



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2022 – 12:48 AM JST

PDB ID : 7EXK
Title : An AA9 LPMO of Ceriporiopsis subvermispora
Authors : Nguyen, H.; Kondo, K.; Nagata, T.; Katahira, M.; Mikami, B.
Deposited on : 2021-05-27
Resolution : 2.14 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
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)	:	2.28.1

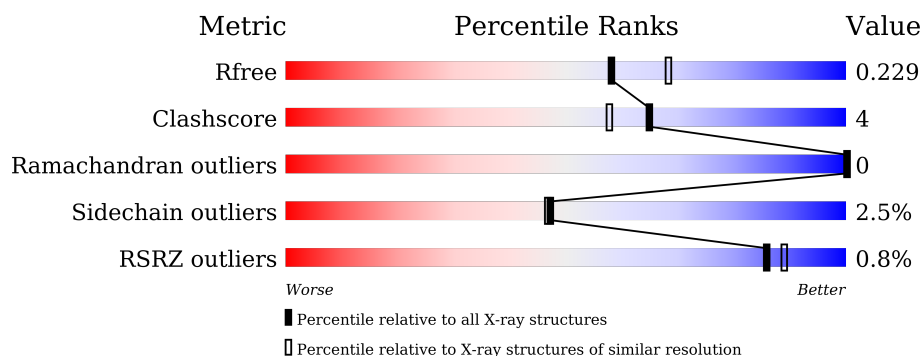
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	217	<div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	B	217	<div> <div>90%</div> <div>10%</div> </div>
1	C	217	<div> <div></div> <div>93%</div> <div>7%</div> </div>
1	D	217	<div> <div>89%</div> <div>10%</div> </div>
1	E	217	<div> <div></div> <div>89%</div> <div>11%</div> </div>
1	F	217	<div> <div>88%</div> <div>12%</div> <div>.</div> </div>

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	EDO	E	303	-	-	X	-

2 Entry composition [i](#)

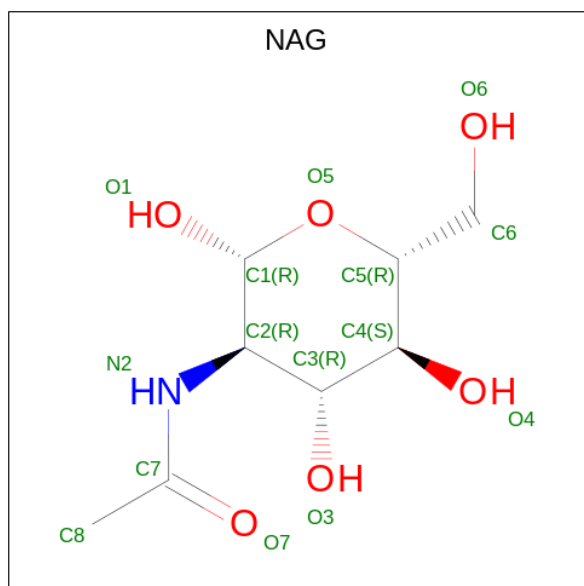
There are 8 unique types of molecules in this entry. The entry contains 10833 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycoside hydrolase family 61 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	1	0
			1634	1045	262	324	3			
1	B	217	Total	C	N	O	S	0	2	0
			1637	1045	263	326	3			
1	C	217	Total	C	N	O	S	0	1	0
			1631	1041	262	325	3			
1	D	217	Total	C	N	O	S	0	1	0
			1631	1041	263	324	3			
1	E	217	Total	C	N	O	S	0	3	0
			1646	1053	263	327	3			
1	F	217	Total	C	N	O	S	0	0	0
			1625	1037	262	323	3			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

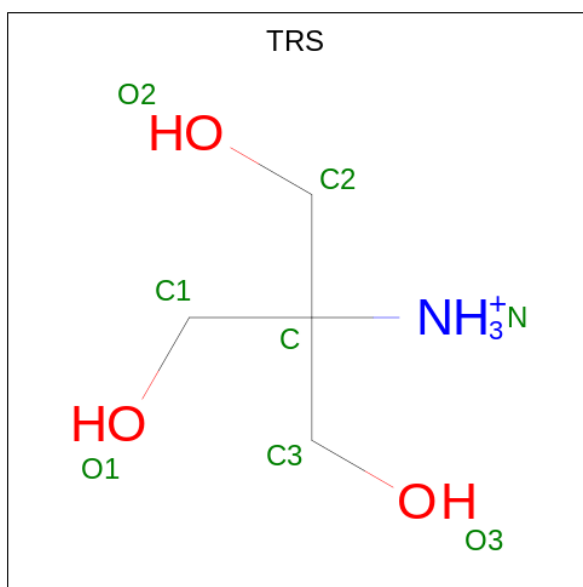


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

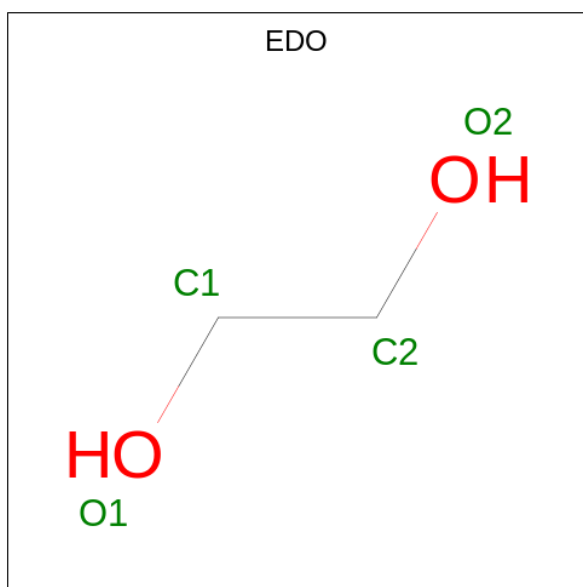
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cu	0	0
			1	1		
3	B	1	Total	Cu	0	0
			1	1		
3	C	1	Total	Cu	0	0
			1	1		
3	D	1	Total	Cu	0	0
			1	1		
3	E	1	Total	Cu	0	0
			1	1		
3	F	1	Total	Cu	0	0
			1	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	C	1	Total	C	N	O	0	0
			8	4	1	3		
4	F	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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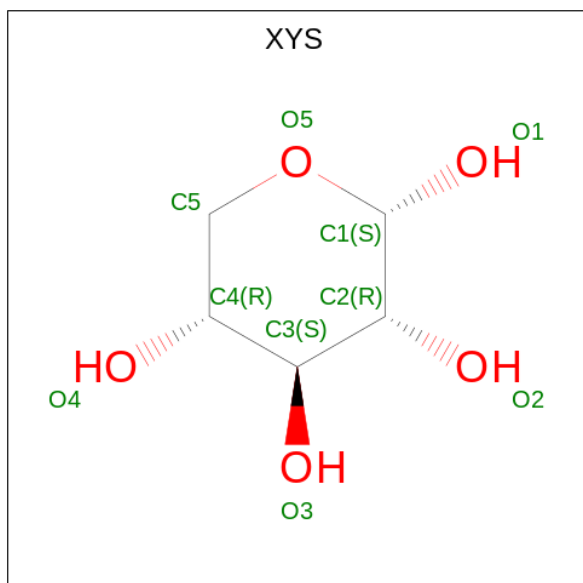
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total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

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

- Molecule 6 is alpha-D-xylopyranose (three-letter code: XYZ) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			9	5	4		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total 1	Ca 1	0	0
7	F	1	Total 1	Ca 1	0	0

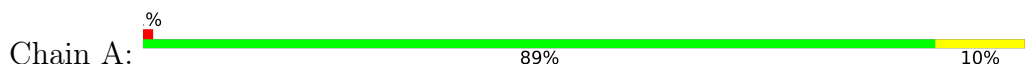
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	84	Total 84	O 84	0	0
8	B	118	Total 118	O 118	0	0
8	C	79	Total 79	O 79	0	0
8	D	142	Total 142	O 142	0	0
8	E	84	Total 84	O 84	0	0
8	F	109	Total 109	O 109	0	0

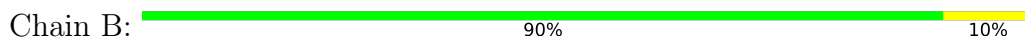
3 Residue-property plots [i](#)

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: Glycoside hydrolase family 61 protein



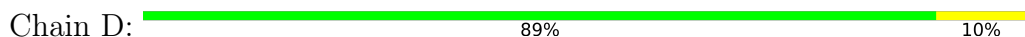
- Molecule 1: Glycoside hydrolase family 61 protein



- Molecule 1: Glycoside hydrolase family 61 protein



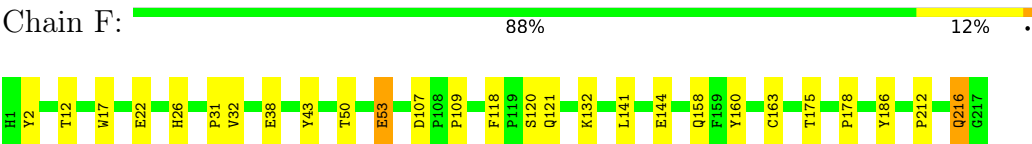
- Molecule 1: Glycoside hydrolase family 61 protein



- Molecule 1: Glycoside hydrolase family 61 protein



- Molecule 1: Glycoside hydrolase family 61 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.06Å 52.43Å 134.62Å 90.00° 90.55° 90.00°	Depositor
Resolution (Å)	48.85 – 2.14 48.85 – 2.14	Depositor EDS
% Data completeness (in resolution range)	95.5 (48.85-2.14) 95.5 (48.85-2.14)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.172 , 0.230 0.172 , 0.229	Depositor DCC
R_{free} test set	3100 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10833	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6415e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CA, XYS, TRS, EDO, CU, NAG

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	0.39	0/1690	0.59	0/2324
1	B	0.41	0/1695	0.60	0/2330
1	C	0.37	0/1686	0.58	0/2318
1	D	0.42	0/1686	0.59	0/2318
1	E	0.39	0/1708	0.57	0/2348
1	F	0.41	0/1677	0.60	0/2306
All	All	0.40	0/10142	0.59	0/13944

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	1634	0	1519	17	0
1	B	1637	0	1523	15	0
1	C	1631	0	1516	9	0
1	D	1631	0	1518	15	0
1	E	1646	0	1533	14	0
1	F	1625	0	1510	15	0
2	A	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	16	0	24	1	0
4	B	16	0	24	0	0
4	C	8	0	12	0	0
4	F	8	0	12	1	0
5	A	40	0	60	7	0
5	B	76	0	114	6	0
5	C	20	0	30	1	0
5	D	40	0	60	4	0
5	E	40	0	60	4	0
5	F	48	0	72	4	0
6	B	9	0	8	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	A	84	0	0	2	0
8	B	118	0	0	1	0
8	C	79	0	0	1	0
8	D	142	0	0	1	0
8	E	84	0	0	2	0
8	F	109	0	0	2	0
All	All	10833	0	9673	82	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 4.

The worst 5 of 82 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:F:32:VAL:HG13	5:F:307:EDO:H21	1.64	0.79
1:D:153:THR:HA	5:D:303:EDO:H12	1.66	0.75
1:F:216:GLN:NE2	8:F:401:HOH:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:ASP:OD1	4:F:303:TRS:N	2.25	0.69
1:B:76:PRO:HA	5:B:307:EDO:H22	1.76	0.68

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	216/217 (100%)	213 (99%)	3 (1%)	0	100	100
1	B	217/217 (100%)	213 (98%)	4 (2%)	0	100	100
1	C	216/217 (100%)	213 (99%)	3 (1%)	0	100	100
1	D	216/217 (100%)	212 (98%)	4 (2%)	0	100	100
1	E	218/217 (100%)	214 (98%)	4 (2%)	0	100	100
1	F	215/217 (99%)	212 (99%)	3 (1%)	0	100	100
All	All	1298/1302 (100%)	1277 (98%)	21 (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	169/168 (101%)	164 (97%)	5 (3%)	41	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	170/168 (101%)	167 (98%)	3 (2%)	59	60
1	C	169/168 (101%)	166 (98%)	3 (2%)	59	60
1	D	169/168 (101%)	166 (98%)	3 (2%)	59	60
1	E	171/168 (102%)	168 (98%)	3 (2%)	59	60
1	F	168/168 (100%)	160 (95%)	8 (5%)	25	21
All	All	1016/1008 (101%)	991 (98%)	25 (2%)	47	47

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2	TYR
1	F	2	TYR
1	F	216	GLN
1	E	112	GLU
1	F	12	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 8 are monoatomic - leaving 79 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	$\# Z > 2$
5	EDO	B	308	-	3,3,3	0.57	0	2,2,2	0.23	0
4	TRS	F	303	-	7,7,7	0.50	0	9,9,9	0.90	0
5	EDO	F	315	-	3,3,3	0.47	0	2,2,2	0.40	0
4	TRS	B	303	-	7,7,7	0.35	0	9,9,9	0.50	0
5	EDO	E	310	-	3,3,3	0.56	0	2,2,2	0.26	0
5	EDO	D	309	-	3,3,3	0.67	0	2,2,2	0.19	0
5	EDO	A	314	-	3,3,3	0.46	0	2,2,2	0.39	0
5	EDO	A	308	-	3,3,3	0.51	0	2,2,2	0.24	0
6	XYX	B	324	-	9,9,10	1.76	2 (22%)	10,12,14	2.49	3 (30%)
5	EDO	E	303	-	3,3,3	0.35	0	2,2,2	0.03	0
5	EDO	B	305	-	3,3,3	0.42	0	2,2,2	0.44	0
5	EDO	E	309	-	3,3,3	0.45	0	2,2,2	0.53	0
5	EDO	D	303	-	3,3,3	0.51	0	2,2,2	0.44	0
5	EDO	D	312	-	3,3,3	0.65	0	2,2,2	0.18	0
5	EDO	E	307	-	3,3,3	0.61	0	2,2,2	0.16	0
5	EDO	A	312	-	3,3,3	0.54	0	2,2,2	0.20	0
4	TRS	B	304	-	7,7,7	0.24	0	9,9,9	0.41	0
5	EDO	C	305	-	3,3,3	0.49	0	2,2,2	0.34	0
5	EDO	D	310	-	3,3,3	0.54	0	2,2,2	0.33	0
5	EDO	F	306	-	3,3,3	0.49	0	2,2,2	0.26	0
5	EDO	D	304	-	3,3,3	0.59	0	2,2,2	0.08	0
5	EDO	E	305	-	3,3,3	0.46	0	2,2,2	0.78	0
5	EDO	B	322	-	3,3,3	0.50	0	2,2,2	0.12	0
5	EDO	F	311	-	3,3,3	0.54	0	2,2,2	0.29	0
5	EDO	F	309	-	3,3,3	0.64	0	2,2,2	0.51	0
5	EDO	C	306	-	3,3,3	0.67	0	2,2,2	0.18	0
5	EDO	A	305	-	3,3,3	0.49	0	2,2,2	0.13	0
5	EDO	F	310	-	3,3,3	0.42	0	2,2,2	0.47	0
5	EDO	D	305	-	3,3,3	0.62	0	2,2,2	0.21	0
2	NAG	D	301	1	14,14,15	0.43	0	17,19,21	0.56	0
5	EDO	D	308	-	3,3,3	0.55	0	2,2,2	0.19	0
5	EDO	B	309	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	B	323	-	3,3,3	0.45	0	2,2,2	0.39	0
5	EDO	E	312	-	3,3,3	0.54	0	2,2,2	0.27	0
4	TRS	A	304	-	7,7,7	0.37	0	9,9,9	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	306	-	3,3,3	0.54	0	2,2,2	0.22	0
5	EDO	B	307	-	3,3,3	0.30	0	2,2,2	0.27	0
5	EDO	B	310	-	3,3,3	0.43	0	2,2,2	0.46	0
5	EDO	B	315	-	3,3,3	0.52	0	2,2,2	0.27	0
2	NAG	B	301	1	14,14,15	0.25	0	17,19,21	0.53	0
2	NAG	F	301	1	14,14,15	0.24	0	17,19,21	0.53	0
5	EDO	C	304	-	3,3,3	0.60	0	2,2,2	0.07	0
5	EDO	B	312	-	3,3,3	0.49	0	2,2,2	0.49	0
5	EDO	F	312	-	3,3,3	0.51	0	2,2,2	0.25	0
5	EDO	B	311	-	3,3,3	0.48	0	2,2,2	0.57	0
4	TRS	C	303	-	7,7,7	0.31	0	9,9,9	0.92	0
5	EDO	E	308	-	3,3,3	0.55	0	2,2,2	0.23	0
5	EDO	A	307	-	3,3,3	0.56	0	2,2,2	0.11	0
5	EDO	B	320	-	3,3,3	0.54	0	2,2,2	0.39	0
5	EDO	F	307	-	3,3,3	0.58	0	2,2,2	0.25	0
2	NAG	A	301	1	14,14,15	0.42	0	17,19,21	0.43	0
5	EDO	C	308	-	3,3,3	0.50	0	2,2,2	0.35	0
5	EDO	B	316	-	3,3,3	0.46	0	2,2,2	0.46	0
5	EDO	F	305	-	3,3,3	0.56	0	2,2,2	0.23	0
5	EDO	B	314	-	3,3,3	0.50	0	2,2,2	0.32	0
5	EDO	F	308	-	3,3,3	0.66	0	2,2,2	0.18	0
5	EDO	B	321	-	3,3,3	0.63	0	2,2,2	0.13	0
5	EDO	B	313	-	3,3,3	0.41	0	2,2,2	0.46	0
5	EDO	B	319	-	3,3,3	0.55	0	2,2,2	0.41	0
4	TRS	A	303	-	7,7,7	0.52	0	9,9,9	0.49	0
5	EDO	E	304	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	A	311	-	3,3,3	0.50	0	2,2,2	0.29	0
5	EDO	A	309	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	D	306	-	3,3,3	0.48	0	2,2,2	0.48	0
5	EDO	A	310	-	3,3,3	0.50	0	2,2,2	0.42	0
2	NAG	E	301	1	14,14,15	0.52	0	17,19,21	0.62	0
5	EDO	B	306	-	3,3,3	0.58	0	2,2,2	0.14	0
5	EDO	F	304	-	3,3,3	0.57	0	2,2,2	0.17	0
5	EDO	B	317	-	3,3,3	0.49	0	2,2,2	0.26	0
5	EDO	E	306	-	3,3,3	0.46	0	2,2,2	0.36	0
5	EDO	F	314	-	3,3,3	0.55	0	2,2,2	0.21	0
5	EDO	F	313	-	3,3,3	0.48	0	2,2,2	0.30	0
5	EDO	C	307	-	3,3,3	0.53	0	2,2,2	0.24	0
5	EDO	A	313	-	3,3,3	0.63	0	2,2,2	0.15	0
2	NAG	C	301	1	14,14,15	0.34	0	17,19,21	0.45	0
5	EDO	E	311	-	3,3,3	0.50	0	2,2,2	0.39	0
5	EDO	D	311	-	3,3,3	0.41	0	2,2,2	0.37	0
5	EDO	D	307	-	3,3,3	0.49	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	318	-	3,3,3	0.46	0	2,2,2	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	308	-	-	0/1/1/1	-
4	TRS	F	303	-	-	3/9/9/9	-
5	EDO	F	315	-	-	0/1/1/1	-
4	TRS	B	303	-	-	0/9/9/9	-
5	EDO	E	310	-	-	0/1/1/1	-
5	EDO	D	309	-	-	1/1/1/1	-
5	EDO	A	314	-	-	0/1/1/1	-
5	EDO	A	308	-	-	0/1/1/1	-
6	XYS	B	324	-	-	-	0/1/1/1
5	EDO	E	303	-	-	0/1/1/1	-
5	EDO	B	305	-	-	0/1/1/1	-
5	EDO	E	309	-	-	0/1/1/1	-
5	EDO	D	303	-	-	0/1/1/1	-
5	EDO	D	312	-	-	0/1/1/1	-
5	EDO	E	307	-	-	1/1/1/1	-
5	EDO	A	312	-	-	0/1/1/1	-
4	TRS	B	304	-	-	3/9/9/9	-
5	EDO	C	305	-	-	0/1/1/1	-
5	EDO	D	310	-	-	1/1/1/1	-
5	EDO	F	306	-	-	0/1/1/1	-
5	EDO	D	304	-	-	1/1/1/1	-
5	EDO	E	305	-	-	1/1/1/1	-
5	EDO	B	322	-	-	0/1/1/1	-
5	EDO	F	311	-	-	0/1/1/1	-
5	EDO	F	309	-	-	1/1/1/1	-
5	EDO	C	306	-	-	0/1/1/1	-
5	EDO	A	305	-	-	0/1/1/1	-
5	EDO	F	310	-	-	0/1/1/1	-
5	EDO	D	305	-	-	0/1/1/1	-
2	NAG	D	301	1	-	0/6/23/26	0/1/1/1
5	EDO	D	308	-	-	0/1/1/1	-
5	EDO	B	309	-	-	1/1/1/1	-
5	EDO	B	323	-	-	0/1/1/1	-
5	EDO	E	312	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	A	304	-	-	5/9/9/9	-
5	EDO	A	306	-	-	0/1/1/1	-
5	EDO	B	307	-	-	1/1/1/1	-
5	EDO	B	310	-	-	1/1/1/1	-
5	EDO	B	315	-	-	0/1/1/1	-
2	NAG	B	301	1	-	0/6/23/26	0/1/1/1
2	NAG	F	301	1	-	2/6/23/26	0/1/1/1
5	EDO	C	304	-	-	0/1/1/1	-
5	EDO	B	312	-	-	0/1/1/1	-
5	EDO	F	312	-	-	0/1/1/1	-
5	EDO	B	311	-	-	1/1/1/1	-
4	TRS	C	303	-	-	4/9/9/9	-
5	EDO	E	308	-	-	0/1/1/1	-
5	EDO	A	307	-	-	0/1/1/1	-
5	EDO	B	320	-	-	0/1/1/1	-
5	EDO	F	307	-	-	1/1/1/1	-
2	NAG	A	301	1	-	4/6/23/26	0/1/1/1
5	EDO	C	308	-	-	1/1/1/1	-
5	EDO	B	316	-	-	1/1/1/1	-
5	EDO	F	305	-	-	0/1/1/1	-
5	EDO	B	314	-	-	0/1/1/1	-
5	EDO	F	308	-	-	1/1/1/1	-
5	EDO	B	321	-	-	0/1/1/1	-
5	EDO	B	313	-	-	1/1/1/1	-
5	EDO	B	319	-	-	1/1/1/1	-
4	TRS	A	303	-	-	4/9/9/9	-
5	EDO	E	304	-	-	0/1/1/1	-
5	EDO	A	311	-	-	1/1/1/1	-
5	EDO	A	309	-	-	1/1/1/1	-
5	EDO	D	306	-	-	0/1/1/1	-
5	EDO	A	310	-	-	0/1/1/1	-
2	NAG	E	301	1	-	2/6/23/26	0/1/1/1
5	EDO	B	306	-	-	0/1/1/1	-
5	EDO	F	304	-	-	0/1/1/1	-
5	EDO	B	317	-	-	1/1/1/1	-
5	EDO	E	306	-	-	0/1/1/1	-
5	EDO	F	314	-	-	0/1/1/1	-
5	EDO	F	313	-	-	0/1/1/1	-
5	EDO	C	307	-	-	0/1/1/1	-
5	EDO	A	313	-	-	0/1/1/1	-
2	NAG	C	301	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	E	311	-	-	0/1/1/1	-
5	EDO	D	311	-	-	1/1/1/1	-
5	EDO	D	307	-	-	0/1/1/1	-
5	EDO	B	318	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	324	XYS	O5-C1	3.30	1.49	1.42
6	B	324	XYS	O5-C5	2.92	1.48	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	324	XYS	C5-C4-C3	5.28	116.15	109.67
6	B	324	XYS	C1-C2-C3	-4.68	103.91	109.67
6	B	324	XYS	O2-C2-C3	2.64	115.43	110.14

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	TRS	N-C-C2-O2
4	A	303	TRS	C1-C-C3-O3
4	A	303	TRS	C2-C-C3-O3
4	A	303	TRS	N-C-C3-O3
4	A	304	TRS	C2-C-C1-O1

There are no ring outliers.

20 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	303	TRS	1	0
5	D	309	EDO	1	0
5	A	314	EDO	1	0
5	E	303	EDO	4	0
5	D	303	EDO	1	0
5	C	305	EDO	1	0
5	D	310	EDO	1	0
5	A	305	EDO	2	0
5	B	307	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	310	EDO	3	0
5	B	311	EDO	1	0
5	B	320	EDO	1	0
5	F	307	EDO	1	0
2	A	301	NAG	1	0
5	F	308	EDO	3	0
4	A	303	TRS	1	0
5	A	311	EDO	1	0
5	A	309	EDO	2	0
5	A	313	EDO	1	0
5	D	307	EDO	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 [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	217/217 (100%)	-0.26	3 (1%) 75 80	20, 32, 51, 66	0
1	B	217/217 (100%)	-0.55	1 (0%) 91 93	15, 25, 42, 51	0
1	C	217/217 (100%)	-0.24	3 (1%) 75 80	25, 34, 50, 62	0
1	D	217/217 (100%)	-0.56	1 (0%) 91 93	16, 25, 36, 48	0
1	E	217/217 (100%)	-0.27	3 (1%) 75 80	21, 32, 53, 70	0
1	F	217/217 (100%)	-0.50	0 100 100	16, 25, 41, 58	0
All	All	1302/1302 (100%)	-0.40	11 (0%) 86 89	15, 29, 48, 70	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	113	ASN	3.9
1	C	216	GLN	3.7
1	E	114	GLY	3.2
1	A	202	ALA	3.1
1	D	202	ALA	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
5	EDO	D	312	4/4	0.66	0.23	37,43,47,50	0
5	EDO	C	306	4/4	0.71	0.20	37,44,45,48	0
5	EDO	A	308	4/4	0.71	0.14	36,42,45,51	0
5	EDO	D	309	4/4	0.72	0.25	34,34,35,36	0
4	TRS	B	304	8/8	0.74	0.16	51,59,61,62	0
5	EDO	B	321	4/4	0.75	0.17	39,41,44,47	0
5	EDO	A	310	4/4	0.75	0.28	38,38,39,47	0
5	EDO	D	305	4/4	0.77	0.15	36,40,41,48	0
6	XYS	B	324	9/10	0.79	0.19	37,46,53,59	0
5	EDO	F	312	4/4	0.81	0.11	38,42,45,45	0
5	EDO	F	308	4/4	0.81	0.28	32,35,35,37	0
5	EDO	D	308	4/4	0.82	0.11	41,43,46,49	0
5	EDO	F	309	4/4	0.82	0.26	29,31,35,38	0
5	EDO	D	304	4/4	0.82	0.16	37,38,48,54	0
2	NAG	E	301	14/15	0.82	0.29	56,60,64,65	0
5	EDO	B	312	4/4	0.83	0.14	36,41,49,61	0
4	TRS	A	303	8/8	0.83	0.13	29,40,51,54	0
4	TRS	C	303	8/8	0.84	0.10	46,50,52,55	0
4	TRS	F	303	8/8	0.84	0.15	19,40,46,58	0
5	EDO	E	306	4/4	0.84	0.15	58,61,61,66	0
5	EDO	E	308	4/4	0.84	0.16	40,43,45,53	0
5	EDO	B	315	4/4	0.85	0.21	35,39,42,42	0
5	EDO	B	310	4/4	0.85	0.20	30,35,35,37	0
5	EDO	B	317	4/4	0.86	0.18	36,38,42,48	0
5	EDO	E	312	4/4	0.86	0.17	38,40,43,46	0
5	EDO	B	309	4/4	0.87	0.12	39,41,49,59	0
5	EDO	A	307	4/4	0.87	0.14	35,39,39,42	0
5	EDO	E	310	4/4	0.87	0.19	37,41,41,45	0
5	EDO	B	311	4/4	0.87	0.17	30,39,43,47	0
4	TRS	A	304	8/8	0.87	0.15	28,45,53,56	0
5	EDO	B	313	4/4	0.87	0.18	37,39,46,46	0
2	NAG	A	301	14/15	0.87	0.14	42,48,55,56	0
5	EDO	A	311	4/4	0.87	0.16	36,40,42,45	0
5	EDO	D	303	4/4	0.88	0.16	25,33,37,41	0
5	EDO	E	305	4/4	0.88	0.14	42,43,43,45	0
5	EDO	A	313	4/4	0.89	0.20	32,38,40,43	0
5	EDO	A	312	4/4	0.89	0.17	37,44,49,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	C	307	4/4	0.89	0.21	41,42,43,46	0
5	EDO	F	307	4/4	0.90	0.20	29,32,35,37	0
5	EDO	B	319	4/4	0.90	0.17	30,33,35,45	0
5	EDO	A	309	4/4	0.90	0.35	44,44,55,60	0
5	EDO	B	318	4/4	0.90	0.13	35,37,46,54	0
5	EDO	F	305	4/4	0.90	0.14	36,38,41,42	0
5	EDO	C	305	4/4	0.91	0.26	38,39,40,43	0
5	EDO	B	320	4/4	0.91	0.23	28,35,44,47	0
5	EDO	B	316	4/4	0.91	0.20	32,38,44,45	0
5	EDO	B	322	4/4	0.91	0.17	39,42,46,53	0
4	TRS	B	303	8/8	0.92	0.10	48,54,58,59	0
5	EDO	E	307	4/4	0.93	0.16	28,28,36,40	0
5	EDO	C	308	4/4	0.93	0.11	41,41,42,47	0
5	EDO	E	309	4/4	0.93	0.14	28,34,37,40	0
5	EDO	A	306	4/4	0.93	0.13	32,32,37,40	0
5	EDO	F	311	4/4	0.93	0.12	36,37,40,50	0
5	EDO	D	310	4/4	0.93	0.13	29,41,42,45	0
5	EDO	F	314	4/4	0.93	0.15	28,30,40,42	0
5	EDO	F	304	4/4	0.93	0.17	25,27,33,35	0
5	EDO	B	323	4/4	0.94	0.11	31,33,37,40	0
5	EDO	A	305	4/4	0.94	0.20	26,29,35,47	0
5	EDO	D	306	4/4	0.94	0.08	40,44,51,51	0
5	EDO	D	307	4/4	0.94	0.17	32,33,37,43	0
5	EDO	F	310	4/4	0.94	0.28	42,43,47,48	0
5	EDO	B	314	4/4	0.94	0.12	32,37,42,47	0
2	NAG	C	301	14/15	0.94	0.12	41,46,52,56	0
5	EDO	F	313	4/4	0.94	0.15	39,42,43,49	0
2	NAG	F	301	14/15	0.94	0.13	29,34,42,51	0
5	EDO	F	315	4/4	0.94	0.14	40,46,47,53	0
5	EDO	B	305	4/4	0.94	0.14	26,28,30,30	0
5	EDO	D	311	4/4	0.95	0.12	32,34,39,39	0
5	EDO	B	307	4/4	0.95	0.27	23,28,28,30	0
5	EDO	E	303	4/4	0.95	0.25	35,35,37,38	0
5	EDO	A	314	4/4	0.95	0.24	46,46,48,49	0
5	EDO	E	311	4/4	0.95	0.26	32,40,46,47	0
5	EDO	C	304	4/4	0.95	0.11	33,34,37,39	0
7	CA	D	313	1/1	0.95	0.09	56,56,56,56	0
5	EDO	F	306	4/4	0.96	0.17	20,28,31,33	0
5	EDO	B	308	4/4	0.96	0.16	29,29,30,32	0
2	NAG	D	301	14/15	0.96	0.09	25,34,40,41	0
2	NAG	B	301	14/15	0.97	0.10	27,31,35,47	0
5	EDO	E	304	4/4	0.97	0.11	37,38,39,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CA	F	316	1/1	0.97	0.07	52,52,52,52	0
5	EDO	B	306	4/4	0.98	0.10	21,23,24,25	0
3	CU	C	302	1/1	0.98	0.05	34,34,34,34	0
3	CU	A	302	1/1	0.99	0.08	28,28,28,28	0
3	CU	B	302	1/1	0.99	0.08	22,22,22,22	0
3	CU	D	302	1/1	1.00	0.09	23,23,23,23	0
3	CU	E	302	1/1	1.00	0.08	26,26,26,26	0
3	CU	F	302	1/1	1.00	0.09	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.