



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:27 PM UTC

PDB ID : 7SF2 / pdb_00007sf2
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 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

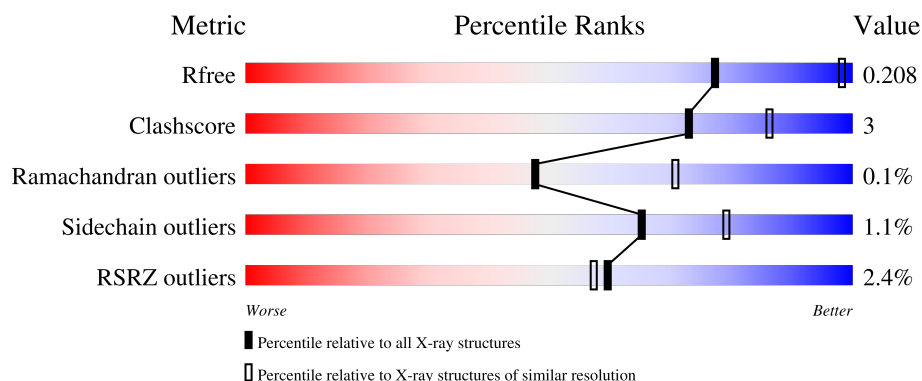
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	588	 2% 89% 10%
1	B	588	 3% 90% 10%
1	C	588	 2% 90% 10% .
1	D	588	 2% 89% 10%
1	E	588	 2% 88% 11%

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Mol	Chain	Length	Quality of chain
1	F	588	3% 92% 8%

2 Entry composition

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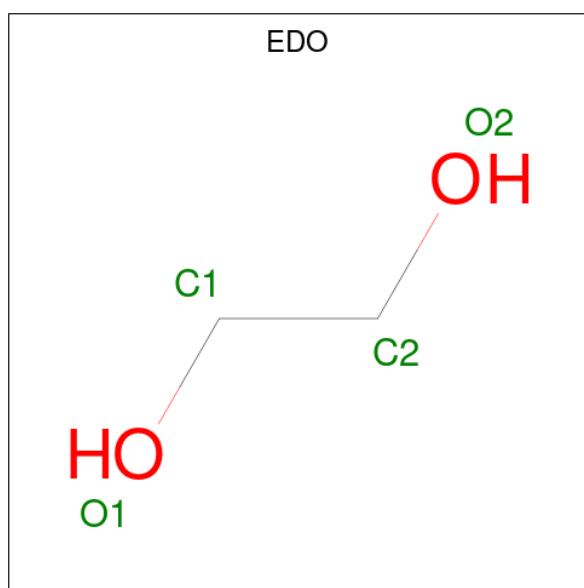
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Chain	Residue	Modelled	Actual	Comment	Reference
E	19	ASN	-	expression tag	UNP E2NBY7
E	20	ALA	-	expression tag	UNP E2NBY7
E	436	HIS	TYR	conflict	UNP E2NBY7
F	18	SER	-	expression tag	UNP E2NBY7
F	19	ASN	-	expression tag	UNP E2NBY7
F	20	ALA	-	expression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

- Molecule 2 is MAGNESIUM ION (CCD ID: 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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

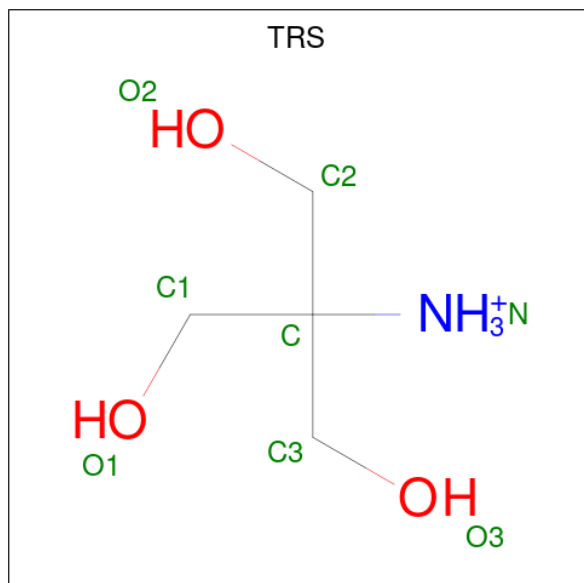
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Cl 4 4	0	0
4	B	3	Total Cl 3 3	0	0
4	C	3	Total Cl 3 3	0	0
4	D	2	Total Cl 2 2	0	0

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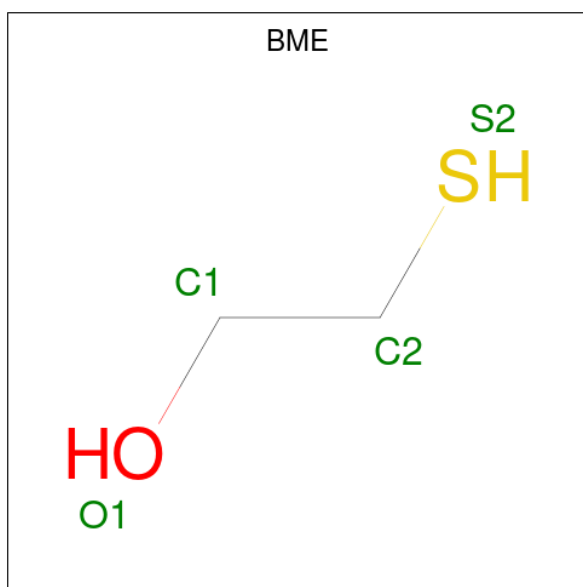
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		

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



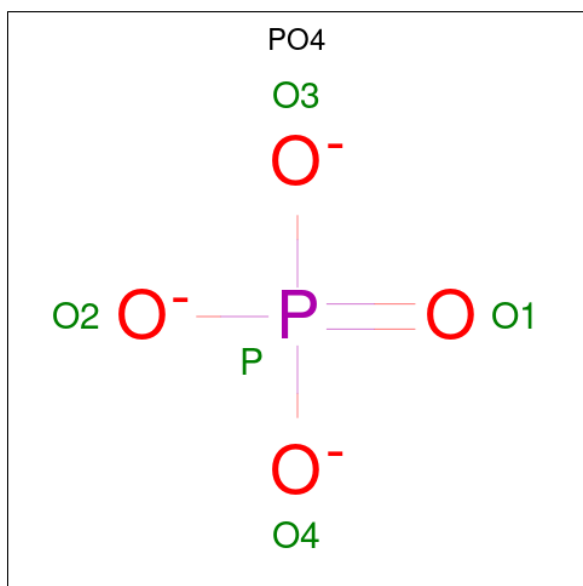
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	B	1	Total	C	N	O	0	0
			8	4	1	3		
5	C	1	Total	C	N	O	0	0
			8	4	1	3		
5	D	1	Total	C	N	O	0	0
			8	4	1	3		
5	E	1	Total	C	N	O	0	0
			8	4	1	3		
5	F	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



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

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

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

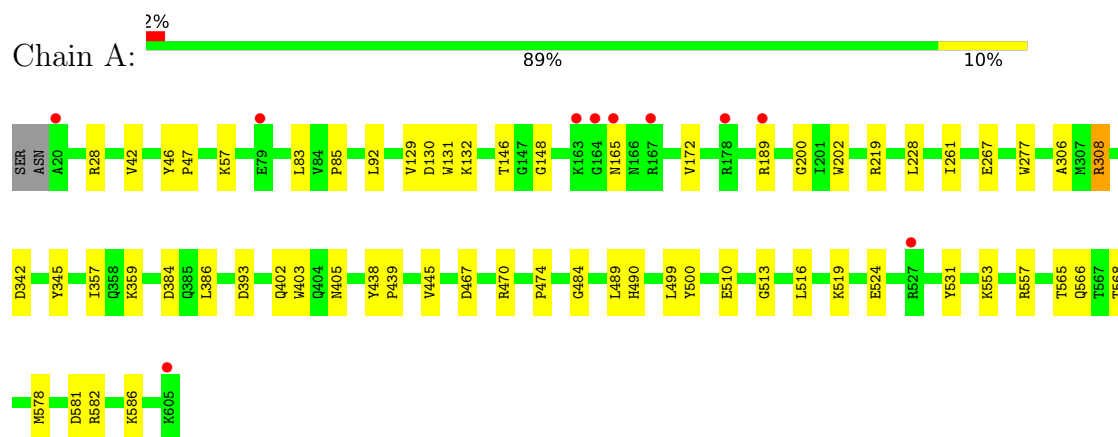
- Molecule 8 is water.

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

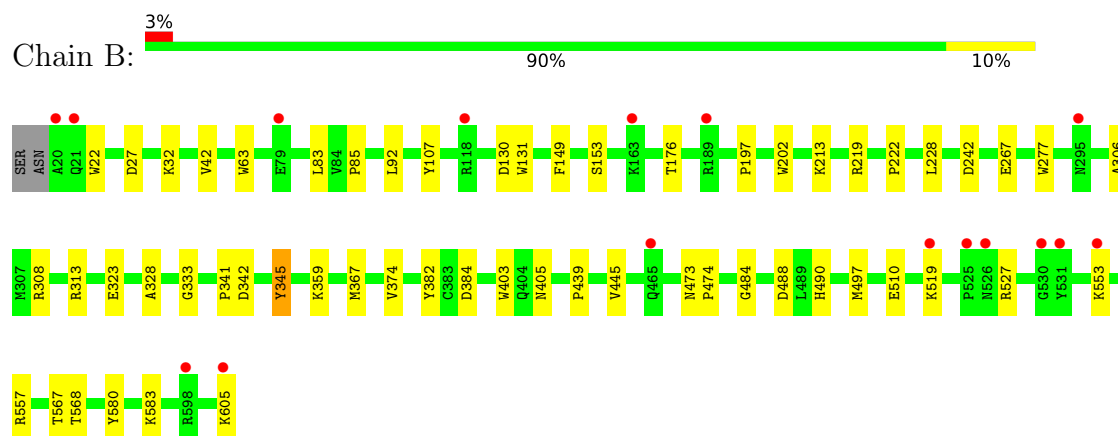
3 Residue-property plots [i](#)

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.

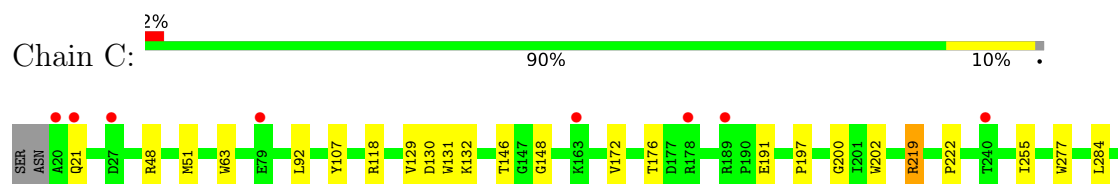
- Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

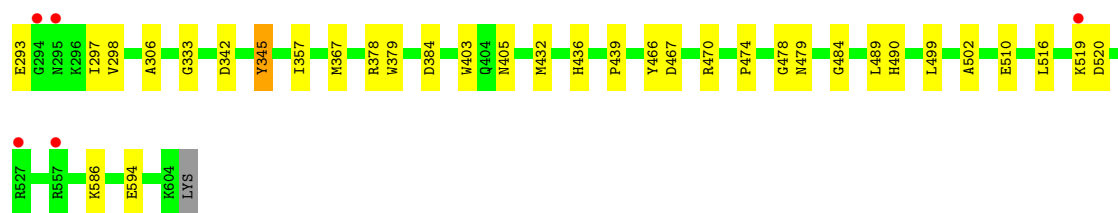


- Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

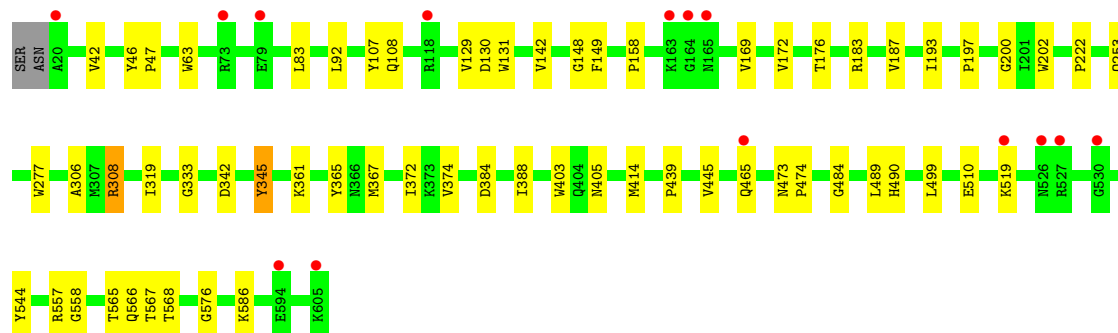
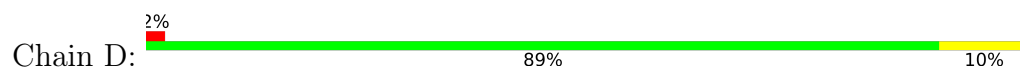


- Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

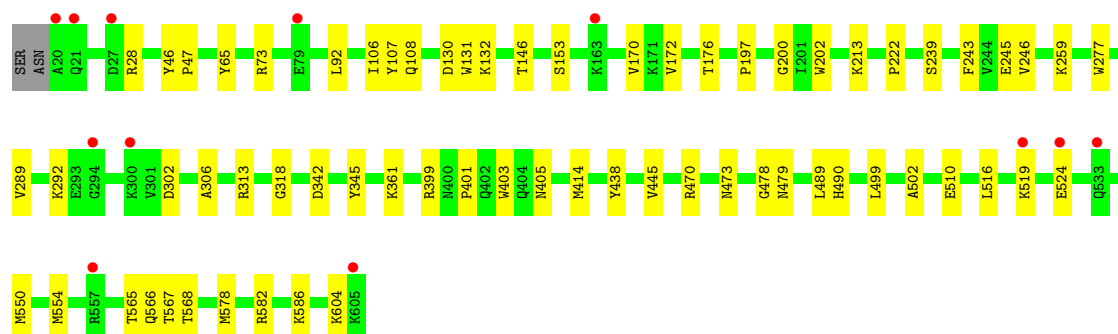
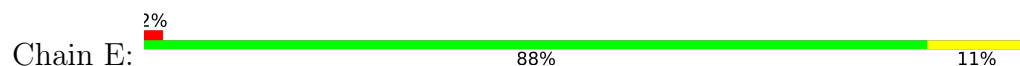




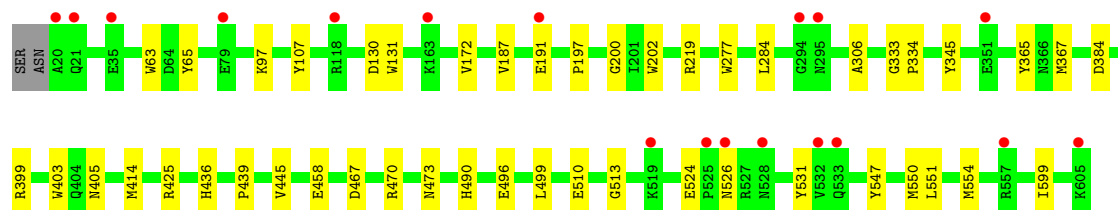
- Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein



- 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

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
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.182 , 0.209 0.182 , 0.208	Depositor DCC
R_{free} test set	12548 reflections (4.74%)	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)	0.33 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, CL, EDO, 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	0.10	0/4982	0.29	0/6753
1	B	0.11	0/4999	0.29	0/6777
1	C	0.10	0/4980	0.28	0/6753
1	D	0.10	0/4992	0.28	0/6766
1	E	0.09	0/4950	0.29	0/6712
1	F	0.10	0/4949	0.29	0/6711
All	All	0.10	0/29852	0.29	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	38	0
1	B	4876	0	4729	33	0
1	C	4857	0	4706	30	0
1	D	4869	0	4728	33	0
1	E	4827	0	4684	33	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	187	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 (187) 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:D:365:TYR:OH	1:D:544:TYR:OH	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:LYS:NZ	1:E:239:SER:OG	2.40	0.46
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:F:384:ASP:CG	1:F:439:PRO:HD2	2.42	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:C:384:ASP:CG	1:C:439:PRO:HD2	2.42	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:384:ASP:CG	1:A:439:PRO:HD2	2.42	0.44
1:A:565:THR:HG23	1:A:566:GLN:HB3	1.99	0.44
1:B:213:LYS:NZ	1:B:242:ASP:OD1	2.51	0.44
1:C:357:ILE:HD11	1:C:379:TRP:CD1	2.53	0.43
1:E:516:LEU:O	1:E:586:LYS:NZ	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:384:ASP:CG	1:D:439:PRO:HD2	2.44	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:E:478:GLY:HA2	1:E:479:ASN:C	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:384:ASP:CG	1:B:439:PRO:HD2	2.46	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:478:GLY:HA2	1:C:479:ASN:C	2.46	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
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: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%)	43	64
1	B	597/588 (102%)	575 (96%)	21 (4%)	1 (0%)	43	64
1	C	595/588 (101%)	576 (97%)	19 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	596/588 (101%)	574 (96%)	21 (4%)	1 (0%)	43	64
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%)	48	71

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 ⓘ

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%)	514 (99%)	5 (1%)	68	81
1	B	521/499 (104%)	513 (98%)	8 (2%)	57	74
1	C	519/499 (104%)	510 (98%)	9 (2%)	53	71
1	D	520/499 (104%)	510 (98%)	10 (2%)	50	70
1	E	516/499 (103%)	509 (99%)	7 (1%)	59	75
1	F	516/499 (103%)	512 (99%)	4 (1%)	73	84
All	All	3111/2994 (104%)	3068 (99%)	43 (1%)	65	75

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	ARG
1	A	308[A]	ARG
1	A	308[B]	ARG
1	A	519[A]	LYS
1	A	519[B]	LYS

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Mol	Chain	Res	Type
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	527	ARG
1	B	605	LYS
1	C	21	GLN
1	C	118	ARG
1	C	191	GLU
1	C	219[A]	ARG
1	C	219[B]	ARG
1	C	255	ILE
1	C	297	ILE
1	C	345	TYR
1	C	594	GLU
1	D	253	GLN
1	D	308[A]	ARG
1	D	308[B]	ARG
1	D	345	TYR
1	D	465[A]	GLN
1	D	465[B]	GLN
1	D	465[C]	GLN
1	D	519[A]	LYS
1	D	519[B]	LYS
1	D	557	ARG
1	E	73	ARG
1	E	108	GLN
1	E	153	SER
1	E	302	ASP
1	E	313	ARG
1	E	361	LYS
1	E	604	LYS
1	F	191	GLU
1	F	499	LEU
1	F	524	GLU
1	F	526	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	54	ASN
1	A	358	GLN
1	A	503	GLN
1	A	528	ASN
1	A	533	GLN
1	B	54	ASN
1	B	102	ASN
1	B	108	GLN
1	B	238	ASN
1	B	252	ASN
1	C	247	ASN
1	C	526	ASN
1	D	121	GLN
1	D	247	ASN
1	D	528	ASN
1	E	54	ASN
1	E	121	GLN
1	E	214	HIS
1	F	54	ASN
1	F	214	HIS
1	F	533	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	708	-	3,3,3	0.44	0	2,2,2	0.26	0
3	EDO	F	709	-	3,3,3	0.42	0	2,2,2	0.38	0
3	EDO	C	703	-	3,3,3	0.41	0	2,2,2	0.42	0
5	TRS	E	706	-	7,7,7	0.34	0	9,9,9	0.33	0
7	PO4	E	712	-	4,4,4	0.95	0	6,6,6	0.47	0
7	PO4	B	720	-	4,4,4	0.98	0	6,6,6	0.45	0
7	PO4	E	711	-	4,4,4	0.95	0	6,6,6	0.45	0
3	EDO	B	713	-	3,3,3	0.44	0	2,2,2	0.30	0
3	EDO	A	703	-	3,3,3	0.41	0	2,2,2	0.44	0
7	PO4	C	713	-	4,4,4	0.95	0	6,6,6	0.46	0
3	EDO	A	710	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	C	706	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	B	707	-	3,3,3	0.44	0	2,2,2	0.33	0
3	EDO	B	712	-	3,3,3	0.43	0	2,2,2	0.36	0
3	EDO	C	712	-	3,3,3	0.45	0	2,2,2	0.25	0
3	EDO	A	702	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	F	705	-	3,3,3	0.43	0	2,2,2	0.37	0
7	PO4	F	704	-	4,4,4	0.95	0	6,6,6	0.46	0
3	EDO	A	713	-	3,3,3	0.42	0	2,2,2	0.41	0
7	PO4	F	711	-	4,4,4	0.96	0	6,6,6	0.46	0
3	EDO	C	709	-	3,3,3	0.43	0	2,2,2	0.36	0
3	EDO	D	707	-	3,3,3	0.43	0	2,2,2	0.34	0
3	EDO	F	710	-	3,3,3	0.39	0	2,2,2	0.33	0
3	EDO	B	717	-	3,3,3	0.41	0	2,2,2	0.23	0
3	EDO	A	715	-	3,3,3	0.41	0	2,2,2	0.17	0
3	EDO	B	708	-	3,3,3	0.43	0	2,2,2	0.40	0
3	EDO	A	709	-	3,3,3	0.45	0	2,2,2	0.28	0
3	EDO	F	707	-	3,3,3	0.43	0	2,2,2	0.30	0
3	EDO	E	704	-	3,3,3	0.42	0	2,2,2	0.38	0
3	EDO	B	711	-	3,3,3	0.45	0	2,2,2	0.26	0
5	TRS	D	705	-	7,7,7	0.33	0	9,9,9	0.41	0
3	EDO	C	705	-	3,3,3	0.43	0	2,2,2	0.38	0
7	PO4	E	703	-	4,4,4	0.95	0	6,6,6	0.47	0
3	EDO	B	702	-	3,3,3	0.39	0	2,2,2	0.51	0
3	EDO	D	704	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	C	711	-	3,3,3	0.44	0	2,2,2	0.29	0
3	EDO	A	717	-	3,3,3	0.41	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	E	708	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	B	710	-	3,3,3	0.43	0	2,2,2	0.33	0
3	EDO	A	708	-	3,3,3	0.43	0	2,2,2	0.36	0
3	EDO	B	714	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	D	702	-	3,3,3	0.44	0	2,2,2	0.27	0
3	EDO	E	710	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	A	705	-	3,3,3	0.42	0	2,2,2	0.40	0
3	EDO	C	710	-	3,3,3	0.44	0	2,2,2	0.31	0
3	EDO	A	707	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	A	712	-	3,3,3	0.44	0	2,2,2	0.24	0
3	EDO	B	715	-	3,3,3	0.41	0	2,2,2	0.28	0
3	EDO	A	711	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	B	719	-	3,3,3	0.42	0	2,2,2	0.32	0
3	EDO	D	708	-	3,3,3	0.44	0	2,2,2	0.31	0
3	EDO	D	709	-	3,3,3	0.43	0	2,2,2	0.30	0
3	EDO	B	709	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	D	706	-	3,3,3	0.42	0	2,2,2	0.40	0
3	EDO	E	702	-	3,3,3	0.40	0	2,2,2	0.44	0
3	EDO	E	707	-	3,3,3	0.43	0	2,2,2	0.35	0
5	TRS	A	706	-	7,7,7	0.34	0	9,9,9	0.34	0
5	TRS	C	707	-	7,7,7	0.35	0	9,9,9	0.35	0
7	PO4	D	710	-	4,4,4	0.95	0	6,6,6	0.52	0
3	EDO	B	716	-	3,3,3	0.43	0	2,2,2	0.29	0
3	EDO	B	703	-	3,3,3	0.43	0	2,2,2	0.32	0
5	TRS	F	706	-	7,7,7	0.34	0	9,9,9	0.31	0
3	EDO	C	702	-	3,3,3	0.43	0	2,2,2	0.36	0
6	BME	B	718	-	3,3,3	0.28	0	2,2,2	0.23	0
3	EDO	A	714	-	3,3,3	0.46	0	2,2,2	0.30	0
3	EDO	F	708	-	3,3,3	0.42	0	2,2,2	0.43	0
5	TRS	B	706	-	7,7,7	0.34	0	9,9,9	0.32	0
3	EDO	D	703	-	3,3,3	0.41	0	2,2,2	0.42	0
3	EDO	B	705	-	3,3,3	0.44	0	2,2,2	0.35	0
3	EDO	E	709	-	3,3,3	0.43	0	2,2,2	0.34	0
7	PO4	C	704	-	4,4,4	0.95	0	6,6,6	0.47	0
3	EDO	F	702	-	3,3,3	0.41	0	2,2,2	0.45	0
3	EDO	E	705	-	3,3,3	0.44	0	2,2,2	0.29	0
3	EDO	A	716	-	3,3,3	0.41	0	2,2,2	0.36	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	C	708	-	-	0/1/1/1	-
3	EDO	F	709	-	-	0/1/1/1	-
3	EDO	C	703	-	-	0/1/1/1	-
5	TRS	E	706	-	-	2/9/9/9	-
3	EDO	B	713	-	-	1/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-
3	EDO	A	710	-	-	0/1/1/1	-
3	EDO	C	706	-	-	0/1/1/1	-
3	EDO	B	707	-	-	0/1/1/1	-
3	EDO	B	712	-	-	0/1/1/1	-
3	EDO	C	712	-	-	0/1/1/1	-
3	EDO	A	702	-	-	1/1/1/1	-
3	EDO	F	705	-	-	0/1/1/1	-
3	EDO	A	713	-	-	0/1/1/1	-
3	EDO	C	709	-	-	0/1/1/1	-
3	EDO	D	707	-	-	0/1/1/1	-
3	EDO	F	710	-	-	0/1/1/1	-
3	EDO	B	717	-	-	1/1/1/1	-
3	EDO	A	715	-	-	0/1/1/1	-
3	EDO	B	708	-	-	0/1/1/1	-
3	EDO	A	709	-	-	0/1/1/1	-
3	EDO	F	707	-	-	0/1/1/1	-
3	EDO	E	704	-	-	0/1/1/1	-
3	EDO	B	711	-	-	1/1/1/1	-
5	TRS	D	705	-	-	3/9/9/9	-
3	EDO	C	705	-	-	0/1/1/1	-
3	EDO	B	702	-	-	0/1/1/1	-
3	EDO	D	704	-	-	1/1/1/1	-
3	EDO	C	711	-	-	0/1/1/1	-
3	EDO	A	717	-	-	0/1/1/1	-
3	EDO	E	708	-	-	0/1/1/1	-
3	EDO	B	710	-	-	0/1/1/1	-
3	EDO	A	708	-	-	0/1/1/1	-
3	EDO	B	714	-	-	0/1/1/1	-
3	EDO	D	702	-	-	0/1/1/1	-
3	EDO	E	710	-	-	0/1/1/1	-
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	C	710	-	-	0/1/1/1	-
3	EDO	A	707	-	-	0/1/1/1	-
3	EDO	A	712	-	-	0/1/1/1	-
3	EDO	B	715	-	-	0/1/1/1	-
3	EDO	A	711	-	-	1/1/1/1	-
3	EDO	B	719	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	708	-	-	0/1/1/1	-
3	EDO	D	709	-	-	1/1/1/1	-
3	EDO	B	709	-	-	0/1/1/1	-
3	EDO	D	706	-	-	0/1/1/1	-
3	EDO	E	702	-	-	0/1/1/1	-
3	EDO	E	707	-	-	1/1/1/1	-
5	TRS	A	706	-	-	0/9/9/9	-
5	TRS	C	707	-	-	2/9/9/9	-
3	EDO	B	716	-	-	1/1/1/1	-
3	EDO	B	703	-	-	0/1/1/1	-
5	TRS	F	706	-	-	3/9/9/9	-
3	EDO	C	702	-	-	0/1/1/1	-
6	BME	B	718	-	-	1/1/1/1	-
3	EDO	A	714	-	-	0/1/1/1	-
3	EDO	F	708	-	-	0/1/1/1	-
5	TRS	B	706	-	-	1/9/9/9	-
3	EDO	D	703	-	-	0/1/1/1	-
3	EDO	B	705	-	-	0/1/1/1	-
3	EDO	E	709	-	-	0/1/1/1	-
3	EDO	F	702	-	-	0/1/1/1	-
3	EDO	E	705	-	-	0/1/1/1	-
3	EDO	A	716	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) 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
5	F	706	TRS	C3-C-C2-O2
3	A	711	EDO	O1-C1-C2-O2
3	E	707	EDO	O1-C1-C2-O2
3	B	716	EDO	O1-C1-C2-O2
5	D	705	TRS	N-C-C3-O3
5	E	706	TRS	N-C-C1-O1
5	D	705	TRS	C2-C-C3-O3
3	D	709	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	D	705	TRS	C1-C-C3-O3
5	F	706	TRS	N-C-C2-O2
3	A	702	EDO	O1-C1-C2-O2
3	B	713	EDO	O1-C1-C2-O2
3	B	717	EDO	O1-C1-C2-O2
5	B	706	TRS	C2-C-C3-O3
5	C	707	TRS	C2-C-C1-O1
5	E	706	TRS	C2-C-C1-O1
3	B	711	EDO	O1-C1-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	C	703	EDO	1	0
3	B	713	EDO	1	0
3	B	707	EDO	2	0
3	C	712	EDO	1	0
5	D	705	TRS	1	0
3	C	705	EDO	1	0
3	B	702	EDO	1	0
3	A	707	EDO	1	0
3	E	702	EDO	1	0
3	B	716	EDO	1	0
3	A	714	EDO	2	0
3	D	703	EDO	1	0
3	B	705	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, 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	574/588 (97%)	-0.33	10 (1%) 69 67	10, 24, 54, 92	11 (1%)
1	B	574/588 (97%)	-0.29	16 (2%) 55 53	11, 25, 54, 90	13 (2%)
1	C	573/588 (97%)	-0.19	13 (2%) 61 59	14, 28, 55, 85	12 (2%)
1	D	574/588 (97%)	-0.28	14 (2%) 59 57	9, 25, 57, 87	11 (1%)
1	E	574/588 (97%)	-0.25	12 (2%) 63 61	13, 27, 54, 87	8 (1%)
1	F	574/588 (97%)	-0.12	18 (3%) 51 49	15, 31, 62, 86	8 (1%)
All	All	3443/3528 (97%)	-0.24	83 (2%) 59 57	9, 27, 57, 92	63 (1%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519[A]	LYS	6.4
1	B	20	ALA	5.3
1	F	557[A]	ARG	4.9
1	E	20	ALA	4.9
1	C	189[A]	ARG	4.8
1	D	20	ALA	4.7
1	A	163	LYS	4.6
1	F	20	ALA	4.5
1	D	519[A]	LYS	4.3
1	D	163	LYS	4.0
1	B	189[A]	ARG	3.8
1	F	519[A]	LYS	3.8
1	B	598[A]	ARG	3.8
1	E	519[A]	LYS	3.7
1	D	465[A]	GLN	3.6
1	B	605	LYS	3.6
1	B	163	LYS	3.6
1	D	605	LYS	3.5
1	C	295	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	164	GLY	3.4
1	F	528	ASN	3.4
1	C	519[A]	LYS	3.3
1	F	605	LYS	3.3
1	C	178[A]	ARG	3.2
1	C	557[A]	ARG	3.2
1	C	20	ALA	3.1
1	D	530	GLY	3.1
1	E	605	LYS	3.1
1	F	351[A]	GLU	3.0
1	C	240	THR	3.0
1	F	79	GLU	3.0
1	C	21	GLN	3.0
1	C	27	ASP	2.9
1	E	557[A]	ARG	2.9
1	C	294	GLY	2.9
1	D	164	GLY	2.9
1	F	163	LYS	2.9
1	F	118	ARG	2.9
1	A	527	ARG	2.8
1	A	20	ALA	2.8
1	E	163	LYS	2.8
1	B	525	PRO	2.7
1	B	465[A]	GLN	2.7
1	E	79	GLU	2.7
1	E	294	GLY	2.6
1	B	553	LYS	2.6
1	D	526	ASN	2.5
1	E	21[A]	GLN	2.5
1	F	525	PRO	2.5
1	F	21	GLN	2.4
1	F	532	VAL	2.4
1	A	165	ASN	2.4
1	B	526	ASN	2.4
1	C	79	GLU	2.4
1	B	531	TYR	2.4
1	F	526	ASN	2.4
1	B	79	GLU	2.4
1	E	27	ASP	2.4
1	A	178[A]	ARG	2.4
1	F	533	GLN	2.4
1	D	165	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	191	GLU	2.3
1	A	605	LYS	2.3
1	F	295	ASN	2.2
1	A	167	ARG	2.2
1	A	189	ARG	2.2
1	D	527	ARG	2.2
1	E	524	GLU	2.2
1	F	35	GLU	2.2
1	E	533	GLN	2.2
1	C	163	LYS	2.2
1	A	79	GLU	2.1
1	C	527	ARG	2.1
1	D	118[A]	ARG	2.1
1	B	21	GLN	2.1
1	E	300	LYS	2.1
1	B	118[A]	ARG	2.1
1	D	73[A]	ARG	2.1
1	B	295[A]	ASN	2.1
1	D	79	GLU	2.1
1	D	594	GLU	2.1
1	B	530	GLY	2.0
1	F	294	GLY	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 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
3	EDO	A	708	4/4	0.55	0.30	47,62,66,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PO4	E	712	5/5	0.59	0.16	95,108,130,155	0
3	EDO	B	717	4/4	0.65	0.29	65,68,76,80	0
7	PO4	C	713	5/5	0.71	0.18	93,93,117,137	0
3	EDO	A	715	4/4	0.72	0.34	48,71,81,91	0
7	PO4	C	704	5/5	0.73	0.24	72,89,103,125	0
3	EDO	E	708	4/4	0.78	0.28	41,44,49,55	0
3	EDO	F	707	4/4	0.79	0.25	48,51,51,64	0
3	EDO	C	712	4/4	0.80	0.25	30,42,46,65	0
3	EDO	B	719	4/4	0.80	0.28	45,53,58,72	0
3	EDO	C	708	4/4	0.80	0.26	39,46,48,51	0
6	BME	B	718	4/4	0.81	0.26	72,77,78,84	0
3	EDO	B	712	4/4	0.81	0.24	38,55,57,69	0
7	PO4	F	711	5/5	0.82	0.23	81,89,113,123	0
3	EDO	A	714	4/4	0.83	0.27	35,45,45,61	0
3	EDO	C	705	4/4	0.84	0.20	43,46,51,53	0
3	EDO	A	702	4/4	0.84	0.22	38,46,51,65	0
3	EDO	B	709	4/4	0.85	0.21	36,40,41,45	0
3	EDO	A	711	4/4	0.85	0.28	45,45,48,54	0
3	EDO	B	715	4/4	0.85	0.21	40,54,63,67	0
3	EDO	B	716	4/4	0.86	0.25	52,59,71,74	0
5	TRS	D	705	8/8	0.86	0.17	31,42,46,59	0
7	PO4	E	711	5/5	0.86	0.19	76,84,100,127	0
5	TRS	F	706	8/8	0.86	0.19	35,48,53,55	0
3	EDO	F	705	4/4	0.86	0.23	45,54,57,64	0
3	EDO	C	710	4/4	0.87	0.24	50,54,63,70	0
4	CL	A	720	1/1	0.87	0.15	70,70,70,70	0
3	EDO	A	709	4/4	0.87	0.24	46,53,75,77	0
3	EDO	B	711	4/4	0.87	0.27	42,47,52,65	0
3	EDO	A	712	4/4	0.87	0.24	49,58,61,70	0
3	EDO	C	706	4/4	0.88	0.21	47,51,54,56	0
3	EDO	B	714	4/4	0.88	0.22	41,41,45,54	0
3	EDO	D	702	4/4	0.88	0.18	53,53,56,68	0
3	EDO	E	705	4/4	0.88	0.17	37,49,51,59	0
4	CL	B	704	1/1	0.90	0.10	38,38,38,38	0
4	CL	B	721	1/1	0.90	0.15	66,66,66,66	0
4	CL	D	711	1/1	0.90	0.12	40,40,40,40	0
3	EDO	B	703	4/4	0.90	0.19	34,40,43,57	0
3	EDO	E	707	4/4	0.90	0.17	44,48,49,57	0
3	EDO	B	708	4/4	0.90	0.15	24,24,25,25	4
7	PO4	B	720	5/5	0.90	0.24	41,50,72,129	0
3	EDO	E	710	4/4	0.90	0.16	42,43,45,46	0
3	EDO	A	713	4/4	0.90	0.17	22,22,22,22	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	717	4/4	0.90	0.23	50,61,63,67	0
3	EDO	F	709	4/4	0.90	0.20	47,49,54,66	0
7	PO4	F	704	5/5	0.90	0.14	48,76,78,95	0
3	EDO	D	706	4/4	0.90	0.21	33,40,56,64	0
7	PO4	D	710	5/5	0.91	0.24	36,45,63,143	0
7	PO4	E	703	5/5	0.91	0.15	53,58,72,99	0
4	CL	C	716	1/1	0.91	0.18	61,61,61,61	0
3	EDO	B	707	4/4	0.91	0.21	38,45,50,53	0
3	EDO	A	710	4/4	0.91	0.18	32,36,46,48	0
3	EDO	A	716	4/4	0.91	0.17	50,58,62,64	0
3	EDO	B	713	4/4	0.92	0.21	42,43,49,55	0
3	EDO	A	705	4/4	0.92	0.12	36,40,45,47	0
5	TRS	C	707	8/8	0.92	0.16	34,38,48,49	0
4	CL	A	719	1/1	0.92	0.10	51,51,51,51	0
5	TRS	E	706	8/8	0.92	0.13	35,39,48,54	0
3	EDO	D	704	4/4	0.92	0.19	27,41,47,52	0
3	EDO	C	711	4/4	0.92	0.18	43,53,55,59	0
3	EDO	D	708	4/4	0.92	0.21	40,43,45,46	0
3	EDO	F	710	4/4	0.93	0.16	55,62,63,69	0
4	CL	A	704	1/1	0.93	0.12	39,39,39,39	0
4	CL	D	712	1/1	0.93	0.12	64,64,64,64	0
5	TRS	A	706	8/8	0.93	0.14	30,32,34,37	0
3	EDO	B	705	4/4	0.93	0.16	39,47,54,54	0
4	CL	C	715	1/1	0.93	0.14	74,74,74,74	0
3	EDO	E	704	4/4	0.94	0.17	40,41,50,63	0
3	EDO	A	707	4/4	0.94	0.13	28,42,42,43	0
3	EDO	C	702	4/4	0.94	0.14	50,54,58,58	0
3	EDO	F	708	4/4	0.94	0.13	33,43,45,48	0
3	EDO	D	709	4/4	0.94	0.14	40,57,66,74	0
4	CL	F	703	1/1	0.95	0.10	51,51,51,51	0
3	EDO	A	703	4/4	0.95	0.13	22,23,26,39	0
3	EDO	C	703	4/4	0.95	0.14	25,27,33,35	0
4	CL	E	713	1/1	0.95	0.10	50,50,50,50	0
5	TRS	B	706	8/8	0.96	0.12	28,39,45,47	0
4	CL	A	718	1/1	0.96	0.11	57,57,57,57	0
3	EDO	D	703	4/4	0.96	0.15	25,29,32,35	0
3	EDO	D	707	4/4	0.96	0.13	28,34,40,48	0
3	EDO	B	710	4/4	0.96	0.12	38,40,44,53	0
3	EDO	E	709	4/4	0.97	0.09	27,32,34,39	0
4	CL	B	722	1/1	0.97	0.08	56,56,56,56	0
4	CL	C	714	1/1	0.97	0.18	67,67,67,67	0
3	EDO	B	702	4/4	0.97	0.11	20,22,26,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	E	702	4/4	0.97	0.09	26,27,29,33	0
3	EDO	F	702	4/4	0.98	0.07	26,26,30,40	0
3	EDO	C	709	4/4	0.98	0.12	31,37,43,52	0
2	MG	D	701	1/1	0.98	0.03	19,19,19,19	0
2	MG	E	701	1/1	1.00	0.03	23,23,23,23	0
2	MG	F	701	1/1	1.00	0.02	25,25,25,25	0
2	MG	B	701	1/1	1.00	0.01	18,18,18,18	0
2	MG	C	701	1/1	1.00	0.01	21,21,21,21	0
2	MG	A	701	1/1	1.00	0.01	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.