CA	2.04	121.55	113.45

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1003	GLY	O-C-CA-N
2	A	1003	GLY	OXT-C-CA-N
2	A	1004	GLY	O-C-CA-N
2	A	1004	GLY	OXT-C-CA-N
6	A	1017	BCN	N1-C5-C6-O6
2	A	1001	GLY	OXT-C-CA-N
2	B	1001	GLY	OXT-C-CA-N
2	A	1001	GLY	O-C-CA-N
2	B	1001	GLY	O-C-CA-N
5	B	1012	EDO	O1-C1-C2-O2
2	A	1002	GLY	OXT-C-CA-N
5	A	1015	EDO	O1-C1-C2-O2
5	B	1013	EDO	O1-C1-C2-O2
5	B	1011	EDO	O1-C1-C2-O2
5	B	1014	EDO	O1-C1-C2-O2
2	A	1002	GLY	O-C-CA-N

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1013	EDO	2	0
5	A	1013	EDO	1	0
2	A	1004	GLY	1	0
5	B	1012	EDO	1	0
5	B	1006	EDO	2	0
5	A	1014	EDO	1	0
5	B	1011	EDO	2	0
6	A	1017	BCN	7	0
2	B	1001	GLY	1	0
5	A	1011	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^{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	941/983 (95%)	-0.33	20 (2%)	63	66	9, 16, 39, 62	2 (0%)
1	B	941/983 (95%)	-0.20	37 (3%)	39	42	9, 17, 43, 86	0
All	All	1882/1966 (95%)	-0.27	57 (3%)	50	53	9, 17, 41, 86	2 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	ILE	6.7
1	B	644	GLY	5.7
1	B	14	GLU	5.5
1	A	16	ILE	5.3
1	B	469	THR	4.3
1	B	828	ASN	4.3
1	B	15	ALA	4.3
1	B	185	LYS	4.2
1	A	969	HIS	4.1
1	A	17	ALA	4.1
1	A	469	THR	4.0
1	B	18	VAL	4.0
1	B	969	HIS	3.8
1	B	968	ARG	3.8
1	A	474	TRP	3.7
1	A	15	ALA	3.4
1	B	465	ASN	3.4
1	A	18	VAL	3.4
1	B	187	LYS	3.3
1	A	470	PRO	3.2
1	B	474	TRP	3.1
1	B	478	LYS	3.1
1	A	467	PRO	3.0
1	B	470	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	313	ARG	2.9
1	A	662	ASP	2.9
1	B	17	ALA	2.9
1	B	20	LEU	2.8
1	B	22	LYS	2.8
1	A	19	ASP	2.7
1	B	19	ASP	2.7
1	B	23	LEU	2.6
1	B	463	LYS	2.6
1	B	468	PHE	2.6
1	B	466	LEU	2.5
1	B	467	PRO	2.5
1	B	965	TYR	2.5
1	A	644	GLY	2.4
1	B	643	ASP	2.4
1	A	20	LEU	2.3
1	B	349	THR	2.3
1	B	975	GLU	2.3
1	B	662	ASP	2.3
1	A	965	TYR	2.2
1	B	977	MET	2.2
1	A	651	GLU	2.2
1	A	755	THR	2.2
1	A	471	GLU	2.2
1	B	472	GLU	2.2
1	A	475	SER	2.2
1	B	462	GLY	2.1
1	B	477	VAL	2.1
1	B	475	SER	2.1
1	B	645	GLU	2.1
1	A	466	LEU	2.1
1	A	472	GLU	2.0
1	B	326	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{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	B-factors(Å^2)	Q<0.9
1	LLP	B	726	24/25	0.96	0.14	10,19,24,25	9
1	LLP	A	726	24/25	0.97	0.08	7,17,24,27	0

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^{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	B-factors(Å^2)	Q<0.9
2	GLY	B	1001	5/5	0.75	0.21	44,51,60,61	0
5	EDO	A	1013	4/4	0.75	0.18	49,50,54,60	0
5	EDO	B	1013	4/4	0.77	0.21	40,45,51,52	0
5	EDO	B	1011	4/4	0.79	0.26	20,23,27,27	4
6	BCN	A	1017	11/11	0.79	0.34	32,45,64,67	11
5	EDO	B	1008	4/4	0.80	0.33	19,22,26,34	4
2	GLY	A	1003	5/5	0.82	0.19	35,36,41,43	5
5	EDO	A	1014	4/4	0.82	0.15	34,40,43,43	0
2	GLY	A	1002	5/5	0.82	0.20	44,47,48,51	0
2	GLY	A	1001	5/5	0.87	0.21	31,35,51,52	0
4	PO4	B	1005	5/5	0.87	0.18	23,29,38,43	5
5	EDO	A	1012	4/4	0.87	0.15	34,37,42,42	0
5	EDO	A	1011	4/4	0.88	0.26	19,21,29,33	4
5	EDO	B	1010	4/4	0.89	0.31	42,43,47,51	0
5	EDO	A	1015	4/4	0.89	0.14	25,32,32,34	4
5	EDO	B	1012	4/4	0.90	0.28	10,11,21,25	4
3	BCT	A	1006	4/4	0.91	0.12	40,41,44,50	4
5	EDO	B	1014	4/4	0.91	0.18	40,42,43,47	0
3	BCT	B	1002	4/4	0.91	0.13	18,35,37,40	4
4	PO4	A	1009	5/5	0.92	0.21	16,19,31,37	5
2	GLY	A	1004	5/5	0.92	0.20	53,56,58,61	0
5	EDO	B	1006	4/4	0.93	0.16	29,34,41,56	0
4	PO4	B	1003	5/5	0.94	0.13	25,45,47,51	0
5	EDO	A	1016	4/4	0.94	0.13	21,23,37,40	2
4	PO4	A	1008	5/5	0.94	0.12	24,27,32,35	5
5	EDO	B	1007	4/4	0.94	0.18	16,36,38,41	0
3	BCT	A	1005	4/4	0.94	0.11	16,30,32,32	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	B	1009	4/4	0.94	0.18	25,27,32,32	0
4	PO4	B	1004	5/5	0.95	0.09	22,23,29,29	5
5	EDO	A	1010	4/4	0.95	0.19	26,26,27,35	0
4	PO4	A	1007	5/5	0.96	0.12	14,32,39,41	5

6.5 Other polymers (i)

There are no such residues in this entry.