



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:56 PM UTC

PDB ID : 7LR1 / pdb_00007lr1
Title : Crystal structure of GH5_18 from Bifidobacterium longum subsp. longum ATCC 55813
Authors : Higgins, M.A.; Ryan, K.S.
Deposited on : 2021-02-15
Resolution : 1.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

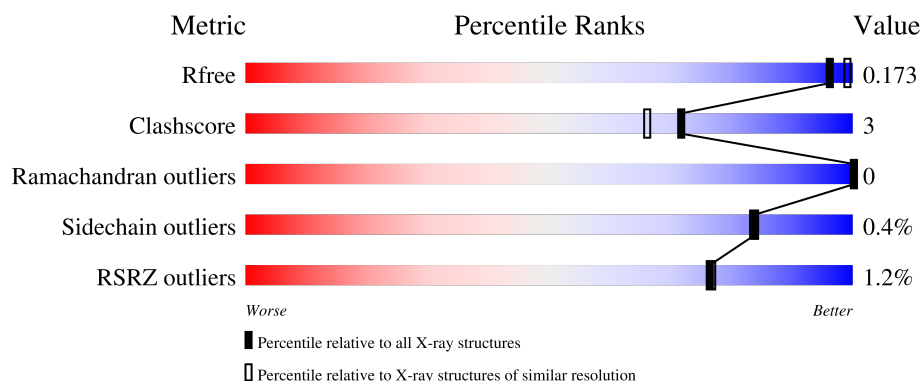
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	446	2% 90% 6%
1	B	446	2% 87% 6% 6%
1	C	446	2% 87% 8% 5%
1	D	446	2% 90% 5%

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	PO4	D	501	-	-	X	-
2	PO4	D	503	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15807 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 Glycosyl hydrolase BlGH5_18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	2	0
			3281	2090	559	617	15			
1	B	418	Total	C	N	O	S	0	5	0
			3310	2106	564	625	15			
1	C	424	Total	C	N	O	S	0	6	0
			3362	2139	568	640	15			
1	D	424	Total	C	N	O	S	0	3	0
			3329	2119	564	631	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP C2GY91
A	-18	GLY	-	expression tag	UNP C2GY91
A	-17	SER	-	expression tag	UNP C2GY91
A	-16	SER	-	expression tag	UNP C2GY91
A	-15	HIS	-	expression tag	UNP C2GY91
A	-14	HIS	-	expression tag	UNP C2GY91
A	-13	HIS	-	expression tag	UNP C2GY91
A	-12	HIS	-	expression tag	UNP C2GY91
A	-11	HIS	-	expression tag	UNP C2GY91
A	-10	HIS	-	expression tag	UNP C2GY91
A	-9	SER	-	expression tag	UNP C2GY91
A	-8	SER	-	expression tag	UNP C2GY91
A	-7	GLY	-	expression tag	UNP C2GY91
A	-6	LEU	-	expression tag	UNP C2GY91
A	-5	VAL	-	expression tag	UNP C2GY91
A	-4	PRO	-	expression tag	UNP C2GY91
A	-3	ARG	-	expression tag	UNP C2GY91
A	-2	GLY	-	expression tag	UNP C2GY91
A	-1	SER	-	expression tag	UNP C2GY91
A	0	HIS	-	expression tag	UNP C2GY91
B	-19	MET	-	initiating methionine	UNP C2GY91

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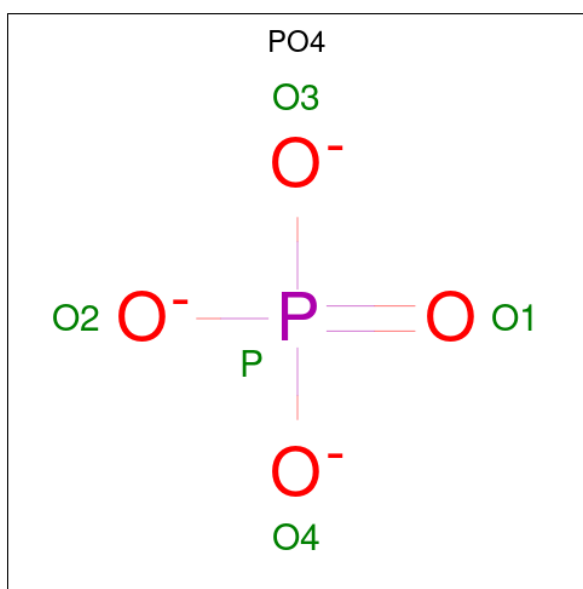
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP C2GY91
B	-17	SER	-	expression tag	UNP C2GY91
B	-16	SER	-	expression tag	UNP C2GY91
B	-15	HIS	-	expression tag	UNP C2GY91
B	-14	HIS	-	expression tag	UNP C2GY91
B	-13	HIS	-	expression tag	UNP C2GY91
B	-12	HIS	-	expression tag	UNP C2GY91
B	-11	HIS	-	expression tag	UNP C2GY91
B	-10	HIS	-	expression tag	UNP C2GY91
B	-9	SER	-	expression tag	UNP C2GY91
B	-8	SER	-	expression tag	UNP C2GY91
B	-7	GLY	-	expression tag	UNP C2GY91
B	-6	LEU	-	expression tag	UNP C2GY91
B	-5	VAL	-	expression tag	UNP C2GY91
B	-4	PRO	-	expression tag	UNP C2GY91
B	-3	ARG	-	expression tag	UNP C2GY91
B	-2	GLY	-	expression tag	UNP C2GY91
B	-1	SER	-	expression tag	UNP C2GY91
B	0	HIS	-	expression tag	UNP C2GY91
C	-19	MET	-	initiating methionine	UNP C2GY91
C	-18	GLY	-	expression tag	UNP C2GY91
C	-17	SER	-	expression tag	UNP C2GY91
C	-16	SER	-	expression tag	UNP C2GY91
C	-15	HIS	-	expression tag	UNP C2GY91
C	-14	HIS	-	expression tag	UNP C2GY91
C	-13	HIS	-	expression tag	UNP C2GY91
C	-12	HIS	-	expression tag	UNP C2GY91
C	-11	HIS	-	expression tag	UNP C2GY91
C	-10	HIS	-	expression tag	UNP C2GY91
C	-9	SER	-	expression tag	UNP C2GY91
C	-8	SER	-	expression tag	UNP C2GY91
C	-7	GLY	-	expression tag	UNP C2GY91
C	-6	LEU	-	expression tag	UNP C2GY91
C	-5	VAL	-	expression tag	UNP C2GY91
C	-4	PRO	-	expression tag	UNP C2GY91
C	-3	ARG	-	expression tag	UNP C2GY91
C	-2	GLY	-	expression tag	UNP C2GY91
C	-1	SER	-	expression tag	UNP C2GY91
C	0	HIS	-	expression tag	UNP C2GY91
D	-19	MET	-	initiating methionine	UNP C2GY91
D	-18	GLY	-	expression tag	UNP C2GY91
D	-17	SER	-	expression tag	UNP C2GY91

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP C2GY91
D	-15	HIS	-	expression tag	UNP C2GY91
D	-14	HIS	-	expression tag	UNP C2GY91
D	-13	HIS	-	expression tag	UNP C2GY91
D	-12	HIS	-	expression tag	UNP C2GY91
D	-11	HIS	-	expression tag	UNP C2GY91
D	-10	HIS	-	expression tag	UNP C2GY91
D	-9	SER	-	expression tag	UNP C2GY91
D	-8	SER	-	expression tag	UNP C2GY91
D	-7	GLY	-	expression tag	UNP C2GY91
D	-6	LEU	-	expression tag	UNP C2GY91
D	-5	VAL	-	expression tag	UNP C2GY91
D	-4	PRO	-	expression tag	UNP C2GY91
D	-3	ARG	-	expression tag	UNP C2GY91
D	-2	GLY	-	expression tag	UNP C2GY91
D	-1	SER	-	expression tag	UNP C2GY91
D	0	HIS	-	expression tag	UNP C2GY91

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



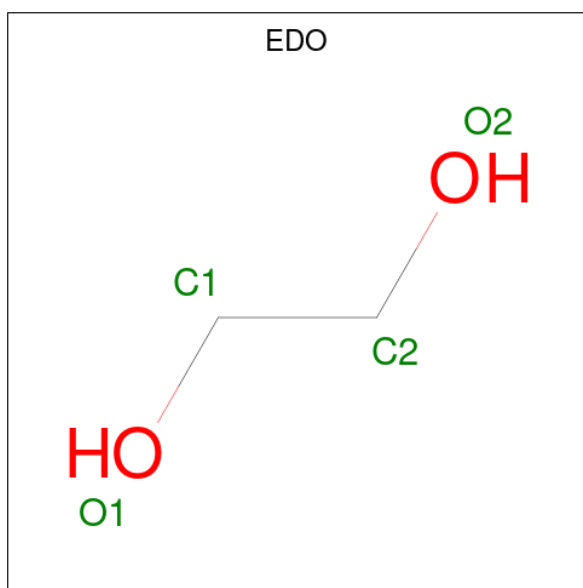
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

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

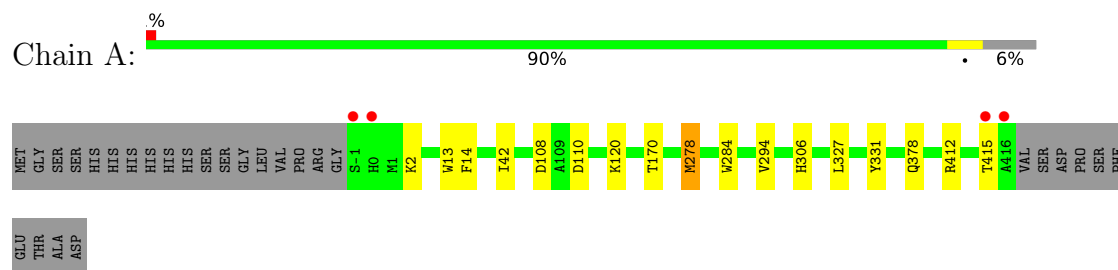
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	614	Total O 614 614	0	0
4	B	581	Total O 581 581	0	0
4	C	566	Total O 566 566	0	0
4	D	577	Total O 577 577	0	0

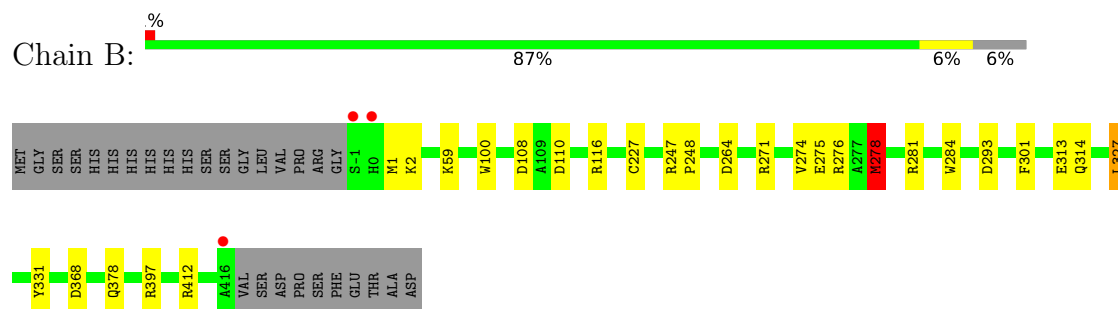
3 Residue-property plots

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.

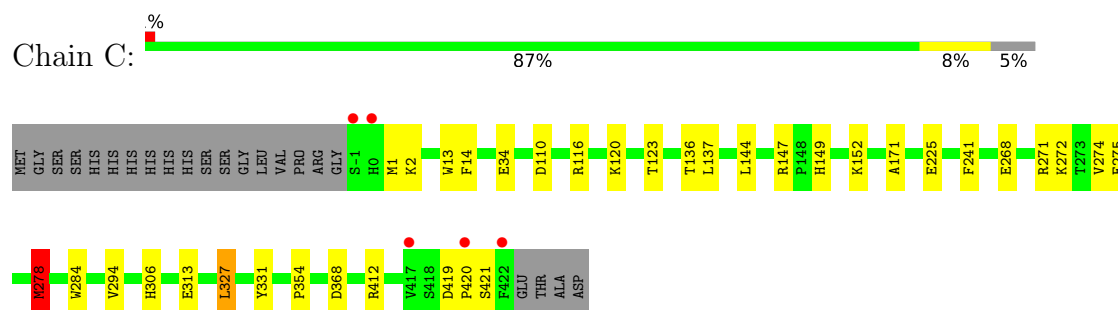
- Molecule 1: Glycosyl hydrolase BlGH5_18



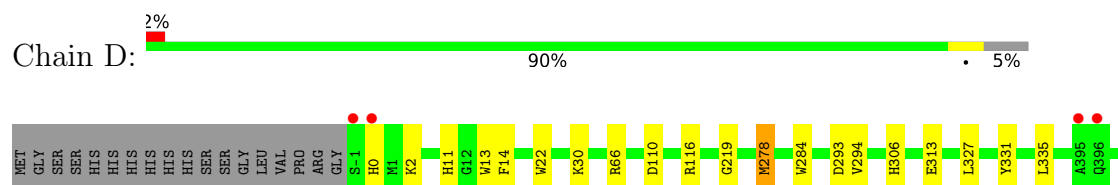
- Molecule 1: Glycosyl hydrolase BlGH5_18

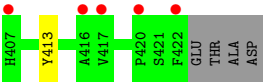


- Molecule 1: Glycosyl hydrolase BlGH5_18



- Molecule 1: Glycosyl hydrolase BlGH5_18





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.42Å 143.73Å 155.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.48 – 1.80 55.48 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.48-1.80) 99.9 (55.48-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.139 , 0.173 0.140 , 0.173	Depositor DCC
R_{free} test set	10914 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15807	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 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, EDO

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	0.89	1/3383 (0.0%)	0.87	1/4619 (0.0%)
1	B	0.90	1/3409 (0.0%)	0.86	2/4653 (0.0%)
1	C	0.84	1/3463 (0.0%)	0.87	0/4728
1	D	0.87	0/3433	0.88	3/4690 (0.1%)
All	All	0.87	3/13688 (0.0%)	0.87	6/18690 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	MET	SD-CE	-12.28	1.48	1.79
1	C	278	MET	SD-CE	-8.06	1.59	1.79
1	A	42	ILE	CB-CG1	-5.48	1.42	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	MET	CA-CB-CG	-6.80	100.49	114.10
1	D	11	HIS	CA-C-N	-5.34	115.06	122.86
1	D	11	HIS	C-N-CA	-5.34	115.06	122.86
1	D	278	MET	CA-CB-CG	-5.17	103.77	114.10
1	B	227	CYS	CA-C-N	-5.02	111.90	121.94
1	B	227	CYS	C-N-CA	-5.02	111.90	121.94

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	3281	0	3101	12	0
1	B	3310	0	3114	25	0
1	C	3362	0	3157	31	0
1	D	3329	0	3126	15	0
2	A	15	0	0	0	0
2	B	10	0	0	1	0
2	C	25	0	0	0	0
2	D	25	0	0	4	0
3	A	36	0	54	0	0
3	B	36	0	54	3	0
3	C	20	0	30	1	0
3	D	20	0	30	2	0
4	A	614	0	0	5	3
4	B	581	0	0	11	3
4	C	566	0	0	8	0
4	D	577	0	0	9	0
All	All	15807	0	12666	87	3

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 (87) 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)
3:B:509:EDO:H11	3:B:510:EDO:H21	1.45	0.98
1:C:110[B]:ASP:OD1	4:C:601:HOH:O	1.82	0.98
1:C:271:ARG:HD3	3:C:510:EDO:H21	1.57	0.85
1:B:108:ASP:HB3	4:B:939:HOH:O	1.74	0.85
1:C:225:GLU:OE2	4:C:602:HOH:O	1.98	0.80
1:A:108:ASP:HB3	4:A:958:HOH:O	1.84	0.77
1:B:313[B]:GLU:H	1:B:313[B]:GLU:CD	1.92	0.76
1:D:110[A]:ASP:OD2	4:D:602:HOH:O	2.05	0.75
1:D:335:LEU:HD23	4:D:929:HOH:O	1.88	0.73
1:B:1:MET:HG2	1:B:278:MET:HE1	1.72	0.70
1:C:1:MET:HE3	1:C:278:MET:HE1	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264[A]:ASP:OD1	4:B:601:HOH:O	2.10	0.69
1:C:116:ARG:NH2	4:C:605:HOH:O	2.26	0.69
1:C:1:MET:HG2	1:C:278:MET:HE1	1.76	0.67
2:D:501:PO4:O4	4:D:603:HOH:O	2.12	0.67
1:D:2:LYS:HD2	1:D:284:TRP:CZ2	2.30	0.66
1:C:120:LYS:HE3	4:C:774:HOH:O	1.95	0.66
1:D:313:GLU:HB2	4:D:641:HOH:O	1.95	0.65
1:A:412:ARG:NH2	4:A:601:HOH:O	2.14	0.65
1:B:301:PHE:O	4:B:602:HOH:O	2.15	0.64
1:C:2:LYS:HD2	1:C:284:TRP:CZ2	2.33	0.64
1:C:1:MET:HE3	1:C:278:MET:CE	2.27	0.63
1:B:281:ARG:HD2	4:B:787:HOH:O	1.98	0.62
1:B:116:ARG:NH2	4:B:611:HOH:O	2.33	0.61
1:A:278:MET:HE1	1:A:331:TYR:CG	2.35	0.60
1:C:274:VAL:O	1:C:278:MET:HG2	2.02	0.59
1:A:415:THR:HG22	4:A:658:HOH:O	2.03	0.59
1:B:108:ASP:OD1	4:B:603:HOH:O	2.17	0.58
2:D:503:PO4:O2	4:D:604:HOH:O	2.17	0.58
1:D:116:ARG:NH1	4:D:609:HOH:O	2.37	0.58
1:B:264[A]:ASP:OD1	4:B:604:HOH:O	2.17	0.57
1:B:1:MET:HE3	1:B:278:MET:CE	2.34	0.57
1:C:147:ARG:HG3	1:C:152:LYS:HE2	1.86	0.56
1:C:116:ARG:NH2	4:C:603:HOH:O	2.17	0.56
1:B:2:LYS:HD2	1:B:284:TRP:CZ2	2.43	0.54
1:D:2:LYS:HD2	1:D:284:TRP:CH2	2.42	0.54
1:B:59:LYS:HE3	4:B:679:HOH:O	2.09	0.53
1:C:419:ASP:OD2	1:C:421:SER:HB2	2.09	0.52
1:D:313:GLU:HB2	4:D:688:HOH:O	2.10	0.51
1:B:276:ARG:NH2	3:B:510:EDO:H11	2.25	0.51
1:C:34:GLU:OE1	4:C:604:HOH:O	2.19	0.51
1:B:275:GLU:HG2	1:B:331:TYR:OH	2.11	0.50
1:C:313:GLU:HB2	4:C:684:HOH:O	2.11	0.49
1:B:274:VAL:O	1:B:278:MET:HG2	2.15	0.47
1:B:368:ASP:OD2	1:B:412:ARG:NH2	2.47	0.47
1:C:1:MET:CE	1:C:278:MET:HE1	2.43	0.47
1:C:123[B]:THR:HG21	1:C:171:ALA:HA	1.97	0.47
1:C:271:ARG:HA	1:C:327:LEU:HD21	1.97	0.47
1:A:110:ASP:HB2	4:A:958:HOH:O	2.15	0.46
1:B:397:ARG:HD3	4:B:605:HOH:O	2.15	0.46
1:A:2:LYS:HD2	1:A:284:TRP:CZ2	2.51	0.46
1:B:110:ASP:HB2	4:B:939:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:MET:HB3	1:B:278:MET:HE2	1.80	0.45
1:B:271[B]:ARG:HA	1:B:327:LEU:HD21	1.97	0.45
2:D:501:PO4:O1	3:D:507:EDO:O2	2.33	0.45
1:B:378:GLN:HG3	3:B:505:EDO:H22	1.99	0.45
1:C:368:ASP:OD2	1:C:412:ARG:NH2	2.49	0.45
1:D:0:HIS:CE1	4:D:929:HOH:O	2.70	0.44
1:D:293:ASP:OD2	2:D:503:PO4:O3	2.35	0.44
1:D:278:MET:HE1	1:D:331:TYR:CG	2.52	0.44
1:B:293:ASP:OD2	2:B:502:PO4:O2	2.36	0.44
1:A:294:VAL:HB	1:A:306:HIS:HA	2.00	0.43
1:B:314:GLN:HG2	4:B:948:HOH:O	2.18	0.43
1:C:241:PHE:CE1	1:C:354:PRO:HG3	2.53	0.43
1:C:13:TRP:CG	1:C:14:PHE:H	2.36	0.43
1:A:120:LYS:HB2	1:A:170[A]:THR:CG2	2.48	0.43
1:A:278:MET:HE1	1:A:331:TYR:CD2	2.53	0.43
1:C:1:MET:CG	1:C:278:MET:HE1	2.43	0.43
1:C:294:VAL:HB	1:C:306:HIS:HA	2.01	0.43
1:A:378:GLN:NE2	4:A:603:HOH:O	2.44	0.43
1:C:278:MET:HB3	1:C:278:MET:HE2	1.75	0.43
1:D:294:VAL:HB	1:D:306:HIS:HA	2.01	0.43
1:D:30:LYS:HD2	4:D:648:HOH:O	2.18	0.43
1:C:268:GLU:HG2	1:C:272:LYS:HE2	2.00	0.42
1:D:13:TRP:CG	1:D:14:PHE:H	2.37	0.42
1:C:1:MET:SD	1:C:278:MET:HE1	2.59	0.42
1:D:219:GLY:HA3	1:D:413:TYR:CD2	2.54	0.42
1:C:420:PRO:HD3	4:C:1036:HOH:O	2.18	0.42
1:C:2:LYS:HD2	1:C:284:TRP:CH2	2.54	0.42
1:A:13:TRP:CG	1:A:14:PHE:H	2.38	0.42
1:C:275:GLU:HG2	1:C:331:TYR:OH	2.21	0.41
1:A:120:LYS:HB2	1:A:170[A]:THR:HG23	2.03	0.41
1:D:22:TRP:CE2	1:D:66:ARG:HD2	2.56	0.41
1:B:100:TRP:CD2	3:D:507:EDO:H22	2.56	0.41
1:C:136:THR:O	1:C:137:LEU:C	2.65	0.40
1:C:144:LEU:HD23	1:C:149:HIS:CE1	2.56	0.40
1:B:247:ARG:HA	1:B:248:PRO:HD3	1.98	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:863:HOH:O	4:B:602:HOH:O[2_665]	1.95	0.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:836:HOH:O	4:B:853:HOH:O[2_665]	2.16	0.04
4:A:1197:HOH:O	4:B:1161:HOH:O[2_665]	2.18	0.02

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	418/446 (94%)	409 (98%)	9 (2%)	0	100	100
1	B	421/446 (94%)	413 (98%)	8 (2%)	0	100	100
1	C	428/446 (96%)	420 (98%)	8 (2%)	0	100	100
1	D	425/446 (95%)	418 (98%)	7 (2%)	0	100	100
All	All	1692/1784 (95%)	1660 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	341/368 (93%)	340 (100%)	1 (0%)	86	86
1	B	343/368 (93%)	341 (99%)	2 (1%)	78	77
1	C	351/368 (95%)	349 (99%)	2 (1%)	78	77
1	D	347/368 (94%)	346 (100%)	1 (0%)	86	86
All	All	1382/1472 (94%)	1376 (100%)	6 (0%)	84	83

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

Mol	Chain	Res	Type
1	A	327	LEU
1	B	278	MET
1	B	327	LEU
1	C	278	MET
1	C	327	LEU
1	D	327	LEU

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	338	GLN
1	B	330	GLN
1	B	407	HIS
1	C	378	GLN
1	C	407	HIS
1	D	11	HIS
1	D	338	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

43 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	$\# Z > 2$
3	EDO	A	509	-	3,3,3	0.59	0	2,2,2	0.64	0
2	PO4	B	501	-	4,4,4	1.11	0	6,6,6	1.05	0
2	PO4	A	501	-	4,4,4	1.13	0	6,6,6	1.56	2 (33%)
3	EDO	A	505	-	3,3,3	0.56	0	2,2,2	0.72	0
3	EDO	B	509	-	3,3,3	0.26	0	2,2,2	0.90	0
3	EDO	B	508	-	3,3,3	0.50	0	2,2,2	0.37	0
3	EDO	A	504	-	3,3,3	0.54	0	2,2,2	0.45	0
3	EDO	A	506	-	3,3,3	0.52	0	2,2,2	0.78	0
2	PO4	D	502	-	4,4,4	0.94	0	6,6,6	1.19	0
3	EDO	A	508	-	3,3,3	0.43	0	2,2,2	1.25	0
3	EDO	B	507	-	3,3,3	0.38	0	2,2,2	1.35	0
2	PO4	D	503	-	4,4,4	1.51	1 (25%)	6,6,6	0.95	0
3	EDO	A	507	-	3,3,3	0.55	0	2,2,2	0.73	0
3	EDO	C	509	-	3,3,3	0.75	0	2,2,2	0.70	0
2	PO4	D	501	-	4,4,4	0.69	0	6,6,6	1.71	1 (16%)
2	PO4	C	501	-	4,4,4	1.24	0	6,6,6	1.67	1 (16%)
2	PO4	D	505	-	4,4,4	1.00	0	6,6,6	0.70	0
2	PO4	C	505	-	4,4,4	0.85	0	6,6,6	0.78	0
3	EDO	B	503	-	3,3,3	0.69	0	2,2,2	0.41	0
2	PO4	D	504	-	4,4,4	0.65	0	6,6,6	1.29	1 (16%)
3	EDO	D	506	-	3,3,3	0.57	0	2,2,2	0.45	0
3	EDO	D	508	-	3,3,3	0.53	0	2,2,2	1.22	0
3	EDO	B	511	-	3,3,3	0.43	0	2,2,2	0.99	0
3	EDO	A	511	-	3,3,3	0.32	0	2,2,2	1.34	0
2	PO4	A	503	-	4,4,4	3.12	2 (50%)	6,6,6	1.39	1 (16%)
3	EDO	B	504	-	3,3,3	0.48	0	2,2,2	0.63	0
3	EDO	B	506	-	3,3,3	0.21	0	2,2,2	1.03	0
3	EDO	C	506	-	3,3,3	0.76	0	2,2,2	0.29	0
3	EDO	D	510	-	3,3,3	0.45	0	2,2,2	0.54	0
3	EDO	B	505	-	3,3,3	0.47	0	2,2,2	0.10	0
3	EDO	A	510	-	3,3,3	0.24	0	2,2,2	1.15	0
3	EDO	D	507	-	3,3,3	0.54	0	2,2,2	0.64	0
3	EDO	C	507	-	3,3,3	0.55	0	2,2,2	0.61	0
2	PO4	C	502	-	4,4,4	1.11	0	6,6,6	0.42	0
3	EDO	B	510	-	3,3,3	0.33	0	2,2,2	0.70	0
2	PO4	C	504	-	4,4,4	1.38	1 (25%)	6,6,6	0.78	0
3	EDO	A	512	-	3,3,3	0.46	0	2,2,2	0.37	0
2	PO4	A	502	-	4,4,4	0.71	0	6,6,6	0.82	0
3	EDO	D	509	-	3,3,3	0.59	0	2,2,2	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	C	503	-	4,4,4	1.22	0	6,6,6	1.17	0
3	EDO	C	508	-	3,3,3	0.54	0	2,2,2	0.75	0
3	EDO	C	510	-	3,3,3	0.44	0	2,2,2	0.30	0
2	PO4	B	502	-	4,4,4	2.55	1 (25%)	6,6,6	1.96	2 (33%)

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
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-
3	EDO	B	509	-	-	0/1/1/1	-
3	EDO	B	508	-	-	1/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	506	-	-	0/1/1/1	-
3	EDO	A	508	-	-	1/1/1/1	-
3	EDO	B	507	-	-	1/1/1/1	-
3	EDO	A	507	-	-	1/1/1/1	-
3	EDO	C	509	-	-	1/1/1/1	-
3	EDO	B	503	-	-	0/1/1/1	-
3	EDO	D	506	-	-	0/1/1/1	-
3	EDO	D	508	-	-	0/1/1/1	-
3	EDO	B	511	-	-	1/1/1/1	-
3	EDO	A	511	-	-	0/1/1/1	-
3	EDO	B	504	-	-	0/1/1/1	-
3	EDO	B	506	-	-	0/1/1/1	-
3	EDO	C	506	-	-	0/1/1/1	-
3	EDO	D	510	-	-	0/1/1/1	-
3	EDO	B	505	-	-	1/1/1/1	-
3	EDO	A	510	-	-	0/1/1/1	-
3	EDO	D	507	-	-	0/1/1/1	-
3	EDO	C	507	-	-	0/1/1/1	-
3	EDO	B	510	-	-	1/1/1/1	-
3	EDO	A	512	-	-	0/1/1/1	-
3	EDO	D	509	-	-	1/1/1/1	-
3	EDO	C	508	-	-	0/1/1/1	-
3	EDO	C	510	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	PO4	P-O2	-4.85	1.40	1.54
2	A	503	PO4	P-O2	-4.42	1.41	1.54
2	A	503	PO4	P-O1	4.14	1.60	1.50
2	D	503	PO4	P-O3	-2.77	1.46	1.54
2	C	504	PO4	P-O3	-2.03	1.48	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	PO4	O4-P-O3	3.59	119.09	107.91
2	C	501	PO4	O4-P-O2	2.83	116.73	107.91
2	D	501	PO4	O4-P-O3	-2.79	99.23	107.91
2	B	502	PO4	O4-P-O1	-2.74	101.25	110.95
2	A	503	PO4	O4-P-O3	2.70	116.32	107.91
2	D	504	PO4	O4-P-O3	2.50	115.69	107.91
2	A	501	PO4	O3-P-O2	2.16	114.64	107.91
2	A	501	PO4	O4-P-O1	-2.14	103.40	110.95

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	508	EDO	O1-C1-C2-O2
3	B	511	EDO	O1-C1-C2-O2
3	B	505	EDO	O1-C1-C2-O2
3	B	507	EDO	O1-C1-C2-O2
3	B	510	EDO	O1-C1-C2-O2
3	A	507	EDO	O1-C1-C2-O2
3	A	508	EDO	O1-C1-C2-O2
3	A	509	EDO	O1-C1-C2-O2
3	C	509	EDO	O1-C1-C2-O2
3	D	509	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	509	EDO	1	0
2	D	503	PO4	2	0
2	D	501	PO4	2	0
3	B	505	EDO	1	0
3	D	507	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	510	EDO	2	0
3	C	510	EDO	1	0
2	B	502	PO4	1	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, 95th 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	418/446 (93%)	-0.80	4 (0%) 79 80	9, 16, 32, 67	2 (0%)
1	B	418/446 (93%)	-0.79	3 (0%) 84 85	8, 15, 32, 61	5 (1%)
1	C	424/446 (95%)	-0.70	5 (1%) 76 77	7, 17, 34, 73	6 (1%)
1	D	424/446 (95%)	-0.70	9 (2%) 63 64	8, 16, 38, 64	3 (0%)
All	All	1684/1784 (94%)	-0.75	21 (1%) 76 77	7, 16, 35, 73	16 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-1	SER	5.6
1	B	-1	SER	5.2
1	A	416	ALA	4.5
1	C	0	HIS	4.3
1	B	416	ALA	3.9
1	C	-1	SER	3.8
1	A	415	THR	3.3
1	D	395	ALA	3.2
1	C	422	PHE	2.8
1	A	-1	SER	2.7
1	A	0	HIS	2.7
1	D	0	HIS	2.5
1	D	416	ALA	2.5
1	C	420	PRO	2.4
1	D	422	PHE	2.3
1	B	0	HIS	2.2
1	D	407	HIS	2.2
1	C	417	VAL	2.1
1	D	417	VAL	2.1
1	D	420	PRO	2.1
1	D	396	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	PO4	C	505	5/5	0.79	0.19	105,107,107,109	0
3	EDO	B	508	4/4	0.80	0.18	56,56,56,56	0
3	EDO	C	510	4/4	0.80	0.18	47,49,51,55	0
3	EDO	B	510	4/4	0.82	0.20	57,57,58,58	0
2	PO4	D	505	5/5	0.83	0.15	87,89,89,90	0
2	PO4	C	504	5/5	0.84	0.16	34,42,49,51	5
3	EDO	B	509	4/4	0.84	0.17	47,49,53,55	0
3	EDO	B	511	4/4	0.85	0.18	45,46,46,48	0
2	PO4	D	504	5/5	0.86	0.15	29,30,38,45	5
3	EDO	B	505	4/4	0.87	0.13	47,47,50,50	0
2	PO4	D	501	5/5	0.87	0.15	46,54,56,56	0
3	EDO	D	509	4/4	0.87	0.14	37,39,42,47	0
2	PO4	A	502	5/5	0.89	0.11	56,60,65,66	0
3	EDO	A	510	4/4	0.89	0.13	27,36,36,44	0
2	PO4	C	501	5/5	0.89	0.12	39,44,48,55	0
3	EDO	A	506	4/4	0.90	0.10	25,26,37,39	0
3	EDO	A	508	4/4	0.91	0.11	33,34,35,40	0
3	EDO	B	507	4/4	0.91	0.13	33,36,37,38	0
2	PO4	C	503	5/5	0.91	0.10	21,24,31,38	5
3	EDO	A	512	4/4	0.91	0.13	40,41,41,44	0
2	PO4	D	503	5/5	0.92	0.12	16,26,37,38	5
3	EDO	C	508	4/4	0.93	0.09	26,27,29,30	0
2	PO4	A	503	5/5	0.93	0.10	10,18,20,32	5
3	EDO	A	509	4/4	0.93	0.14	15,23,26,33	0
3	EDO	A	507	4/4	0.94	0.12	29,33,34,36	0
2	PO4	B	501	5/5	0.94	0.08	26,31,36,36	5
2	PO4	C	502	5/5	0.94	0.08	10,25,27,28	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	B	502	5/5	0.94	0.10	14,21,25,31	5
3	EDO	A	511	4/4	0.94	0.09	25,25,26,28	0
3	EDO	A	505	4/4	0.94	0.09	24,24,31,33	0
3	EDO	B	504	4/4	0.94	0.09	21,23,27,28	0
2	PO4	D	502	5/5	0.94	0.09	9,21,27,31	5
3	EDO	C	507	4/4	0.95	0.08	19,25,26,27	0
3	EDO	D	507	4/4	0.95	0.08	20,23,29,30	0
3	EDO	D	508	4/4	0.95	0.09	22,28,31,31	0
2	PO4	A	501	5/5	0.95	0.08	19,20,26,27	5
3	EDO	D	510	4/4	0.96	0.11	15,18,24,31	0
3	EDO	C	509	4/4	0.97	0.09	16,16,27,27	0
3	EDO	B	506	4/4	0.97	0.07	24,29,31,32	0
3	EDO	A	504	4/4	0.98	0.04	13,14,16,17	0
3	EDO	B	503	4/4	0.98	0.04	13,14,14,15	0
3	EDO	C	506	4/4	0.99	0.03	16,17,17,17	0
3	EDO	D	506	4/4	0.99	0.03	13,15,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.