



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:06 AM UTC

PDB ID : 8DGE / pdb_00008dge
Title : BoGH13ASus from Bacteroides ovatus
Authors : Brown, H.A.; DeVeaux, A.L.; Koropatkin, N.M.
Deposited on : 2022-06-23
Resolution : 1.89 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

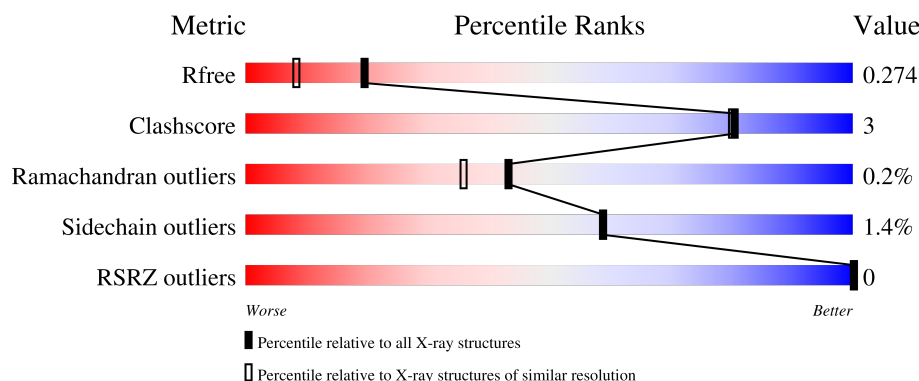
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 $\leq 5\%$. 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	738	
1	B	738	
1	C	738	
1	D	738	

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
5	PEG	A	831	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24832 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 Alpha amylase, catalytic domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	707	Total	C	N	O	S	0	1	0
			5661	3612	929	1098	22			
1	B	711	Total	C	N	O	S	0	3	0
			5719	3651	941	1105	22			
1	C	712	Total	C	N	O	S	0	3	0
			5721	3650	939	1110	22			
1	D	712	Total	C	N	O	S	0	1	0
			5689	3627	931	1109	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	expression tag	UNP A7M087
B	21	GLY	-	expression tag	UNP A7M087
C	21	GLY	-	expression tag	UNP A7M087
D	21	GLY	-	expression tag	UNP A7M087

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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

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

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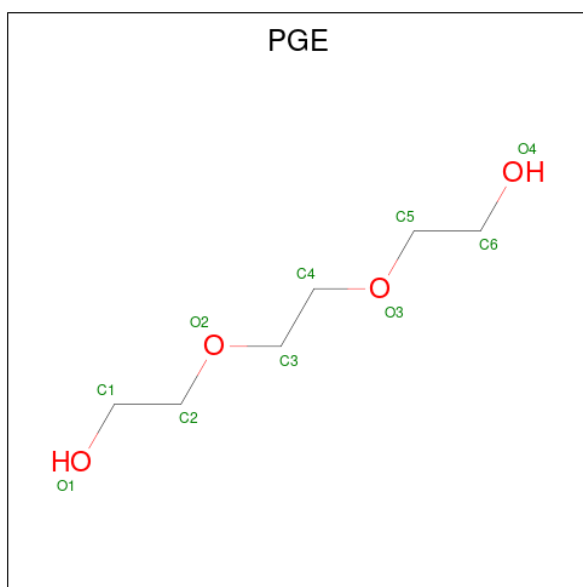
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



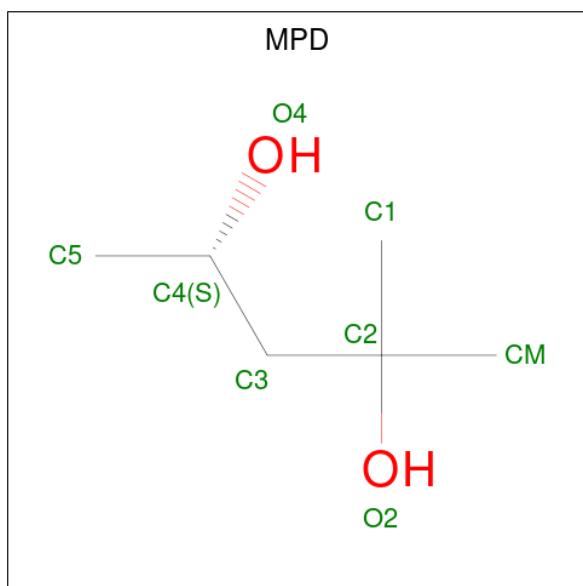
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total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

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



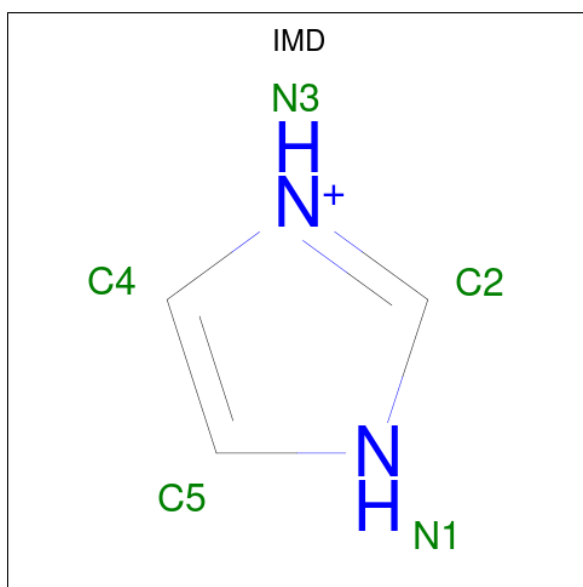
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			8	6	2		
7	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	N	0	0
			5	3	2		
8	D	1	Total	C	N	0	0
			5	3	2		

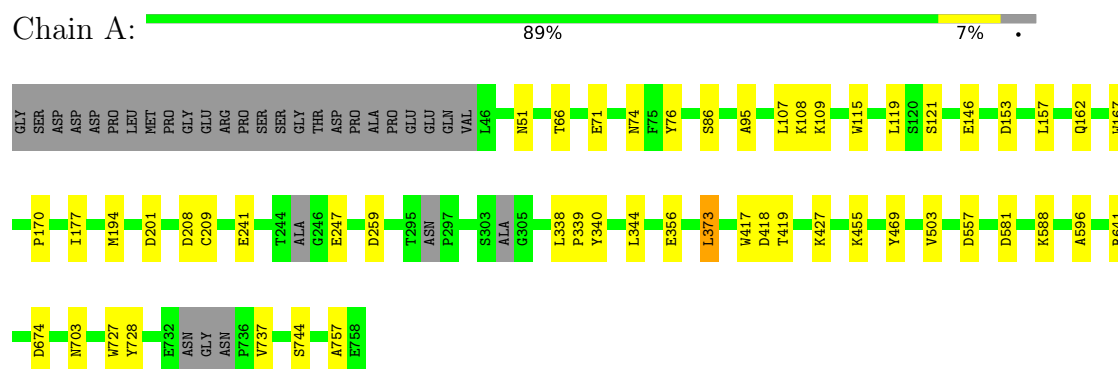
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	379	Total	O	0	0
			379	379		
9	B	417	Total	O	0	0
			417	417		
9	C	377	Total	O	0	0
			377	377		
9	D	391	Total	O	0	0
			391	391		

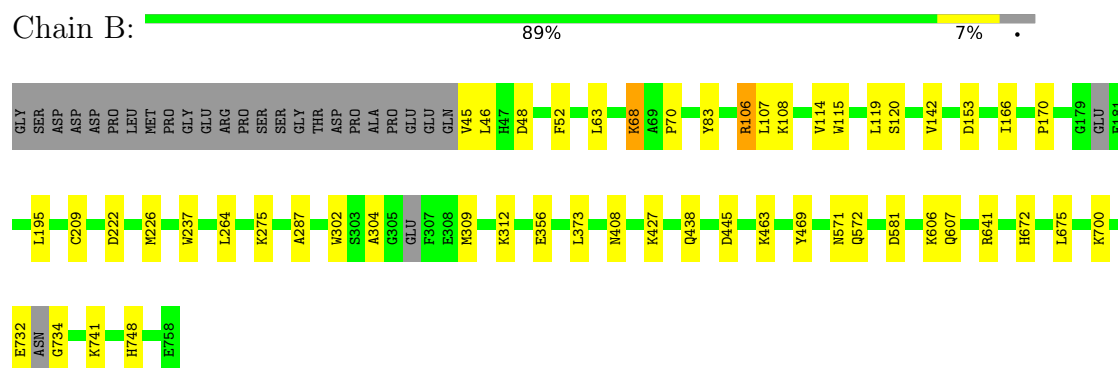
3 Residue-property plots

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.

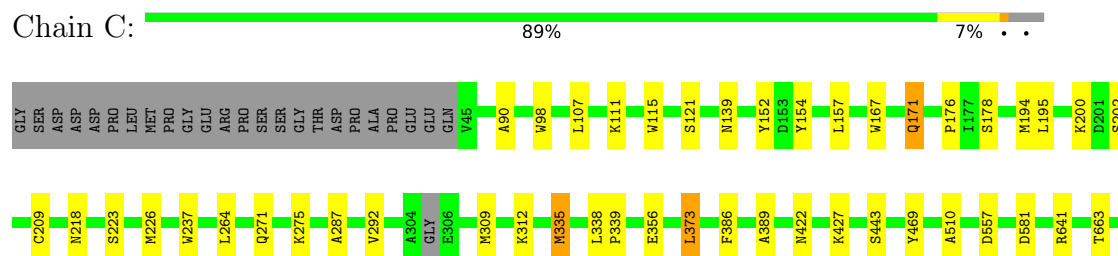
- Molecule 1: Alpha amylase, catalytic domain protein



- Molecule 1: Alpha amylase, catalytic domain protein

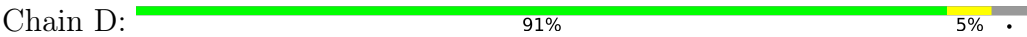


- Molecule 1: Alpha amylase, catalytic domain protein





- Molecule 1: Alpha amylase, catalytic domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.39Å 148.44Å 112.77Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	62.00 – 1.89 62.00 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.6 (62.00-1.89) 94.8 (62.00-1.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.271 0.214 , 0.274	Depositor DCC
R_{free} test set	13119 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.297 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24832	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, MPD, EDO, CA, PEG, PGE, MN

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	0.98	0/5827	1.30	0/7929
1	B	0.99	0/5893	1.29	2/8015 (0.0%)
1	C	0.98	0/5895	1.29	0/8023
1	D	0.99	0/5855	1.30	0/7972
All	All	0.99	0/23470	1.29	2/31939 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ASP	CA-C-N	5.05	127.30	120.38
1	B	222	ASP	C-N-CA	5.05	127.30	120.38

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	5661	0	5257	32	0
1	B	5719	0	5352	26	0
1	C	5721	0	5331	31	1
1	D	5689	0	5284	24	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	112	0	168	5	0
4	B	88	0	132	0	0
4	C	116	0	174	3	0
4	D	48	0	72	4	0
5	A	21	0	30	4	0
5	B	21	0	30	2	0
5	C	7	0	10	1	0
5	D	21	0	30	0	0
6	A	10	0	14	2	0
7	C	16	0	28	4	0
8	D	10	0	10	0	0
9	A	379	0	0	5	0
9	B	417	0	0	5	0
9	C	377	0	0	4	0
9	D	391	0	0	5	1
All	All	24832	0	21922	116	1

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 (116) 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:641:ARG:NH2	9:D:902:HOH:O	2.11	0.82
1:A:417:TRP:O	5:A:831:PEG:H42	1.83	0.78
1:B:571:ASN:HB2	5:B:825:PEG:H42	1.68	0.76
7:C:834:MPD:H12	7:C:834:MPD:H52	1.69	0.73
1:D:111:LYS:NZ	9:D:903:HOH:O	2.22	0.72
1:B:120:SER:O	9:B:902:HOH:O	2.09	0.70
1:B:606:LYS:NZ	9:B:903:HOH:O	2.25	0.70
1:B:153:ASP:OD2	9:B:901:HOH:O	2.08	0.69
1:A:744:SER:O	9:A:902:HOH:O	2.11	0.68
1:C:663:THR:HG21	7:C:834:MPD:HM1	1.74	0.68
1:A:728:TYR:OH	9:A:901:HOH:O	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ILE:HG21	1:A:194:MET:HE1	1.80	0.64
1:C:735:ASN:HB2	1:C:736:PRO:HD2	1.80	0.64
1:A:581:ASP:O	1:A:641:ARG:NH2	2.31	0.62
1:D:68:LYS:NZ	9:D:908:HOH:O	2.33	0.61
1:D:124:ARG:NH2	1:D:133:THR:O	2.35	0.60
1:C:735:ASN:HB2	1:C:736:PRO:CD	2.31	0.59
1:B:209:CYS:HB2	1:B:226:MET:HE3	1.83	0.59
1:C:335:MET:HE1	1:C:386:PHE:HA	1.85	0.59
1:C:758:GLU:O	9:C:901:HOH:O	2.17	0.59
1:C:735:ASN:CB	1:C:736:PRO:CD	2.82	0.58
1:B:581:ASP:O	1:B:641:ARG:NH1	2.40	0.55
1:A:153:ASP:HB3	4:A:805:EDO:H21	1.89	0.54
1:A:170:PRO:HG2	1:A:208:ASP:O	2.09	0.53
1:A:727:TRP:HB2	1:A:737:VAL:CG1	2.39	0.52
1:D:373:LEU:HD22	1:D:469:TYR:CZ	2.45	0.52
1:D:106:ARG:NH1	9:D:915:HOH:O	2.39	0.51
1:A:419:THR:H	5:A:831:PEG:H21	1.76	0.50
1:D:463:LYS:NZ	1:D:467:ASP:OD2	2.45	0.50
7:C:834:MPD:H53	9:C:1086:HOH:O	2.13	0.49
1:B:607:GLN:OE1	1:B:748:HIS:HA	2.13	0.49
1:C:157:LEU:HB3	1:C:167:TRP:CZ2	2.48	0.49
1:D:697:LEU:HD12	1:D:697:LEU:C	2.38	0.49
1:D:630:MET:O	1:D:655:ARG:HG3	2.14	0.48
1:C:275:LYS:HD3	1:C:287:ALA:HB2	1.95	0.48
1:C:176:PRO:HG2	1:C:194:MET:HE1	1.94	0.48
1:C:107:LEU:HB3	1:C:115:TRP:HB3	1.95	0.48
1:D:107:LEU:HB3	1:D:115:TRP:HB3	1.95	0.48
1:A:674:ASP:OD2	1:A:703:ASN:ND2	2.46	0.48
1:B:275:LYS:HD3	1:B:287:ALA:HB2	1.96	0.47
1:B:572:GLN:HG2	5:B:825:PEG:H41	1.96	0.47
1:C:335:MET:HE1	1:C:389:ALA:HB3	1.95	0.47
1:B:83:TYR:CE2	1:B:106:ARG:HD3	2.49	0.47
1:C:90:ALA:HB2	4:C:821:EDO:H22	1.96	0.47
1:A:86:SER:O	1:A:95:ALA:HA	2.15	0.47
1:B:463:LYS:NZ	9:B:925:HOH:O	2.48	0.47
1:B:68:LYS:HG2	1:B:114:VAL:HG22	1.96	0.46
1:B:408:ASN:ND2	1:B:445:ASP:OD2	2.49	0.46
1:A:107:LEU:HB3	1:A:115:TRP:HB3	1.97	0.46
1:B:373:LEU:HD22	1:B:469:TYR:CZ	2.51	0.45
1:C:152:TYR:CD2	1:C:422:ASN:HB2	2.51	0.45
1:B:438:GLN:CD	9:B:1068:HOH:O	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:674:ASP:OD2	1:D:703:ASN:ND2	2.48	0.45
1:C:373:LEU:HD22	1:C:469:TYR:CZ	2.52	0.45
1:A:340:TYR:CD1	4:A:825:EDO:H12	2.51	0.45
1:C:209:CYS:SG	7:C:833:MPD:HM2	2.57	0.45
1:D:751:ARG:HA	4:D:813:EDO:C2	2.47	0.45
1:B:45:VAL:CB	1:B:68:LYS:HG3	2.48	0.44
1:B:52:PHE:HB3	1:B:63:LEU:HD11	2.00	0.44
1:D:82:LEU:HD13	1:D:142:VAL:HG11	1.98	0.44
1:B:170:PRO:HG3	1:B:226:MET:HE1	1.99	0.44
1:C:271[B]:GLN:HG3	1:C:292:VAL:O	2.18	0.44
1:C:139:ASN:HA	1:C:154:TYR:O	2.18	0.44
1:A:157:LEU:HB3	1:A:167:TRP:CZ2	2.53	0.43
1:C:309:MET:O	1:C:312:LYS:HG3	2.18	0.43
1:B:119:LEU:N	1:B:119:LEU:HD12	2.33	0.43
1:C:510:ALA:O	4:C:808:EDO:O1	2.32	0.43
1:D:192:SER:HA	1:D:240:LEU:O	2.18	0.43
1:A:373:LEU:HD22	1:A:469:TYR:CZ	2.54	0.43
1:B:672:HIS:O	1:B:675:LEU:HB2	2.19	0.43
1:D:751:ARG:HA	4:D:813:EDO:H22	1.99	0.43
1:C:335:MET:CE	1:C:389:ALA:HB3	2.49	0.43
1:B:107:LEU:HB3	1:B:115:TRP:HB3	2.01	0.42
1:C:338:LEU:N	1:C:339:PRO:CD	2.82	0.42
1:D:211:PHE:CZ	1:D:226:MET:HE2	2.53	0.42
1:A:201:ASP:HB2	1:A:427:LYS:O	2.19	0.42
1:D:303:SER:OG	9:D:901:HOH:O	2.03	0.42
1:D:515:LYS:NZ	1:D:517:ASP:OD1	2.47	0.42
1:A:455:LYS:HD3	1:A:503:VAL:HG23	2.01	0.42
1:B:195:LEU:O	1:B:237:TRP:HA	2.20	0.42
1:A:418:ASP:HA	5:A:831:PEG:H21	2.01	0.42
1:A:588:LYS:HD3	4:A:830:EDO:H22	2.02	0.42
1:A:596:ALA:CB	6:A:834:PGE:H12	2.49	0.42
1:B:732:GLU:O	1:B:734:GLY:N	2.53	0.42
1:B:48:ASP:OD2	1:B:70:PRO:HB3	2.19	0.42
1:C:98:TRP:CE3	5:C:832:PEG:H21	2.55	0.42
1:A:74:ASN:ND2	9:A:939:HOH:O	2.52	0.42
1:C:226:MET:HG2	9:C:1099:HOH:O	2.19	0.42
1:C:335:MET:CE	1:C:389:ALA:CB	2.98	0.42
1:B:309:MET:HE3	1:B:312:LYS:HA	2.01	0.41
1:D:459:LYS:NZ	1:D:506:GLU:OE2	2.44	0.41
1:D:287:ALA:HB3	4:D:805:EDO:H21	2.01	0.41
1:A:119:LEU:HD12	1:A:119:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:TRP:CZ2	1:D:139:ASN:HB3	2.56	0.41
1:A:340:TYR:CE1	4:A:825:EDO:H12	2.55	0.41
1:A:109:LYS:NZ	9:A:943:HOH:O	2.53	0.41
1:C:443:SER:HA	4:C:812:EDO:H22	2.02	0.41
1:C:218:ASN:ND2	9:C:937:HOH:O	2.53	0.41
1:C:223:SER:HA	1:C:226:MET:HE2	2.02	0.41
1:D:318:TYR:CZ	1:D:626:GLN:HA	2.56	0.41
1:A:51:ASN:HB2	1:A:66:THR:HB	2.03	0.41
1:A:108:LYS:O	1:A:115:TRP:HA	2.20	0.41
1:A:596:ALA:HB2	6:A:834:PGE:H12	2.03	0.41
1:C:202:SER:OG	1:C:427:LYS:HA	2.20	0.41
1:D:752:LEU:H	4:D:813:EDO:H21	1.85	0.41
1:A:162:GLN:HB2	9:A:917:HOH:O	2.20	0.41
1:A:259:ASP:HA	5:A:831:PEG:H32	2.01	0.41
1:A:338:LEU:N	1:A:339:PRO:CD	2.85	0.40
4:A:817:EDO:O1	4:A:827:EDO:H12	2.20	0.40
1:C:195:LEU:O	1:C:237:TRP:HA	2.22	0.40
1:C:581:ASP:O	1:C:641:ARG:NH1	2.54	0.40
1:C:757:ALA:O	1:C:758:GLU:C	2.64	0.40
1:A:170:PRO:HG3	1:A:209:CYS:HB3	2.03	0.40
1:A:71:GLU:HA	1:A:76:TYR:CD1	2.56	0.40
1:B:119:LEU:N	1:B:119:LEU:CD1	2.85	0.40
1:D:82:LEU:HD13	1:D:142:VAL:CG1	2.52	0.40

All (1) 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)
1:C:171:GLN:OE1	9:D:1111:HOH:O[2_655]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	698/738 (95%)	671 (96%)	25 (4%)	2 (0%)	36	29
1	B	706/738 (96%)	677 (96%)	26 (4%)	3 (0%)	30	22
1	C	709/738 (96%)	679 (96%)	28 (4%)	2 (0%)	36	29
1	D	707/738 (96%)	682 (96%)	25 (4%)	0	100	100
All	All	2820/2952 (96%)	2709 (96%)	104 (4%)	7 (0%)	43	36

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	757	ALA
1	B	302	TRP
1	C	735	ASN
1	B	304	ALA
1	C	121	SER
1	A	121	SER
1	B	46	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/639 (94%)	594 (99%)	7 (1%)	63	63
1	B	610/639 (96%)	599 (98%)	11 (2%)	51	50
1	C	609/639 (95%)	597 (98%)	12 (2%)	48	46
1	D	604/639 (94%)	597 (99%)	7 (1%)	63	63
All	All	2424/2556 (95%)	2387 (98%)	37 (2%)	59	56

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	241	GLU
1	A	247	GLU
1	A	344	LEU

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Mol	Chain	Res	Type
1	A	356	GLU
1	A	373	LEU
1	A	557	ASP
1	B	68	LYS
1	B	106	ARG
1	B	108	LYS
1	B	142	VAL
1	B	166	ILE
1	B	264	LEU
1	B	356	GLU
1	B	427[A]	LYS
1	B	427[B]	LYS
1	B	700	LYS
1	B	741	LYS
1	C	111	LYS
1	C	171	GLN
1	C	178	SER
1	C	200	LYS
1	C	264	LEU
1	C	335	MET
1	C	356	GLU
1	C	373	LEU
1	C	557[A]	ASP
1	C	557[B]	ASP
1	C	741	LYS
1	C	742	LYS
1	D	46	LEU
1	D	112	ASP
1	D	169	GLU
1	D	180	GLU
1	D	356	GLU
1	D	373	LEU
1	D	475	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	GLN
1	A	286	GLN
1	A	380	GLN
1	A	550	GLN
1	A	558	ASN

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Mol	Chain	Res	Type
1	B	102	GLN
1	B	149	GLN
1	B	162	GLN
1	B	233	ASN
1	B	311	ASN
1	B	681	GLN
1	B	689	ASN
1	B	693	ASN
1	C	125	HIS
1	C	162	GLN
1	C	163	ASN
1	C	203	GLN
1	C	392	GLN
1	C	689	ASN
1	C	706	GLN
1	D	91	ASN
1	D	139	ASN
1	D	672	HIS

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](#)

Of 114 ligands modelled in this entry, 8 are monoatomic - leaving 106 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	C	811	-	3,3,3	0.08	0	2,2,2	0.19	0
7	MPD	C	834	-	7,7,7	0.11	0	9,10,10	0.40	0
4	EDO	C	808	-	3,3,3	0.07	0	2,2,2	0.06	0
4	EDO	C	824	-	3,3,3	0.10	0	2,2,2	0.13	0
5	PEG	A	833	-	6,6,6	0.15	0	5,5,5	0.07	0
4	EDO	D	811	-	3,3,3	0.05	0	2,2,2	0.05	0
4	EDO	C	809	-	3,3,3	0.13	0	2,2,2	0.13	0
4	EDO	C	815	-	3,3,3	0.11	0	2,2,2	0.19	0
4	EDO	A	826	-	3,3,3	0.16	0	2,2,2	0.04	0
4	EDO	D	812	-	3,3,3	0.03	0	2,2,2	0.04	0
4	EDO	C	828	-	3,3,3	0.08	0	2,2,2	0.14	0
4	EDO	A	803	-	3,3,3	0.13	0	2,2,2	0.20	0
4	EDO	D	803	-	3,3,3	0.17	0	2,2,2	0.07	0
4	EDO	A	828	-	3,3,3	0.10	0	2,2,2	0.24	0
4	EDO	A	807	-	3,3,3	0.09	0	2,2,2	0.16	0
4	EDO	D	813	-	3,3,3	0.02	0	2,2,2	0.17	0
4	EDO	C	827	-	3,3,3	0.04	0	2,2,2	0.13	0
4	EDO	B	823	-	3,3,3	0.16	0	2,2,2	0.23	0
4	EDO	B	808	-	3,3,3	0.19	0	2,2,2	0.31	0
4	EDO	C	816	-	3,3,3	0.17	0	2,2,2	0.14	0
4	EDO	A	819	-	3,3,3	0.09	0	2,2,2	0.10	0
4	EDO	B	810	-	3,3,3	0.06	0	2,2,2	0.09	0
4	EDO	A	812	-	3,3,3	0.08	0	2,2,2	0.16	0
4	EDO	C	805	-	3,3,3	0.17	0	2,2,2	0.20	0
4	EDO	B	812	-	3,3,3	0.13	0	2,2,2	0.16	0
4	EDO	D	807	-	3,3,3	0.07	0	2,2,2	0.16	0
4	EDO	C	825	-	3,3,3	0.16	0	2,2,2	0.19	0
4	EDO	A	808	-	3,3,3	0.13	0	2,2,2	0.26	0
6	PGE	A	834	-	9,9,9	0.17	0	8,8,8	0.14	0
4	EDO	C	814	-	3,3,3	0.11	0	2,2,2	0.11	0
8	IMD	D	814	-	5,5,5	0.26	0	5,5,5	0.54	0
4	EDO	A	824	-	3,3,3	0.09	0	2,2,2	0.15	0
4	EDO	A	817	-	3,3,3	0.16	0	2,2,2	0.27	0
4	EDO	C	826	-	3,3,3	0.21	0	2,2,2	0.16	0
5	PEG	D	816	-	6,6,6	0.25	0	5,5,5	0.18	0
7	MPD	C	833	-	7,7,7	0.12	0	9,10,10	0.21	0
4	EDO	B	822	-	3,3,3	0.13	0	2,2,2	0.06	0
4	EDO	B	805	-	3,3,3	0.06	0	2,2,2	0.20	0
4	EDO	B	820	-	3,3,3	0.09	0	2,2,2	0.22	0
4	EDO	C	817	-	3,3,3	0.12	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	810	-	3,3,3	0.05	0	2,2,2	0.14	0
4	EDO	C	818	-	3,3,3	0.14	0	2,2,2	0.22	0
4	EDO	B	815	-	3,3,3	0.07	0	2,2,2	0.09	0
4	EDO	A	822	-	3,3,3	0.09	0	2,2,2	0.12	0
4	EDO	C	819	-	3,3,3	0.03	0	2,2,2	0.14	0
4	EDO	C	829	-	3,3,3	0.05	0	2,2,2	0.22	0
4	EDO	A	820	-	3,3,3	0.13	0	2,2,2	0.19	0
4	EDO	C	821	-	3,3,3	0.13	0	2,2,2	0.22	0
4	EDO	B	819	-	3,3,3	0.10	0	2,2,2	0.21	0
5	PEG	A	832	-	6,6,6	0.14	0	5,5,5	0.14	0
4	EDO	A	815	-	3,3,3	0.06	0	2,2,2	0.18	0
4	EDO	A	823	-	3,3,3	0.06	0	2,2,2	0.19	0
4	EDO	C	806	-	3,3,3	0.06	0	2,2,2	0.15	0
4	EDO	A	809	-	3,3,3	0.10	0	2,2,2	0.15	0
4	EDO	A	821	-	3,3,3	0.04	0	2,2,2	0.09	0
4	EDO	B	816	-	3,3,3	0.10	0	2,2,2	0.15	0
4	EDO	A	827	-	3,3,3	0.05	0	2,2,2	0.16	0
4	EDO	A	830	-	3,3,3	0.11	0	2,2,2	0.16	0
4	EDO	D	808	-	3,3,3	0.13	0	2,2,2	0.18	0
4	EDO	B	814	-	3,3,3	0.14	0	2,2,2	0.13	0
4	EDO	A	805	-	3,3,3	0.05	0	2,2,2	0.17	0
4	EDO	C	823	-	3,3,3	0.08	0	2,2,2	0.18	0
4	EDO	A	806	-	3,3,3	0.08	0	2,2,2	0.05	0
4	EDO	A	829	-	3,3,3	0.10	0	2,2,2	0.21	0
4	EDO	D	810	-	3,3,3	0.20	0	2,2,2	0.10	0
5	PEG	D	817	-	6,6,6	0.16	0	5,5,5	0.13	0
4	EDO	A	814	-	3,3,3	0.07	0	2,2,2	0.10	0
5	PEG	D	815	-	6,6,6	0.15	0	5,5,5	0.14	0
4	EDO	D	804	-	3,3,3	0.07	0	2,2,2	0.10	0
4	EDO	D	805	-	3,3,3	0.10	0	2,2,2	0.13	0
4	EDO	D	819	-	3,3,3	0.02	0	2,2,2	0.18	0
4	EDO	C	807	-	3,3,3	0.22	0	2,2,2	0.27	0
4	EDO	C	804	-	3,3,3	0.11	0	2,2,2	0.31	0
4	EDO	A	810	-	3,3,3	0.07	0	2,2,2	0.13	0
8	IMD	D	818	-	5,5,5	0.21	0	5,5,5	0.53	0
4	EDO	A	818	-	3,3,3	0.16	0	2,2,2	0.17	0
4	EDO	C	812	-	3,3,3	0.07	0	2,2,2	0.30	0
4	EDO	D	809	-	3,3,3	0.14	0	2,2,2	0.10	0
4	EDO	C	822	-	3,3,3	0.13	0	2,2,2	0.12	0
4	EDO	C	813	-	3,3,3	0.20	0	2,2,2	0.23	0
5	PEG	B	825	-	6,6,6	0.14	0	5,5,5	0.19	0
4	EDO	C	831	-	3,3,3	0.09	0	2,2,2	0.15	0
4	EDO	B	803	-	3,3,3	0.07	0	2,2,2	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	811	-	3,3,3	0.12	0	2,2,2	0.07	0
5	PEG	A	831	-	6,6,6	0.16	0	5,5,5	0.14	0
5	PEG	B	827	-	6,6,6	0.17	0	5,5,5	0.10	0
4	EDO	B	804	-	3,3,3	0.14	0	2,2,2	0.12	0
4	EDO	B	807	-	3,3,3	0.03	0	2,2,2	0.13	0
5	PEG	C	832	-	6,6,6	0.16	0	5,5,5	0.13	0
4	EDO	B	817	-	3,3,3	0.10	0	2,2,2	0.17	0
4	EDO	A	816	-	3,3,3	0.11	0	2,2,2	0.02	0
4	EDO	D	806	-	3,3,3	0.12	0	2,2,2	0.24	0
4	EDO	A	811	-	3,3,3	0.10	0	2,2,2	0.14	0
5	PEG	B	826	-	6,6,6	0.18	0	5,5,5	0.07	0
4	EDO	A	804	-	3,3,3	0.10	0	2,2,2	0.14	0
4	EDO	B	809	-	3,3,3	0.15	0	2,2,2	0.16	0
4	EDO	B	821	-	3,3,3	0.09	0	2,2,2	0.17	0
4	EDO	A	825	-	3,3,3	0.13	0	2,2,2	0.24	0
4	EDO	A	813	-	3,3,3	0.03	0	2,2,2	0.15	0
4	EDO	C	830	-	3,3,3	0.07	0	2,2,2	0.21	0
4	EDO	B	813	-	3,3,3	0.08	0	2,2,2	0.22	0
4	EDO	B	824	-	3,3,3	0.08	0	2,2,2	0.15	0
4	EDO	C	820	-	3,3,3	0.06	0	2,2,2	0.06	0
4	EDO	B	818	-	3,3,3	0.11	0	2,2,2	0.11	0
4	EDO	C	803	-	3,3,3	0.05	0	2,2,2	0.06	0
4	EDO	B	806	-	3,3,3	0.10	0	2,2,2	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	811	-	-	1/1/1/1	-
7	MPD	C	834	-	-	2/5/5/5	-
4	EDO	C	808	-	-	0/1/1/1	-
4	EDO	C	824	-	-	1/1/1/1	-
5	PEG	A	833	-	-	3/4/4/4	-
4	EDO	D	811	-	-	0/1/1/1	-
4	EDO	C	809	-	-	1/1/1/1	-
4	EDO	C	815	-	-	1/1/1/1	-
4	EDO	A	826	-	-	1/1/1/1	-
4	EDO	D	812	-	-	0/1/1/1	-
4	EDO	C	828	-	-	0/1/1/1	-
4	EDO	A	803	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	803	-	-	0/1/1/1	-
4	EDO	A	828	-	-	1/1/1/1	-
4	EDO	A	807	-	-	1/1/1/1	-
4	EDO	D	813	-	-	1/1/1/1	-
4	EDO	C	827	-	-	0/1/1/1	-
4	EDO	B	823	-	-	1/1/1/1	-
4	EDO	B	808	-	-	0/1/1/1	-
4	EDO	C	816	-	-	1/1/1/1	-
4	EDO	A	819	-	-	1/1/1/1	-
4	EDO	B	810	-	-	1/1/1/1	-
4	EDO	A	812	-	-	1/1/1/1	-
4	EDO	C	805	-	-	0/1/1/1	-
4	EDO	B	812	-	-	1/1/1/1	-
4	EDO	D	807	-	-	1/1/1/1	-
4	EDO	C	825	-	-	1/1/1/1	-
4	EDO	A	808	-	-	1/1/1/1	-
6	PGE	A	834	-	-	3/7/7/7	-
4	EDO	C	814	-	-	0/1/1/1	-
8	IMD	D	814	-	-	-	0/1/1/1
4	EDO	A	824	-	-	0/1/1/1	-
4	EDO	A	817	-	-	1/1/1/1	-
4	EDO	C	826	-	-	1/1/1/1	-
5	PEG	D	816	-	-	1/4/4/4	-
7	MPD	C	833	-	-	0/5/5/5	-
4	EDO	B	822	-	-	1/1/1/1	-
4	EDO	B	805	-	-	0/1/1/1	-
4	EDO	B	820	-	-	1/1/1/1	-
4	EDO	C	817	-	-	0/1/1/1	-
4	EDO	C	810	-	-	1/1/1/1	-
4	EDO	C	818	-	-	1/1/1/1	-
4	EDO	B	815	-	-	1/1/1/1	-
4	EDO	A	822	-	-	1/1/1/1	-
4	EDO	C	819	-	-	1/1/1/1	-
4	EDO	C	829	-	-	1/1/1/1	-
4	EDO	A	820	-	-	1/1/1/1	-
4	EDO	C	821	-	-	1/1/1/1	-
4	EDO	B	819	-	-	1/1/1/1	-
5	PEG	A	832	-	-	3/4/4/4	-
4	EDO	A	815	-	-	1/1/1/1	-
4	EDO	A	823	-	-	1/1/1/1	-
4	EDO	C	806	-	-	1/1/1/1	-
4	EDO	A	809	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	821	-	-	0/1/1/1	-
4	EDO	B	816	-	-	1/1/1/1	-
4	EDO	A	827	-	-	1/1/1/1	-
4	EDO	A	830	-	-	1/1/1/1	-
4	EDO	D	808	-	-	1/1/1/1	-
4	EDO	B	814	-	-	0/1/1/1	-
4	EDO	A	805	-	-	0/1/1/1	-
4	EDO	C	823	-	-	1/1/1/1	-
4	EDO	A	806	-	-	0/1/1/1	-
4	EDO	A	829	-	-	1/1/1/1	-
4	EDO	D	810	-	-	1/1/1/1	-
5	PEG	D	817	-	-	0/4/4/4	-
4	EDO	A	814	-	-	1/1/1/1	-
5	PEG	D	815	-	-	2/4/4/4	-
4	EDO	D	804	-	-	1/1/1/1	-
4	EDO	D	805	-	-	1/1/1/1	-
4	EDO	D	819	-	-	1/1/1/1	-
4	EDO	C	807	-	-	1/1/1/1	-
4	EDO	C	804	-	-	1/1/1/1	-
4	EDO	A	810	-	-	1/1/1/1	-
8	IMD	D	818	-	-	-	0/1/1/1
4	EDO	A	818	-	-	1/1/1/1	-
4	EDO	C	812	-	-	1/1/1/1	-
4	EDO	D	809	-	-	1/1/1/1	-
4	EDO	C	822	-	-	1/1/1/1	-
4	EDO	C	813	-	-	1/1/1/1	-
5	PEG	B	825	-	-	1/4/4/4	-
4	EDO	C	831	-	-	1/1/1/1	-
4	EDO	B	803	-	-	0/1/1/1	-
4	EDO	B	811	-	-	0/1/1/1	-
5	PEG	A	831	-	-	2/4/4/4	-
5	PEG	B	827	-	-	1/4/4/4	-
4	EDO	B	804	-	-	0/1/1/1	-
4	EDO	B	807	-	-	0/1/1/1	-
5	PEG	C	832	-	-	2/4/4/4	-
4	EDO	B	817	-	-	1/1/1/1	-
4	EDO	A	816	-	-	1/1/1/1	-
4	EDO	D	806	-	-	1/1/1/1	-
4	EDO	A	811	-	-	1/1/1/1	-
5	PEG	B	826	-	-	2/4/4/4	-
4	EDO	A	804	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	809	-	-	1/1/1/1	-
4	EDO	B	821	-	-	1/1/1/1	-
4	EDO	A	825	-	-	1/1/1/1	-
4	EDO	A	813	-	-	1/1/1/1	-
4	EDO	C	830	-	-	1/1/1/1	-
4	EDO	B	813	-	-	1/1/1/1	-
4	EDO	B	824	-	-	1/1/1/1	-
4	EDO	C	820	-	-	1/1/1/1	-
4	EDO	B	818	-	-	0/1/1/1	-
4	EDO	C	803	-	-	1/1/1/1	-
4	EDO	B	806	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	834	MPD	C2-C3-C4-O4
7	C	834	MPD	C2-C3-C4-C5
5	B	826	PEG	O2-C3-C4-O4
6	A	834	PGE	O1-C1-C2-O2
5	B	825	PEG	O2-C3-C4-O4
5	D	815	PEG	O2-C3-C4-O4
5	A	833	PEG	O2-C3-C4-O4
5	C	832	PEG	O2-C3-C4-O4
4	A	808	EDO	O1-C1-C2-O2
4	A	825	EDO	O1-C1-C2-O2
4	A	829	EDO	O1-C1-C2-O2
4	B	810	EDO	O1-C1-C2-O2
4	B	819	EDO	O1-C1-C2-O2
4	C	829	EDO	O1-C1-C2-O2
4	D	806	EDO	O1-C1-C2-O2
4	D	808	EDO	O1-C1-C2-O2
4	D	809	EDO	O1-C1-C2-O2
5	A	831	PEG	O2-C3-C4-O4
5	A	832	PEG	O1-C1-C2-O2
5	B	826	PEG	O1-C1-C2-O2
5	A	832	PEG	O2-C3-C4-O4
5	A	833	PEG	O1-C1-C2-O2
5	D	815	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	834	PGE	C6-C5-O3-C4
4	A	810	EDO	O1-C1-C2-O2
4	A	820	EDO	O1-C1-C2-O2
4	B	816	EDO	O1-C1-C2-O2
4	B	823	EDO	O1-C1-C2-O2
4	C	803	EDO	O1-C1-C2-O2
4	C	806	EDO	O1-C1-C2-O2
4	C	816	EDO	O1-C1-C2-O2
4	C	823	EDO	O1-C1-C2-O2
4	C	824	EDO	O1-C1-C2-O2
4	C	826	EDO	O1-C1-C2-O2
4	D	810	EDO	O1-C1-C2-O2
4	A	827	EDO	O1-C1-C2-O2
4	B	813	EDO	O1-C1-C2-O2
4	B	815	EDO	O1-C1-C2-O2
4	B	817	EDO	O1-C1-C2-O2
4	C	818	EDO	O1-C1-C2-O2
4	C	825	EDO	O1-C1-C2-O2
4	D	807	EDO	O1-C1-C2-O2
5	D	816	PEG	O1-C1-C2-O2
5	C	832	PEG	C4-C3-O2-C2
5	A	831	PEG	O1-C1-C2-O2
5	A	832	PEG	C4-C3-O2-C2
4	A	813	EDO	O1-C1-C2-O2
4	A	830	EDO	O1-C1-C2-O2
4	C	809	EDO	O1-C1-C2-O2
4	C	815	EDO	O1-C1-C2-O2
4	C	819	EDO	O1-C1-C2-O2
5	B	827	PEG	C1-C2-O2-C3
4	B	820	EDO	O1-C1-C2-O2
4	C	813	EDO	O1-C1-C2-O2
4	D	805	EDO	O1-C1-C2-O2
4	A	804	EDO	O1-C1-C2-O2
4	A	809	EDO	O1-C1-C2-O2
4	A	812	EDO	O1-C1-C2-O2
4	A	816	EDO	O1-C1-C2-O2
4	A	818	EDO	O1-C1-C2-O2
4	A	826	EDO	O1-C1-C2-O2
4	C	804	EDO	O1-C1-C2-O2
4	C	807	EDO	O1-C1-C2-O2
4	C	810	EDO	O1-C1-C2-O2
4	C	822	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	831	EDO	O1-C1-C2-O2
4	D	804	EDO	O1-C1-C2-O2
4	A	807	EDO	O1-C1-C2-O2
4	A	817	EDO	O1-C1-C2-O2
4	B	812	EDO	O1-C1-C2-O2
4	C	811	EDO	O1-C1-C2-O2
4	C	820	EDO	O1-C1-C2-O2
4	C	821	EDO	O1-C1-C2-O2
4	C	830	EDO	O1-C1-C2-O2
5	A	833	PEG	C4-C3-O2-C2
4	A	811	EDO	O1-C1-C2-O2
4	A	814	EDO	O1-C1-C2-O2
4	A	819	EDO	O1-C1-C2-O2
4	A	823	EDO	O1-C1-C2-O2
4	B	821	EDO	O1-C1-C2-O2
4	B	824	EDO	O1-C1-C2-O2
4	C	812	EDO	O1-C1-C2-O2
4	D	813	EDO	O1-C1-C2-O2
4	A	815	EDO	O1-C1-C2-O2
4	B	806	EDO	O1-C1-C2-O2
4	B	809	EDO	O1-C1-C2-O2
4	A	803	EDO	O1-C1-C2-O2
4	A	822	EDO	O1-C1-C2-O2
4	A	828	EDO	O1-C1-C2-O2
4	B	822	EDO	O1-C1-C2-O2
6	A	834	PGE	O2-C3-C4-O3
4	D	819	EDO	O1-C1-C2-O2

There are no ring outliers.

16 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	834	MPD	3	0
4	C	808	EDO	1	0
4	D	813	EDO	3	0
6	A	834	PGE	2	0
4	A	817	EDO	1	0
7	C	833	MPD	1	0
4	C	821	EDO	1	0
4	A	827	EDO	1	0
4	A	830	EDO	1	0
4	A	805	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	805	EDO	1	0
4	C	812	EDO	1	0
5	B	825	PEG	2	0
5	A	831	PEG	4	0
5	C	832	PEG	1	0
4	A	825	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	707/738 (95%)	-0.82	0 100 100	17, 31, 43, 58	1 (0%)
1	B	711/738 (96%)	-0.82	0 100 100	19, 29, 43, 54	3 (0%)
1	C	712/738 (96%)	-0.83	0 100 100	17, 30, 43, 53	3 (0%)
1	D	712/738 (96%)	-0.82	0 100 100	22, 29, 43, 55	1 (0%)
All	All	2842/2952 (96%)	-0.82	0 100 100	17, 30, 43, 58	8 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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, 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
4	EDO	A	803	4/4	0.92	0.10	39,41,41,47	0
4	EDO	D	805	4/4	0.93	0.09	36,39,39,43	0
4	EDO	D	809	4/4	0.93	0.11	40,41,41,44	0
4	EDO	A	827	4/4	0.94	0.08	35,38,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	820	4/4	0.94	0.08	42,42,45,45	0
4	EDO	C	822	4/4	0.94	0.07	38,39,40,41	0
4	EDO	A	813	4/4	0.94	0.08	42,44,46,47	0
4	EDO	A	821	4/4	0.94	0.10	41,42,45,47	0
4	EDO	A	823	4/4	0.95	0.09	36,40,42,44	0
4	EDO	B	822	4/4	0.95	0.07	33,35,35,38	0
4	EDO	A	826	4/4	0.95	0.10	33,35,36,37	0
4	EDO	C	828	4/4	0.95	0.10	31,34,36,37	0
4	EDO	D	803	4/4	0.95	0.08	34,34,35,36	0
4	EDO	D	804	4/4	0.95	0.07	38,42,45,46	0
4	EDO	A	820	4/4	0.95	0.08	38,39,40,42	0
4	EDO	D	808	4/4	0.95	0.08	34,37,38,40	0
4	EDO	A	830	4/4	0.95	0.13	34,36,38,40	0
5	PEG	B	826	7/7	0.95	0.07	42,44,46,49	0
5	PEG	D	815	7/7	0.95	0.07	39,43,44,44	0
6	PGE	A	834	10/10	0.95	0.08	41,46,48,49	0
4	EDO	B	817	4/4	0.96	0.09	39,43,44,44	0
4	EDO	A	817	4/4	0.96	0.06	41,41,42,43	0
4	EDO	B	821	4/4	0.96	0.07	38,39,40,40	0
4	EDO	A	806	4/4	0.96	0.07	42,45,46,47	0
4	EDO	B	823	4/4	0.96	0.08	43,44,45,46	0
4	EDO	C	809	4/4	0.96	0.08	39,41,42,44	0
4	EDO	C	820	4/4	0.96	0.07	41,42,45,50	0
4	EDO	A	809	4/4	0.96	0.07	35,37,40,43	0
4	EDO	C	823	4/4	0.96	0.06	41,42,43,44	0
4	EDO	C	824	4/4	0.96	0.07	36,37,37,40	0
4	EDO	C	826	4/4	0.96	0.17	35,36,36,36	0
4	EDO	A	811	4/4	0.96	0.08	37,39,44,47	0
4	EDO	A	804	4/4	0.96	0.07	40,41,42,44	0
4	EDO	A	814	4/4	0.96	0.07	40,41,42,44	0
4	EDO	A	828	4/4	0.96	0.07	39,39,40,41	0
4	EDO	A	816	4/4	0.96	0.07	40,42,43,46	0
4	EDO	B	812	4/4	0.96	0.08	37,39,40,44	0
4	EDO	D	813	4/4	0.96	0.07	37,39,40,41	0
5	PEG	A	833	7/7	0.96	0.09	42,42,44,46	0
4	EDO	B	814	4/4	0.96	0.07	36,37,39,44	0
5	PEG	B	827	7/7	0.96	0.07	43,44,45,48	0
4	EDO	B	815	4/4	0.96	0.07	44,44,47,48	0
4	EDO	B	816	4/4	0.96	0.07	38,40,40,43	0
8	IMD	D	814	5/5	0.96	0.06	37,37,43,44	0
8	IMD	D	818	5/5	0.96	0.08	33,38,39,39	0
4	EDO	A	819	4/4	0.97	0.08	38,39,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	808	4/4	0.97	0.08	41,42,44,47	0
4	EDO	A	812	4/4	0.97	0.08	44,45,45,52	0
4	EDO	A	829	4/4	0.97	0.08	32,40,42,50	0
4	EDO	C	825	4/4	0.97	0.07	35,35,37,37	0
4	EDO	B	818	4/4	0.97	0.07	39,41,43,47	0
4	EDO	C	827	4/4	0.97	0.06	36,39,43,46	0
4	EDO	B	819	4/4	0.97	0.06	39,42,45,50	0
4	EDO	C	829	4/4	0.97	0.07	35,37,40,45	0
4	EDO	A	810	4/4	0.97	0.07	39,40,41,41	0
4	EDO	B	806	4/4	0.97	0.06	33,35,35,36	0
4	EDO	B	810	4/4	0.97	0.06	42,42,43,44	0
4	EDO	D	807	4/4	0.97	0.08	38,39,39,44	0
4	EDO	B	811	4/4	0.97	0.06	36,36,37,38	0
4	EDO	B	824	4/4	0.97	0.08	39,40,42,43	0
4	EDO	D	812	4/4	0.97	0.07	40,40,43,43	0
4	EDO	C	804	4/4	0.97	0.07	37,37,37,41	0
5	PEG	A	831	7/7	0.97	0.07	35,39,43,45	0
5	PEG	A	832	7/7	0.97	0.07	35,39,45,45	0
4	EDO	C	806	4/4	0.97	0.07	38,41,42,43	0
5	PEG	B	825	7/7	0.97	0.07	35,37,39,39	0
4	EDO	C	808	4/4	0.97	0.06	33,34,35,35	0
4	EDO	A	824	4/4	0.97	0.08	35,37,39,40	0
5	PEG	C	832	7/7	0.97	0.08	41,44,45,46	0
4	EDO	C	812	4/4	0.97	0.07	39,41,42,44	0
5	PEG	D	816	7/7	0.97	0.07	32,37,38,39	0
5	PEG	D	817	7/7	0.97	0.06	33,37,40,40	0
4	EDO	C	816	4/4	0.97	0.07	36,36,37,40	0
7	MPD	C	833	8/8	0.97	0.07	37,38,40,42	0
4	EDO	C	818	4/4	0.97	0.07	36,37,37,40	0
4	EDO	C	819	4/4	0.97	0.07	31,35,41,41	0
4	EDO	A	815	4/4	0.98	0.06	37,39,40,41	0
4	EDO	C	813	4/4	0.98	0.11	33,36,36,38	0
4	EDO	D	806	4/4	0.98	0.06	38,39,39,41	0
4	EDO	C	814	4/4	0.98	0.07	40,41,42,44	0
4	EDO	C	815	4/4	0.98	0.07	36,36,39,40	0
4	EDO	A	818	4/4	0.98	0.05	41,44,44,45	0
4	EDO	D	810	4/4	0.98	0.06	33,37,40,43	0
4	EDO	D	811	4/4	0.98	0.06	33,38,41,43	0
4	EDO	C	817	4/4	0.98	0.06	38,42,42,43	0
4	EDO	B	813	4/4	0.98	0.06	42,43,45,47	0
4	EDO	D	819	4/4	0.98	0.06	38,38,38,41	0
4	EDO	B	805	4/4	0.98	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	822	4/4	0.98	0.10	34,36,36,38	0
4	EDO	C	821	4/4	0.98	0.08	31,31,31,34	0
4	EDO	C	803	4/4	0.98	0.07	36,37,38,42	0
4	EDO	B	807	4/4	0.98	0.07	35,36,37,42	0
4	EDO	C	805	4/4	0.98	0.06	37,40,40,42	0
4	EDO	B	808	4/4	0.98	0.08	36,37,37,38	0
4	EDO	C	807	4/4	0.98	0.08	42,46,46,49	0
4	EDO	B	809	4/4	0.98	0.05	40,40,41,41	0
4	EDO	A	805	4/4	0.98	0.07	41,43,43,43	0
4	EDO	C	810	4/4	0.98	0.06	35,36,39,43	0
4	EDO	C	830	4/4	0.98	0.06	40,42,42,44	0
7	MPD	C	834	8/8	0.98	0.08	38,41,44,48	0
4	EDO	C	831	4/4	0.98	0.06	47,48,48,49	0
4	EDO	C	811	4/4	0.98	0.07	35,39,40,44	0
4	EDO	A	825	4/4	0.99	0.05	32,33,33,35	0
4	EDO	A	807	4/4	0.99	0.04	38,38,41,43	0
4	EDO	B	803	4/4	0.99	0.03	34,35,35,36	0
4	EDO	B	804	4/4	0.99	0.05	31,34,35,39	0
2	CA	C	801	1/1	1.00	0.02	28,28,28,28	0
2	CA	D	801	1/1	1.00	0.02	27,27,27,27	0
3	MN	A	802	1/1	1.00	0.04	35,35,35,35	0
3	MN	B	802	1/1	1.00	0.05	33,33,33,33	0
3	MN	C	802	1/1	1.00	0.03	33,33,33,33	0
3	MN	D	802	1/1	1.00	0.02	30,30,30,30	0
2	CA	A	801	1/1	1.00	0.01	25,25,25,25	0
2	CA	B	801	1/1	1.00	0.01	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.