Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2021 – 06:48 PM EDT

PDB ID	:	7SF2
Title	:	Crystal Structure of Beta-Galactosidase from Bacteroides cellulosilyticus
Authors	:	Kim, Y.; Joachimiak, G.; Endres, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2021-10-02
Resolution	:	2.75 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 following versions of software and data (see references ⓘ) were used in the production of this report:

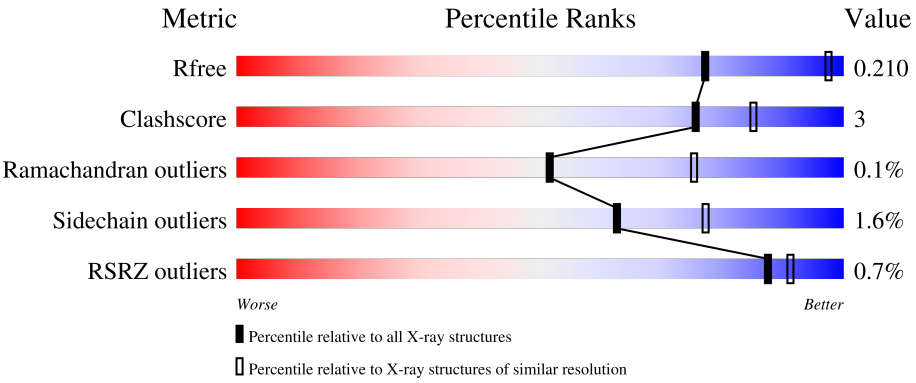
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	588	89% 11%
1	B	588	90% 9%
1	C	588	90% 9%
1	D	588	89% 10%
1	E	588	88% 11%

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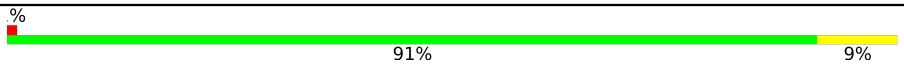
Mol	Chain	Length	Quality of chain
1	F	588	

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
7	PO4	E	712	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 31047 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 family 2, sugar binding domain protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	Se	0	11	0
			4859	3097	843	902	5	12			
1	B	586	Total	C	N	O	S	Se	0	13	0
			4876	3106	848	905	5	12			
1	C	585	Total	C	N	O	S	Se	0	12	0
			4857	3095	842	903	5	12			
1	D	586	Total	C	N	O	S	Se	0	11	0
			4869	3103	847	902	5	12			
1	E	586	Total	C	N	O	S	Se	0	8	0
			4827	3080	833	897	5	12			
1	F	586	Total	C	N	O	S	Se	0	8	0
			4826	3079	832	898	5	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	SER	-	expression tag	UNP E2NBY7
A	19	ASN	-	expression tag	UNP E2NBY7
A	20	ALA	-	expression tag	UNP E2NBY7
A	436	HIS	TYR	conflict	UNP E2NBY7
B	18	SER	-	expression tag	UNP E2NBY7
B	19	ASN	-	expression tag	UNP E2NBY7
B	20	ALA	-	expression tag	UNP E2NBY7
B	436	HIS	TYR	conflict	UNP E2NBY7
C	18	SER	-	expression tag	UNP E2NBY7
C	19	ASN	-	expression tag	UNP E2NBY7
C	20	ALA	-	expression tag	UNP E2NBY7
C	436	HIS	TYR	conflict	UNP E2NBY7
D	18	SER	-	expression tag	UNP E2NBY7
D	19	ASN	-	expression tag	UNP E2NBY7
D	20	ALA	-	expression tag	UNP E2NBY7
D	436	HIS	TYR	conflict	UNP E2NBY7
E	18	SER	-	expression tag	UNP E2NBY7

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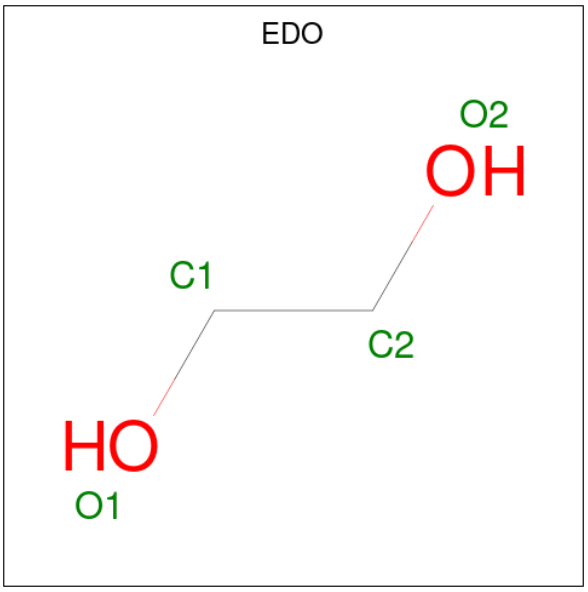
Chain	Residue	Modelled	Actual	Comment	Reference
E	19	ASN	-	expression tag	UNP E2NBY7
E	20	ALA	-	expression tag	UNP E2NBY7
E	436	HIS	TYR	conflict	UNP E2NBY7
F	18	SER	-	expression tag	UNP E2NBY7
F	19	ASN	-	expression tag	UNP E2NBY7
F	20	ALA	-	expression tag	UNP E2NBY7
F	436	HIS	TYR	conflict	UNP E2NBY7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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	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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
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
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

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Cl 4 4	0	0
4	B	3	Total Cl 3 3	0	0
4	C	3	Total Cl 3 3	0	0
4	D	2	Total Cl 2 2	0	0

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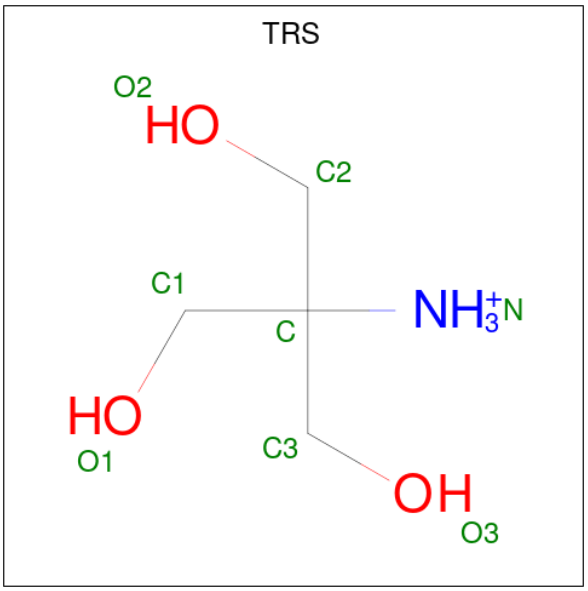
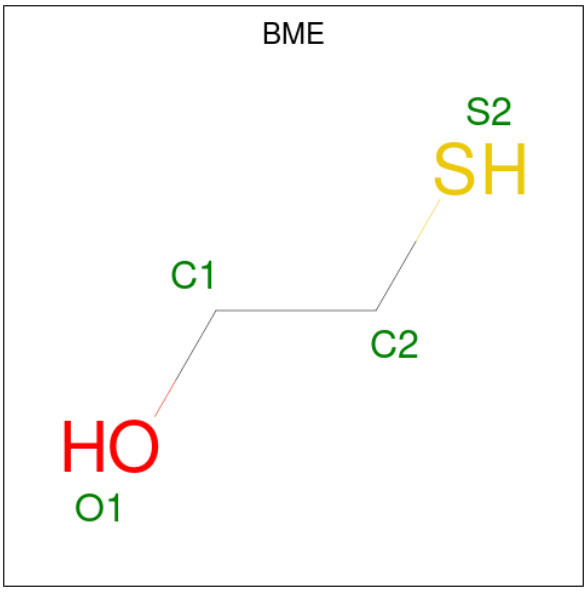
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



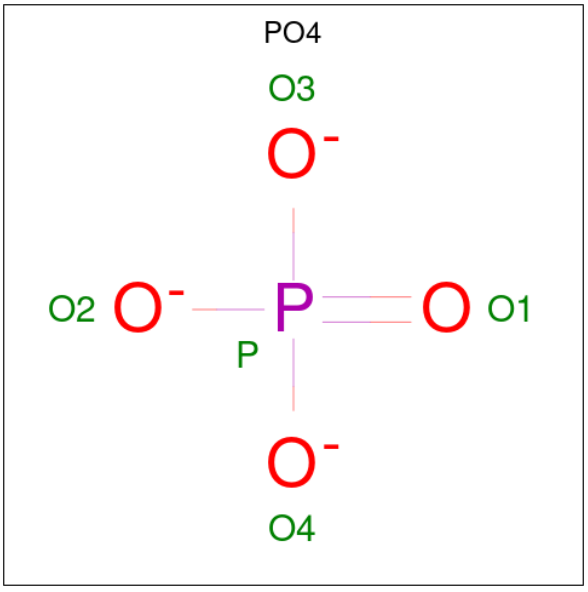
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 8 4 1 3	0	0
5	B	1	Total C N O 8 4 1 3	0	0
5	C	1	Total C N O 8 4 1 3	0	0
5	D	1	Total C N O 8 4 1 3	0	0
5	E	1	Total C N O 8 4 1 3	0	0
5	F	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total O P 5 4 1	0	0
7	E	1	Total O P 5 4 1	0	0
7	E	1	Total O P 5 4 1	0	0
7	E	1	Total O P 5 4 1	0	0
7	F	1	Total O P 5 4 1	0	0
7	F	1	Total O P 5 4 1	0	0

- Molecule 8 is water.

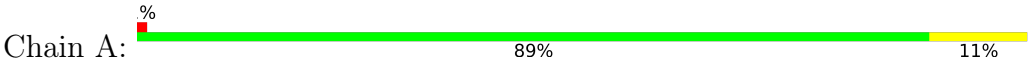
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	295	Total O 295 295	0	0
8	B	292	Total O 292 292	0	0
8	C	233	Total O 233 233	0	0
8	D	277	Total O 277 277	0	0
8	E	253	Total O 253 253	0	0
8	F	234	Total O 234 234	0	0

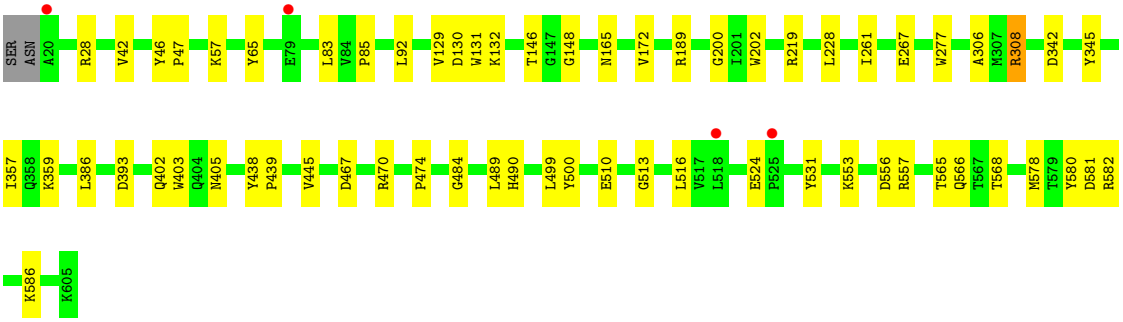
3 Residue-property plots (i)

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: Glycosyl hydrolase family 2, sugar binding domain protein

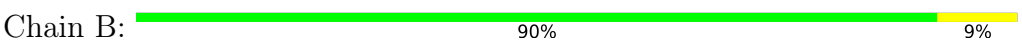
Chain A:

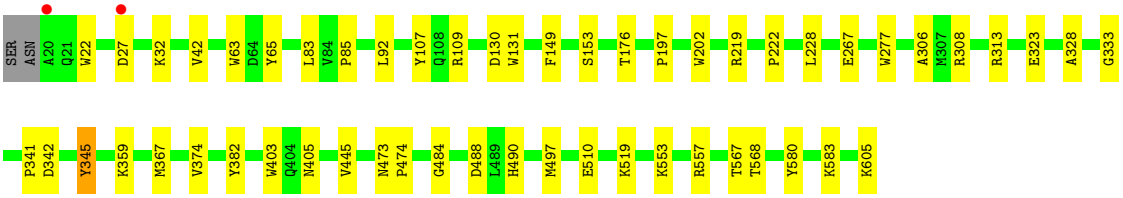




• Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

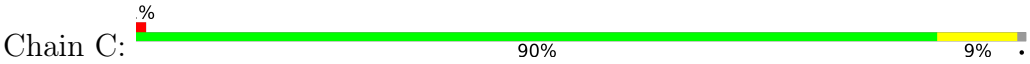
Chain B:

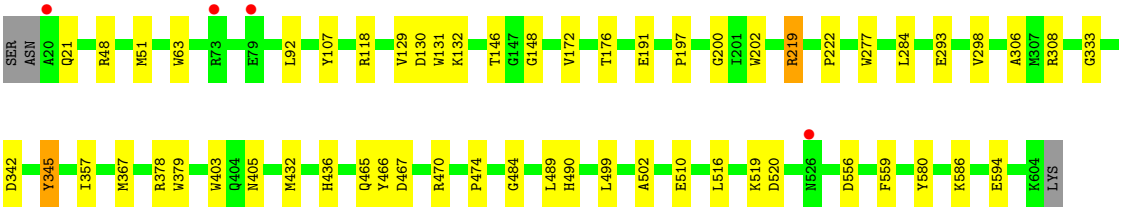




• Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

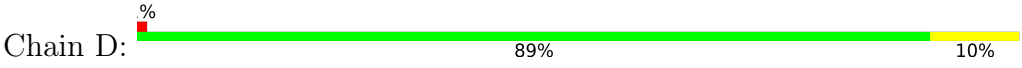
Chain C:

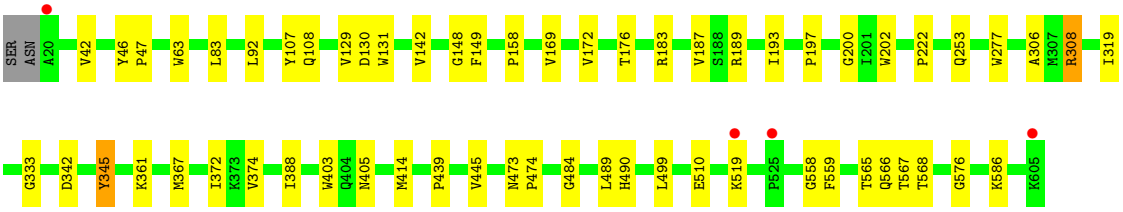




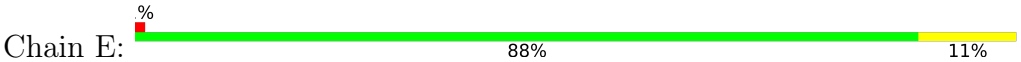
• Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

Chain D:

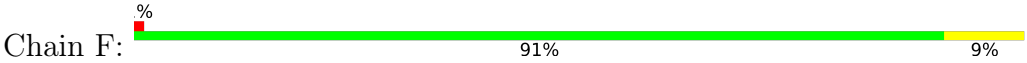


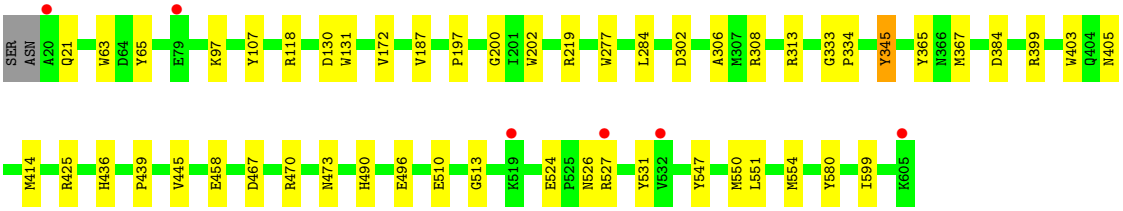


• Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein



• Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	335.85Å 349.40Å 352.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.10 – 2.75 48.10 – 2.75	Depositor EDS
% Data completeness (in resolution range)	90.8 (48.10-2.75) 90.8 (48.10-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.182 , 0.209 0.182 , 0.210	Depositor DCC
R_{free} test set	12548 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for l,-k,h 0.000 for -k,-h,-l 0.000 for -k,-l,h 0.000 for l,-h,-k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31047	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 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.24	0/4982	0.49	0/6753
1	B	0.24	0/4999	0.49	0/6777
1	C	0.24	0/4980	0.49	0/6753
1	D	0.24	0/4992	0.49	0/6766
1	E	0.24	0/4950	0.48	0/6712
1	F	0.24	0/4949	0.48	0/6711
All	All	0.24	0/29852	0.49	0/40472

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	4859	0	4714	37	0
1	B	4876	0	4729	31	0
1	C	4857	0	4706	28	0
1	D	4869	0	4728	31	0
1	E	4827	0	4684	32	0
1	F	4826	0	4680	25	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	56	0	84	3	0
3	B	60	0	90	6	0
3	C	36	0	54	3	0
3	D	28	0	42	1	0
3	E	28	0	42	1	0
3	F	24	0	36	0	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	8	0	12	0	0
5	B	8	0	12	0	0
5	C	8	0	12	0	0
5	D	8	0	12	1	0
5	E	8	0	12	0	0
5	F	8	0	12	0	0
6	B	4	0	6	0	0
7	B	5	0	0	0	0
7	C	10	0	0	0	0
7	D	5	0	0	0	0
7	E	15	0	0	0	0
7	F	10	0	0	0	0
8	A	295	0	0	2	0
8	B	292	0	0	1	0
8	C	233	0	0	0	0
8	D	277	0	0	1	0
8	E	253	0	0	1	0
8	F	234	0	0	1	0
All	All	31047	0	28667	179	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (179) 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:E:222:PRO:HD3	3:E:702:EDO:H11	1.78	0.65
1:A:557[B]:ARG:HD3	1:E:318:GLY:HA3	1.83	0.60
1:C:516:LEU:O	1:C:586:LYS:NZ	2.38	0.56
1:C:474:PRO:HG3	1:C:484:GLY:HA3	1.87	0.56
1:D:474:PRO:HG3	1:D:484:GLY:HA3	1.87	0.56
1:A:57:LYS:HA	3:A:707:EDO:H12	1.89	0.55
1:B:92:LEU:HG	1:B:342:ASP:HB2	1.88	0.55
1:B:219[B]:ARG:NH2	8:B:801:HOH:O	2.28	0.55
1:D:445:VAL:HG22	1:D:473:ASN:HB3	1.90	0.54
1:E:243:PHE:HB3	1:E:292:LYS:HB2	1.89	0.54
1:D:183:ARG:NH2	8:D:803:HOH:O	2.41	0.54
1:F:551:LEU:HD23	1:F:599:ILE:HD13	1.90	0.54
1:B:228:LEU:HD11	1:B:267:GLU:HB3	1.90	0.54
1:D:490:HIS:CD2	1:D:510:GLU:HB2	2.43	0.53
1:F:65:TYR:OH	1:F:97:LYS:NZ	2.42	0.53
1:A:474:PRO:HG3	1:A:484:GLY:HA3	1.91	0.53
1:A:568:THR:HG22	1:A:578:MSE:HE3	1.91	0.53
1:D:42:VAL:HG21	1:D:83:LEU:HD11	1.90	0.53
1:D:567:THR:HG22	1:D:568:THR:HG23	1.91	0.53
1:C:92:LEU:HG	1:C:342:ASP:HB2	1.92	0.52
1:C:219[B]:ARG:HG3	1:C:436:HIS:CD2	2.44	0.52
1:C:293:GLU:HB2	1:C:298:VAL:HG21	1.91	0.52
1:D:92:LEU:HG	1:D:342:ASP:HB2	1.92	0.52
1:B:32:LYS:HD3	3:B:707:EDO:H11	1.92	0.51
1:B:567:THR:HG22	1:B:568:THR:HG23	1.92	0.51
1:E:489:LEU:HD21	1:E:499:LEU:HB2	1.92	0.51
1:B:583:LYS:HA	3:B:707:EDO:H12	1.93	0.51
1:C:490:HIS:CD2	1:C:510:GLU:HB2	2.45	0.51
1:A:219[B]:ARG:NH1	8:A:803:HOH:O	2.44	0.51
1:E:445:VAL:HG22	1:E:473:ASN:HB3	1.93	0.51
1:E:176:THR:HG21	1:E:197:PRO:HB3	1.93	0.50
1:E:578:MSE:HE3	1:E:582:ARG:HD2	1.94	0.50
1:B:473:ASN:ND2	1:B:488:ASP:OD2	2.40	0.50
1:D:202:TRP:CE3	1:D:345:TYR:HB3	2.46	0.50
1:E:132:LYS:HG3	1:E:146:THR:HG22	1.92	0.50
1:B:341:PRO:HG3	1:B:580:TYR:CG	2.47	0.49
1:C:489:LEU:HD21	1:C:499:LEU:HB2	1.93	0.49
1:A:438:TYR:O	1:A:470:ARG:NH2	2.45	0.49
1:A:516:LEU:O	1:A:586:LYS:NZ	2.45	0.49
1:F:333:GLY:HA3	1:F:367:MSE:O	2.12	0.49
1:F:399:ARG:HG3	1:F:414:MSE:HE1	1.94	0.49
1:A:28:ARG:HH12	1:A:524:GLU:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:HIS:CD2	1:B:510:GLU:HB2	2.48	0.49
1:E:92:LEU:HG	1:E:342:ASP:HB2	1.94	0.49
1:F:490:HIS:CG	1:F:510:GLU:HB2	2.48	0.49
1:B:27:ASP:OD1	1:B:27:ASP:N	2.45	0.49
1:C:172:VAL:HG11	1:C:200:GLY:HA2	1.94	0.49
1:C:277:TRP:HB2	1:C:306:ALA:HB1	1.95	0.49
1:B:333:GLY:HA3	1:B:367:MSE:O	2.13	0.49
1:D:222:PRO:HD3	3:D:703:EDO:H22	1.95	0.49
1:C:130:ASP:HA	1:C:131:TRP:HA	1.59	0.48
1:E:438:TYR:O	1:E:470:ARG:NH2	2.47	0.48
1:A:261:ILE:HD11	1:D:142:VAL:HG12	1.96	0.48
1:D:130:ASP:HA	1:D:131:TRP:HA	1.57	0.48
1:B:277:TRP:HB2	1:B:306:ALA:HB1	1.96	0.48
1:D:277:TRP:HB2	1:D:306:ALA:HB1	1.95	0.48
1:C:63:TRP:CE3	1:C:107:TYR:HB3	2.49	0.48
1:D:108:GLN:HG3	1:D:169:VAL:HG22	1.96	0.48
1:A:92:LEU:HG	1:A:342:ASP:HB2	1.96	0.47
1:A:402:GLN:HB2	3:C:712:EDO:H22	1.96	0.47
1:A:42:VAL:HG21	1:A:83:LEU:HD11	1.96	0.47
1:E:130:ASP:HA	1:E:131:TRP:HA	1.57	0.47
1:B:130:ASP:HA	1:B:131:TRP:HA	1.59	0.47
1:C:403:TRP:CE2	1:C:405:ASN:HB3	2.49	0.47
1:B:149:PHE:HB3	1:B:374:VAL:HB	1.97	0.47
1:C:378:ARG:HH21	3:C:705:EDO:H11	1.80	0.47
1:E:28:ARG:HH12	1:E:524:GLU:HG3	1.79	0.47
1:E:172:VAL:HG11	1:E:200:GLY:HA2	1.96	0.47
1:F:172:VAL:HG11	1:F:200:GLY:HA2	1.97	0.47
1:A:172:VAL:HG11	1:A:200:GLY:HA2	1.97	0.47
1:B:42:VAL:HG21	1:B:83:LEU:HD11	1.97	0.47
1:B:474:PRO:HG3	1:B:484:GLY:HA3	1.97	0.47
1:A:359:LYS:HA	1:A:359:LYS:HE2	1.96	0.46
1:E:490:HIS:CD2	1:E:510:GLU:HB2	2.50	0.46
1:D:176:THR:HG21	1:D:197:PRO:HB3	1.97	0.46
1:D:333:GLY:HA3	1:D:367:MSE:O	2.16	0.46
1:A:553:LYS:NZ	8:A:806:HOH:O	2.48	0.46
1:D:403:TRP:CE2	1:D:405:ASN:HB3	2.50	0.46
1:B:557:ARG:HG3	3:B:705:EDO:H12	1.98	0.46
1:A:202:TRP:CE3	1:A:345:TYR:HB3	2.51	0.46
1:B:313:ARG:HG3	3:B:716:EDO:H22	1.98	0.46
1:D:149:PHE:HB3	1:D:374:VAL:HB	1.98	0.46
1:E:213:LYS:NZ	1:E:239:SER:OG	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:TYR:HB2	1:E:170:VAL:HB	1.99	0.45
1:C:202:TRP:CE3	1:C:345:TYR:HB3	2.51	0.45
1:F:496:GLU:HA	1:F:554:MSE:HE1	1.98	0.45
1:E:277:TRP:HB2	1:E:306:ALA:HB1	1.98	0.45
1:B:497:MSE:HE1	1:C:502:ALA:HB1	1.98	0.45
1:C:222:PRO:HD3	3:C:703:EDO:H11	1.98	0.45
1:F:490:HIS:CD2	1:F:510:GLU:HB2	2.51	0.45
1:A:490:HIS:CD2	1:A:510:GLU:HB2	2.52	0.45
1:F:445:VAL:HG22	1:F:473:ASN:HB3	1.98	0.45
1:E:399:ARG:HG3	1:E:414:MSE:HE1	1.98	0.44
1:F:130:ASP:HA	1:F:131:TRP:HA	1.60	0.44
1:F:513:GLY:HA3	1:F:531:TYR:HD2	1.82	0.44
1:A:277:TRP:HB2	1:A:306:ALA:HB1	2.00	0.44
1:B:202:TRP:CE3	1:B:345:TYR:HB3	2.52	0.44
1:F:467:ASP:OD2	1:F:470:ARG:HD3	2.16	0.44
1:E:28:ARG:NH1	1:E:524:GLU:HG3	2.33	0.44
1:E:202:TRP:CE3	1:E:345:TYR:HB3	2.52	0.44
1:F:277:TRP:HB2	1:F:306:ALA:HB1	1.99	0.44
1:B:222:PRO:HD3	3:B:702:EDO:H22	1.98	0.44
1:E:245:GLU:HG2	1:E:259:LYS:HG2	1.99	0.44
1:D:172:VAL:HG11	1:D:200:GLY:HA2	1.99	0.44
1:D:308[B]:ARG:HE	1:D:439:PRO:HA	1.82	0.44
1:F:403:TRP:CE2	1:F:405:ASN:HB3	2.53	0.44
1:A:129:VAL:O	1:A:148:GLY:HA2	2.18	0.44
1:B:553:LYS:O	1:B:557:ARG:HD3	2.17	0.44
1:A:565:THR:HG23	1:A:566:GLN:HB3	1.99	0.44
1:C:357:ILE:HD11	1:C:379:TRP:CD1	2.53	0.43
1:F:284:LEU:HD23	1:F:306:ALA:HB2	2.00	0.43
1:C:132:LYS:HG3	1:C:146:THR:HG22	2.00	0.43
1:E:565:THR:HA	1:E:566:GLN:HA	1.80	0.43
1:F:202:TRP:CE3	1:F:345:TYR:HB3	2.52	0.43
1:B:403:TRP:CE2	1:B:405:ASN:HB3	2.53	0.43
1:E:46:TYR:HA	1:E:47:PRO:HD3	1.88	0.43
1:A:130:ASP:HA	1:A:131:TRP:HA	1.56	0.43
1:A:132:LYS:HG3	1:A:146:THR:HG22	2.00	0.43
1:D:489:LEU:HD11	1:D:499:LEU:O	2.18	0.43
1:A:581:ASP:O	3:A:714:EDO:O2	2.36	0.43
1:B:176:THR:HG21	1:B:197:PRO:HB3	2.01	0.43
1:A:403:TRP:CE2	1:A:405:ASN:HB3	2.53	0.43
1:D:129:VAL:O	1:D:148:GLY:HA2	2.18	0.43
1:A:261:ILE:HD12	1:D:158:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ARG:NH1	1:C:51:MSE:O	2.42	0.43
1:A:46:TYR:HA	1:A:47:PRO:HD3	1.88	0.43
1:A:357:ILE:HG22	1:A:386:LEU:HD12	2.01	0.43
1:B:490:HIS:CG	1:B:510:GLU:HB2	2.54	0.43
1:C:467:ASP:OD2	1:C:470:ARG:HD3	2.19	0.43
1:D:46:TYR:HA	1:D:47:PRO:HD3	1.87	0.43
1:F:187:VAL:O	1:F:197:PRO:HG3	2.19	0.43
1:A:467:ASP:OD2	1:A:470:ARG:HD3	2.19	0.42
1:F:399:ARG:H	1:F:399:ARG:HG2	1.67	0.42
1:D:414:MSE:HE2	1:D:414:MSE:HB3	1.92	0.42
1:E:246:VAL:HG22	1:E:289:VAL:HG22	2.01	0.42
1:E:567:THR:HG22	1:E:568:THR:HG23	2.01	0.42
1:A:513:GLY:HA3	1:A:531:TYR:HD2	1.84	0.42
1:C:333:GLY:HA3	1:C:367:MSE:O	2.19	0.42
1:D:187:VAL:O	1:D:197:PRO:HD3	2.18	0.42
1:D:576:GLY:O	1:D:586:LYS:HE2	2.19	0.42
1:A:582:ARG:O	3:A:714:EDO:H12	2.20	0.42
1:E:401:PRO:HB3	1:E:414:MSE:HB3	2.01	0.42
1:B:359:LYS:HE2	1:B:359:LYS:HA	2.02	0.42
1:C:63:TRP:HE3	1:C:107:TYR:HB3	1.83	0.42
1:D:63:TRP:CE3	1:D:107:TYR:HB3	2.55	0.41
1:F:425:ARG:NH1	8:F:807:HOH:O	2.52	0.41
1:C:176:THR:HG21	1:C:197:PRO:HB3	2.02	0.41
1:F:334:PRO:HD3	1:F:365:TYR:CD2	2.55	0.41
1:D:565:THR:HG23	1:D:566:GLN:HB3	2.03	0.41
1:F:547:TYR:HA	1:F:550:MSE:HE3	2.02	0.41
1:C:519[B]:LYS:HE3	1:C:519[B]:LYS:HB2	1.77	0.41
1:D:361:LYS:HG2	1:D:388:ILE:HD11	2.03	0.41
1:E:516:LEU:O	1:E:586:LYS:NZ	2.51	0.41
1:A:165:ASN:O	1:A:165:ASN:ND2	2.53	0.41
1:A:393:ASP:HA	1:A:445:VAL:HB	2.03	0.41
1:C:129:VAL:O	1:C:148:GLY:HA2	2.20	0.41
1:E:550:MSE:O	1:E:554:MSE:HG3	2.20	0.41
1:D:193:ILE:HB	5:D:705:TRS:H12	2.01	0.41
1:D:319:ILE:HD13	1:D:558:GLY:HA2	2.02	0.41
1:F:219[B]:ARG:HG3	1:F:436:HIS:CD2	2.56	0.41
1:B:445:VAL:HG22	1:B:473:ASN:HB3	2.03	0.41
1:C:432:MSE:HE2	1:C:466:TYR:HD2	1.84	0.41
1:C:519[A]:LYS:HG3	1:C:520[A]:ASP:N	2.35	0.41
1:A:490:HIS:CG	1:A:510:GLU:HB2	2.56	0.41
1:B:22:TRP:CE2	1:B:83:LEU:HD22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LEU:HD11	1:A:499:LEU:O	2.21	0.40
1:C:284:LEU:HD23	1:C:306:ALA:HB2	2.02	0.40
1:E:519[B]:LYS:O	8:E:801:HOH:O	2.22	0.40
1:F:63:TRP:CE3	1:F:107:TYR:HB3	2.56	0.40
1:F:384:ASP:CG	1:F:439:PRO:HD2	2.42	0.40
1:A:228:LEU:HD11	1:A:267:GLU:HB3	2.03	0.40
1:A:308[B]:ARG:HE	1:A:439:PRO:HA	1.86	0.40
1:A:500:TYR:CG	1:E:502:ALA:HB3	2.56	0.40
1:B:63:TRP:HE3	1:B:107:TYR:HB3	1.86	0.40
1:B:382:TYR:CE1	3:B:713:EDO:H12	2.56	0.40
1:E:65:TYR:HA	1:E:106:ILE:O	2.21	0.40
1:B:323:GLU:HG2	1:B:328:ALA:HA	2.02	0.40
1:E:403:TRP:CE2	1:E:405:ASN:HB3	2.56	0.40
1:F:425:ARG:NH2	1:F:458:GLU:OE2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	595/588 (101%)	574 (96%)	20 (3%)	1 (0%)	47	69
1	B	597/588 (102%)	575 (96%)	21 (4%)	1 (0%)	47	69
1	C	595/588 (101%)	576 (97%)	19 (3%)	0	100	100
1	D	596/588 (101%)	574 (96%)	21 (4%)	1 (0%)	47	69
1	E	592/588 (101%)	567 (96%)	25 (4%)	0	100	100
1	F	592/588 (101%)	571 (96%)	21 (4%)	0	100	100
All	All	3567/3528 (101%)	3437 (96%)	127 (4%)	3 (0%)	51	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	372	ILE
1	B	85	PRO
1	A	85	PRO

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	519/499 (104%)	513 (99%)	6 (1%)	71	82
1	B	521/499 (104%)	512 (98%)	9 (2%)	60	76
1	C	519/499 (104%)	506 (98%)	13 (2%)	47	67
1	D	520/499 (104%)	512 (98%)	8 (2%)	65	78
1	E	516/499 (103%)	506 (98%)	10 (2%)	57	73
1	F	516/499 (103%)	506 (98%)	10 (2%)	57	73
All	All	3111/2994 (104%)	3055 (98%)	56 (2%)	62	75

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	TYR
1	A	189	ARG
1	A	308[A]	ARG
1	A	308[B]	ARG
1	A	556	ASP
1	A	580	TYR
1	B	65	TYR
1	B	109	ARG
1	B	153	SER
1	B	308[A]	ARG
1	B	308[B]	ARG
1	B	345	TYR
1	B	519[A]	LYS
1	B	519[B]	LYS
1	B	605	LYS
1	C	21	GLN

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Mol	Chain	Res	Type
1	C	118	ARG
1	C	191	GLU
1	C	219[A]	ARG
1	C	219[B]	ARG
1	C	308	ARG
1	C	345	TYR
1	C	465[A]	GLN
1	C	465[B]	GLN
1	C	556	ASP
1	C	559	PHE
1	C	580	TYR
1	C	594	GLU
1	D	189	ARG
1	D	253	GLN
1	D	308[A]	ARG
1	D	308[B]	ARG
1	D	345	TYR
1	D	519[A]	LYS
1	D	519[B]	LYS
1	D	559	PHE
1	E	27	ASP
1	E	108	GLN
1	E	217	ASN
1	E	275	LYS
1	E	302	ASP
1	E	308	ARG
1	E	313	ARG
1	E	361	LYS
1	E	527	ARG
1	E	580	TYR
1	F	21	GLN
1	F	118	ARG
1	F	302	ASP
1	F	308	ARG
1	F	313	ARG
1	F	345	TYR
1	F	524	GLU
1	F	526	ASN
1	F	527	ARG
1	F	580	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 94 ligands modelled in this entry, 20 are monoatomic - leaving 74 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	$\#\|Z\| > 2$
3	EDO	A	710	-	3,3,3	0.47	0	2,2,2	0.29	0
7	PO4	B	720	-	4,4,4	0.93	0	6,6,6	0.42	0
3	EDO	D	707	-	3,3,3	0.46	0	2,2,2	0.29	0
3	EDO	F	709	-	3,3,3	0.45	0	2,2,2	0.34	0
7	PO4	F	704	-	4,4,4	0.91	0	6,6,6	0.43	0
3	EDO	C	711	-	3,3,3	0.47	0	2,2,2	0.24	0
3	EDO	B	719	-	3,3,3	0.45	0	2,2,2	0.27	0
3	EDO	B	702	-	3,3,3	0.42	0	2,2,2	0.48	0
7	PO4	C	713	-	4,4,4	0.91	0	6,6,6	0.43	0
3	EDO	A	703	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	B	717	-	3,3,3	0.44	0	2,2,2	0.17	0
3	EDO	B	712	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	F	707	-	3,3,3	0.46	0	2,2,2	0.25	0
5	TRS	B	706	-	7,7,7	0.33	0	9,9,9	0.32	0
3	EDO	B	705	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	A	709	-	3,3,3	0.48	0	2,2,2	0.23	0
3	EDO	A	714	-	3,3,3	0.50	0	2,2,2	0.25	0
3	EDO	D	709	-	3,3,3	0.46	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	B	707	-	3,3,3	0.47	0	2,2,2	0.29	0
3	EDO	C	710	-	3,3,3	0.47	0	2,2,2	0.26	0
3	EDO	B	714	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	C	709	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	C	703	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	F	702	-	3,3,3	0.44	0	2,2,2	0.41	0
3	EDO	A	711	-	3,3,3	0.46	0	2,2,2	0.33	0
5	TRS	A	706	-	7,7,7	0.33	0	9,9,9	0.34	0
5	TRS	D	705	-	7,7,7	0.33	0	9,9,9	0.40	0
3	EDO	F	710	-	3,3,3	0.42	0	2,2,2	0.28	0
3	EDO	A	708	-	3,3,3	0.46	0	2,2,2	0.31	0
7	PO4	D	710	-	4,4,4	0.91	0	6,6,6	0.49	0
3	EDO	B	703	-	3,3,3	0.46	0	2,2,2	0.27	0
3	EDO	E	707	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	A	707	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	B	710	-	3,3,3	0.46	0	2,2,2	0.28	0
3	EDO	D	703	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	D	702	-	3,3,3	0.47	0	2,2,2	0.22	0
3	EDO	D	704	-	3,3,3	0.46	0	2,2,2	0.35	0
3	EDO	C	706	-	3,3,3	0.46	0	2,2,2	0.32	0
6	BME	B	718	-	3,3,3	0.28	0	1,2,2	0.31	0
3	EDO	E	705	-	3,3,3	0.47	0	2,2,2	0.24	0
3	EDO	E	708	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	B	716	-	3,3,3	0.46	0	2,2,2	0.24	0
3	EDO	E	709	-	3,3,3	0.46	0	2,2,2	0.29	0
3	EDO	C	712	-	3,3,3	0.48	0	2,2,2	0.20	0
3	EDO	B	709	-	3,3,3	0.46	0	2,2,2	0.35	0
5	TRS	E	706	-	7,7,7	0.33	0	9,9,9	0.33	0
3	EDO	C	705	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	A	702	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	A	717	-	3,3,3	0.44	0	2,2,2	0.13	0
3	EDO	C	708	-	3,3,3	0.48	0	2,2,2	0.21	0
5	TRS	C	707	-	7,7,7	0.34	0	9,9,9	0.35	0
3	EDO	B	715	-	3,3,3	0.44	0	2,2,2	0.23	0
3	EDO	B	713	-	3,3,3	0.47	0	2,2,2	0.25	0
3	EDO	B	708	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	D	708	-	3,3,3	0.47	0	2,2,2	0.26	0
3	EDO	A	715	-	3,3,3	0.44	0	2,2,2	0.11	0
3	EDO	E	702	-	3,3,3	0.43	0	2,2,2	0.40	0
5	TRS	F	706	-	7,7,7	0.33	0	9,9,9	0.32	0
3	EDO	E	704	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	B	711	-	3,3,3	0.49	0	2,2,2	0.21	0
3	EDO	A	716	-	3,3,3	0.44	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	F	705	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	F	708	-	3,3,3	0.45	0	2,2,2	0.39	0
7	PO4	C	704	-	4,4,4	0.91	0	6,6,6	0.44	0
7	PO4	E	703	-	4,4,4	0.90	0	6,6,6	0.43	0
3	EDO	D	706	-	3,3,3	0.45	0	2,2,2	0.35	0
7	PO4	F	711	-	4,4,4	0.91	0	6,6,6	0.42	0
3	EDO	A	705	-	3,3,3	0.45	0	2,2,2	0.35	0
7	PO4	E	711	-	4,4,4	0.91	0	6,6,6	0.42	0
7	PO4	E	712	-	4,4,4	0.91	0	6,6,6	0.44	0
3	EDO	C	702	-	3,3,3	0.46	0	2,2,2	0.31	0
3	EDO	A	713	-	3,3,3	0.45	0	2,2,2	0.37	0
3	EDO	E	710	-	3,3,3	0.46	0	2,2,2	0.34	0
3	EDO	A	712	-	3,3,3	0.48	0	2,2,2	0.19	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
3	EDO	A	710	-	-	0/1/1/1	-
3	EDO	D	707	-	-	0/1/1/1	-
3	EDO	F	709	-	-	0/1/1/1	-
3	EDO	C	711	-	-	0/1/1/1	-
3	EDO	B	719	-	-	0/1/1/1	-
3	EDO	B	702	-	-	0/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-
3	EDO	B	717	-	-	1/1/1/1	-
3	EDO	B	712	-	-	0/1/1/1	-
3	EDO	F	707	-	-	0/1/1/1	-
5	TRS	B	706	-	-	0/9/9/9	-
3	EDO	B	705	-	-	0/1/1/1	-
3	EDO	A	709	-	-	0/1/1/1	-
3	EDO	A	714	-	-	0/1/1/1	-
3	EDO	D	709	-	-	1/1/1/1	-
3	EDO	B	707	-	-	0/1/1/1	-
3	EDO	C	710	-	-	0/1/1/1	-
3	EDO	B	714	-	-	0/1/1/1	-
3	EDO	C	709	-	-	0/1/1/1	-
3	EDO	C	703	-	-	0/1/1/1	-
3	EDO	F	702	-	-	0/1/1/1	-
3	EDO	A	711	-	-	1/1/1/1	-
5	TRS	A	706	-	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRS	D	705	-	-	3/9/9/9	-
3	EDO	F	710	-	-	0/1/1/1	-
3	EDO	A	708	-	-	0/1/1/1	-
3	EDO	B	703	-	-	0/1/1/1	-
3	EDO	E	707	-	-	1/1/1/1	-
3	EDO	A	707	-	-	0/1/1/1	-
3	EDO	B	710	-	-	0/1/1/1	-
3	EDO	D	703	-	-	0/1/1/1	-
3	EDO	D	702	-	-	0/1/1/1	-
3	EDO	D	704	-	-	1/1/1/1	-
3	EDO	C	706	-	-	0/1/1/1	-
6	BME	B	718	-	-	1/1/1/1	-
3	EDO	E	705	-	-	0/1/1/1	-
3	EDO	E	708	-	-	0/1/1/1	-
3	EDO	B	716	-	-	1/1/1/1	-
3	EDO	E	709	-	-	0/1/1/1	-
3	EDO	C	712	-	-	0/1/1/1	-
3	EDO	B	709	-	-	0/1/1/1	-
5	TRS	E	706	-	-	1/9/9/9	-
3	EDO	C	705	-	-	0/1/1/1	-
3	EDO	A	702	-	-	1/1/1/1	-
3	EDO	A	717	-	-	0/1/1/1	-
3	EDO	C	708	-	-	0/1/1/1	-
5	TRS	C	707	-	-	1/9/9/9	-
3	EDO	B	715	-	-	0/1/1/1	-
3	EDO	B	713	-	-	1/1/1/1	-
3	EDO	B	708	-	-	0/1/1/1	-
3	EDO	D	708	-	-	0/1/1/1	-
3	EDO	A	715	-	-	0/1/1/1	-
3	EDO	E	702	-	-	0/1/1/1	-
5	TRS	F	706	-	-	3/9/9/9	-
3	EDO	E	704	-	-	0/1/1/1	-
3	EDO	B	711	-	-	1/1/1/1	-
3	EDO	A	716	-	-	0/1/1/1	-
3	EDO	F	705	-	-	0/1/1/1	-
3	EDO	F	708	-	-	0/1/1/1	-
3	EDO	D	706	-	-	0/1/1/1	-
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	C	702	-	-	0/1/1/1	-
3	EDO	A	713	-	-	0/1/1/1	-
3	EDO	E	710	-	-	0/1/1/1	-
3	EDO	A	712	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	707	TRS	N-C-C1-O1
5	F	706	TRS	C1-C-C2-O2
6	B	718	BME	O1-C1-C2-S2
3	A	711	EDO	O1-C1-C2-O2
3	B	716	EDO	O1-C1-C2-O2
3	E	707	EDO	O1-C1-C2-O2
5	F	706	TRS	C3-C-C2-O2
5	D	705	TRS	N-C-C3-O3
5	E	706	TRS	N-C-C1-O1
3	B	713	EDO	O1-C1-C2-O2
3	B	717	EDO	O1-C1-C2-O2
3	D	709	EDO	O1-C1-C2-O2
5	D	705	TRS	C2-C-C3-O3
3	B	711	EDO	O1-C1-C2-O2
3	A	702	EDO	O1-C1-C2-O2
5	D	705	TRS	C1-C-C3-O3
5	F	706	TRS	N-C-C2-O2
3	D	704	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	EDO	1	0
3	B	705	EDO	1	0
3	A	714	EDO	2	0
3	B	707	EDO	2	0
3	C	703	EDO	1	0
5	D	705	TRS	1	0
3	A	707	EDO	1	0
3	D	703	EDO	1	0
3	B	716	EDO	1	0
3	C	712	EDO	1	0
3	C	705	EDO	1	0
3	B	713	EDO	1	0
3	E	702	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	574/588 (97%)	-0.53	4 (0%)	87	91	15, 24, 54, 92	0
1	B	574/588 (97%)	-0.60	2 (0%)	94	96	15, 26, 54, 90	0
1	C	573/588 (97%)	-0.50	4 (0%)	87	91	18, 28, 57, 85	0
1	D	574/588 (97%)	-0.59	4 (0%)	87	91	14, 26, 57, 87	0
1	E	574/588 (97%)	-0.51	5 (0%)	84	89	18, 27, 55, 87	0
1	F	574/588 (97%)	-0.46	6 (1%)	82	87	18, 31, 62, 86	0
All	All	3443/3528 (97%)	-0.53	25 (0%)	87	91	14, 27, 57, 92	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	605	LYS	3.2
1	C	79	GLU	3.2
1	D	20	ALA	2.9
1	C	20	ALA	2.9
1	A	518[A]	LEU	2.9
1	B	20	ALA	2.9
1	F	519[A]	LYS	2.8
1	F	605	LYS	2.7
1	F	20	ALA	2.7
1	B	27	ASP	2.6
1	D	519[A]	LYS	2.6
1	F	527	ARG	2.5
1	E	79	GLU	2.5
1	A	20	ALA	2.4
1	E	519[A]	LYS	2.4
1	F	79	GLU	2.4
1	D	525	PRO	2.4
1	D	605	LYS	2.3
1	F	532	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	525	PRO	2.2
1	C	73	ARG	2.2
1	E	20	ALA	2.2
1	E	527	ARG	2.1
1	C	526	ASN	2.1
1	A	79	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PO4	E	712	5/5	0.76	0.40	95,108,130,155	0
3	EDO	B	712	4/4	0.77	0.32	38,55,57,69	0
3	EDO	F	707	4/4	0.80	0.30	48,51,51,64	0
3	EDO	C	712	4/4	0.81	0.26	30,42,46,65	0
3	EDO	A	708	4/4	0.81	0.26	47,62,66,76	0
3	EDO	C	708	4/4	0.81	0.27	39,46,48,51	0
3	EDO	B	719	4/4	0.82	0.34	45,53,58,72	0
7	PO4	D	710	5/5	0.83	0.33	36,45,63,143	0
3	EDO	B	707	4/4	0.83	0.27	38,45,50,53	0
3	EDO	D	702	4/4	0.84	0.44	53,53,56,68	0
3	EDO	E	708	4/4	0.84	0.29	41,44,49,55	0
3	EDO	A	702	4/4	0.84	0.23	38,46,51,65	0
3	EDO	A	709	4/4	0.84	0.41	46,53,75,77	0
3	EDO	B	717	4/4	0.84	0.34	65,68,76,80	0
3	EDO	A	712	4/4	0.85	0.26	49,58,61,70	0
3	EDO	A	714	4/4	0.85	0.34	35,45,45,61	0
7	PO4	C	704	5/5	0.85	0.23	72,89,103,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	C	706	4/4	0.85	0.39	47,51,54,56	0
3	EDO	E	705	4/4	0.85	0.26	37,49,51,59	0
3	EDO	B	714	4/4	0.86	0.30	41,41,45,54	0
3	EDO	B	711	4/4	0.86	0.40	42,47,52,65	0
3	EDO	A	715	4/4	0.86	0.28	48,71,81,91	0
7	PO4	E	711	5/5	0.86	0.26	76,84,100,127	0
3	EDO	F	705	4/4	0.86	0.34	45,54,57,64	0
4	CL	B	721	1/1	0.87	0.22	66,66,66,66	0
3	EDO	B	716	4/4	0.87	0.28	52,59,71,74	0
7	PO4	C	713	5/5	0.87	0.29	93,93,117,137	0
7	PO4	B	720	5/5	0.88	0.27	41,50,72,129	0
3	EDO	A	711	4/4	0.88	0.38	45,45,48,54	0
3	EDO	D	709	4/4	0.89	0.27	40,57,66,74	0
4	CL	A	720	1/1	0.89	0.24	70,70,70,70	0
3	EDO	E	707	4/4	0.89	0.23	44,48,49,57	0
4	CL	B	704	1/1	0.90	0.09	38,38,38,38	0
3	EDO	B	709	4/4	0.90	0.27	36,40,41,45	0
6	BME	B	718	4/4	0.90	0.23	72,77,78,84	0
3	EDO	A	717	4/4	0.91	0.50	50,61,63,67	0
3	EDO	D	706	4/4	0.91	0.21	33,40,56,64	0
3	EDO	C	710	4/4	0.91	0.40	50,54,63,70	0
4	CL	C	715	1/1	0.91	0.33	74,74,74,74	0
5	TRS	D	705	8/8	0.91	0.21	31,42,46,59	0
3	EDO	B	715	4/4	0.91	0.20	40,54,63,67	0
3	EDO	A	710	4/4	0.92	0.23	32,36,46,48	0
4	CL	D	712	1/1	0.92	0.14	64,64,64,64	0
7	PO4	F	704	5/5	0.92	0.18	48,76,78,95	0
7	PO4	F	711	5/5	0.92	0.29	81,89,113,123	0
3	EDO	A	716	4/4	0.93	0.23	50,58,62,64	0
3	EDO	A	705	4/4	0.93	0.21	36,40,45,47	0
5	TRS	F	706	8/8	0.93	0.18	35,48,53,55	0
3	EDO	B	703	4/4	0.93	0.21	34,40,43,57	0
3	EDO	A	713	4/4	0.93	0.27	22,22,22,22	4
4	CL	C	716	1/1	0.93	0.15	61,61,61,61	0
3	EDO	B	713	4/4	0.94	0.18	42,43,49,55	0
3	EDO	F	709	4/4	0.94	0.34	47,49,54,66	0
4	CL	D	711	1/1	0.94	0.09	40,40,40,40	0
4	CL	A	719	1/1	0.94	0.09	51,51,51,51	0
7	PO4	E	703	5/5	0.94	0.14	53,58,72,99	0
5	TRS	A	706	8/8	0.94	0.17	30,32,34,37	0
3	EDO	D	708	4/4	0.94	0.21	40,43,45,46	0
3	EDO	D	704	4/4	0.94	0.44	27,41,47,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	E	704	4/4	0.94	0.20	40,41,50,63	0
3	EDO	C	705	4/4	0.95	0.32	43,46,51,53	0
3	EDO	C	711	4/4	0.95	0.29	43,53,55,59	0
3	EDO	F	708	4/4	0.95	0.28	33,43,45,48	0
3	EDO	B	708	4/4	0.95	0.23	24,24,25,25	4
3	EDO	F	710	4/4	0.95	0.42	55,62,63,69	0
4	CL	A	704	1/1	0.95	0.10	39,39,39,39	0
4	CL	F	703	1/1	0.95	0.09	51,51,51,51	0
3	EDO	B	705	4/4	0.95	0.13	39,47,54,54	0
5	TRS	C	707	8/8	0.95	0.18	34,38,48,49	0
3	EDO	E	710	4/4	0.95	0.17	42,43,45,46	0
5	TRS	E	706	8/8	0.95	0.16	35,39,48,54	0
3	EDO	C	702	4/4	0.96	0.16	50,54,58,58	0
4	CL	C	714	1/1	0.96	0.30	67,67,67,67	0
3	EDO	A	703	4/4	0.97	0.18	22,23,26,39	0
3	EDO	D	707	4/4	0.97	0.28	28,34,40,48	0
3	EDO	E	709	4/4	0.97	0.22	27,32,34,39	0
4	CL	A	718	1/1	0.97	0.09	57,57,57,57	0
4	CL	E	713	1/1	0.97	0.11	50,50,50,50	0
3	EDO	C	703	4/4	0.97	0.26	25,27,33,35	0
3	EDO	F	702	4/4	0.97	0.14	26,26,30,40	0
5	TRS	B	706	8/8	0.97	0.15	28,39,45,47	0
2	MG	D	701	1/1	0.97	0.07	19,19,19,19	0
3	EDO	A	707	4/4	0.97	0.14	28,42,42,43	0
3	EDO	B	710	4/4	0.97	0.29	38,40,44,53	0
2	MG	F	701	1/1	0.98	0.04	25,25,25,25	0
4	CL	B	722	1/1	0.98	0.16	56,56,56,56	0
3	EDO	D	703	4/4	0.98	0.14	25,29,32,35	0
2	MG	B	701	1/1	0.98	0.05	18,18,18,18	0
3	EDO	C	709	4/4	0.98	0.36	31,37,43,52	0
2	MG	C	701	1/1	0.99	0.05	21,21,21,21	0
2	MG	A	701	1/1	0.99	0.04	20,20,20,20	0
3	EDO	E	702	4/4	0.99	0.10	26,27,29,33	0
2	MG	E	701	1/1	0.99	0.05	23,23,23,23	0
3	EDO	B	702	4/4	0.99	0.18	20,22,26,31	0

6.5 Other polymers (i)

There are no such residues in this entry.