



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:56 AM UTC

PDB ID : 7NN3 / pdb_00007nn3
Title : A carbohydrate esterase family 15 (CE15) glucuronoyl esterase from Caldicellulosiruptor kristjansonii
Authors : Krska, D.; Mazurkewich, S.; Navarro Poulsen, J.; Larsbrink, J.; Lo Leggio, L.
Deposited on : 2021-02-24
Resolution : 1.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

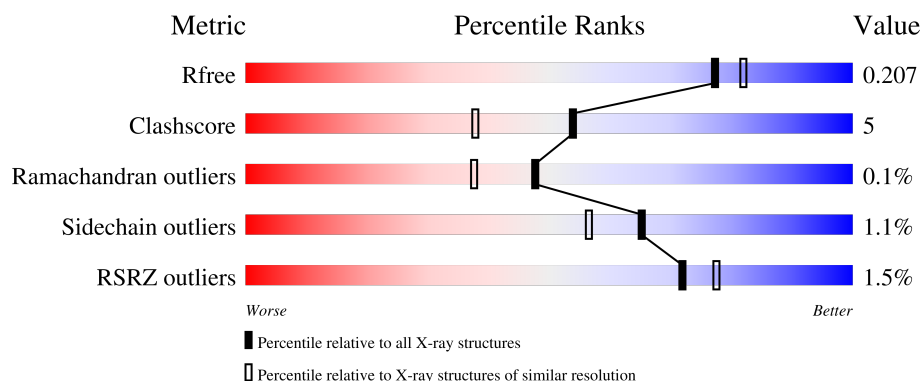
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	399	88% 7% • •
1	B	399	86% 7% 7%
1	C	399	85% 8% • 7%
1	D	399	3% 85% 11% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	405	-	-	X	-
3	EDO	D	401	-	-	X	-
4	PEG	D	409	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13567 atoms, of which 245 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 Beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	4	0
			3058	1961	512	580	5			
1	B	371	Total	C	N	O	S	0	3	0
			2945	1887	492	561	5			
1	C	372	Total	C	N	O	S	0	3	0
			2953	1892	493	563	5			
1	D	381	Total	C	N	O	S	0	6	0
			3059	1960	512	581	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP E4S6E9
A	2	GLY	-	expression tag	UNP E4S6E9
A	3	SER	-	expression tag	UNP E4S6E9
A	4	SER	-	expression tag	UNP E4S6E9
A	5	HIS	-	expression tag	UNP E4S6E9
A	6	HIS	-	expression tag	UNP E4S6E9
A	7	HIS	-	expression tag	UNP E4S6E9
A	8	HIS	-	expression tag	UNP E4S6E9
A	9	HIS	-	expression tag	UNP E4S6E9
A	10	HIS	-	expression tag	UNP E4S6E9
A	11	SER	-	expression tag	UNP E4S6E9
A	12	SER	-	expression tag	UNP E4S6E9
A	13	GLU	-	expression tag	UNP E4S6E9
A	14	ASN	-	expression tag	UNP E4S6E9
A	15	LEU	-	expression tag	UNP E4S6E9
A	16	TYR	-	expression tag	UNP E4S6E9
A	17	PHE	-	expression tag	UNP E4S6E9
A	18	GLN	-	expression tag	UNP E4S6E9
A	19	GLY	-	expression tag	UNP E4S6E9
A	20	HIS	-	expression tag	UNP E4S6E9
A	21	ILE	-	expression tag	UNP E4S6E9

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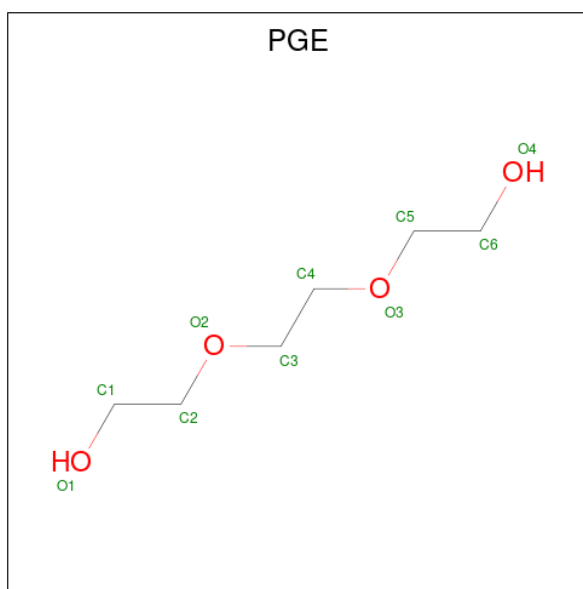
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP E4S6E9
B	2	GLY	-	expression tag	UNP E4S6E9
B	3	SER	-	expression tag	UNP E4S6E9
B	4	SER	-	expression tag	UNP E4S6E9
B	5	HIS	-	expression tag	UNP E4S6E9
B	6	HIS	-	expression tag	UNP E4S6E9
B	7	HIS	-	expression tag	UNP E4S6E9
B	8	HIS	-	expression tag	UNP E4S6E9
B	9	HIS	-	expression tag	UNP E4S6E9
B	10	HIS	-	expression tag	UNP E4S6E9
B	11	SER	-	expression tag	UNP E4S6E9
B	12	SER	-	expression tag	UNP E4S6E9
B	13	GLU	-	expression tag	UNP E4S6E9
B	14	ASN	-	expression tag	UNP E4S6E9
B	15	LEU	-	expression tag	UNP E4S6E9
B	16	TYR	-	expression tag	UNP E4S6E9
B	17	PHE	-	expression tag	UNP E4S6E9
B	18	GLN	-	expression tag	UNP E4S6E9
B	19	GLY	-	expression tag	UNP E4S6E9
B	20	HIS	-	expression tag	UNP E4S6E9
B	21	ILE	-	expression tag	UNP E4S6E9
C	1	MET	-	initiating methionine	UNP E4S6E9
C	2	GLY	-	expression tag	UNP E4S6E9
C	3	SER	-	expression tag	UNP E4S6E9
C	4	SER	-	expression tag	UNP E4S6E9
C	5	HIS	-	expression tag	UNP E4S6E9
C	6	HIS	-	expression tag	UNP E4S6E9
C	7	HIS	-	expression tag	UNP E4S6E9
C	8	HIS	-	expression tag	UNP E4S6E9
C	9	HIS	-	expression tag	UNP E4S6E9
C	10	HIS	-	expression tag	UNP E4S6E9
C	11	SER	-	expression tag	UNP E4S6E9
C	12	SER	-	expression tag	UNP E4S6E9
C	13	GLU	-	expression tag	UNP E4S6E9
C	14	ASN	-	expression tag	UNP E4S6E9
C	15	LEU	-	expression tag	UNP E4S6E9
C	16	TYR	-	expression tag	UNP E4S6E9
C	17	PHE	-	expression tag	UNP E4S6E9
C	18	GLN	-	expression tag	UNP E4S6E9
C	19	GLY	-	expression tag	UNP E4S6E9
C	20	HIS	-	expression tag	UNP E4S6E9
C	21	ILE	-	expression tag	UNP E4S6E9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP E4S6E9
D	2	GLY	-	expression tag	UNP E4S6E9
D	3	SER	-	expression tag	UNP E4S6E9
D	4	SER	-	expression tag	UNP E4S6E9
D	5	HIS	-	expression tag	UNP E4S6E9
D	6	HIS	-	expression tag	UNP E4S6E9
D	7	HIS	-	expression tag	UNP E4S6E9
D	8	HIS	-	expression tag	UNP E4S6E9
D	9	HIS	-	expression tag	UNP E4S6E9
D	10	HIS	-	expression tag	UNP E4S6E9
D	11	SER	-	expression tag	UNP E4S6E9
D	12	SER	-	expression tag	UNP E4S6E9
D	13	GLU	-	expression tag	UNP E4S6E9
D	14	ASN	-	expression tag	UNP E4S6E9
D	15	LEU	-	expression tag	UNP E4S6E9
D	16	TYR	-	expression tag	UNP E4S6E9
D	17	PHE	-	expression tag	UNP E4S6E9
D	18	GLN	-	expression tag	UNP E4S6E9
D	19	GLY	-	expression tag	UNP E4S6E9
D	20	HIS	-	expression tag	UNP E4S6E9
D	21	ILE	-	expression tag	UNP E4S6E9

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			24	6	14	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		

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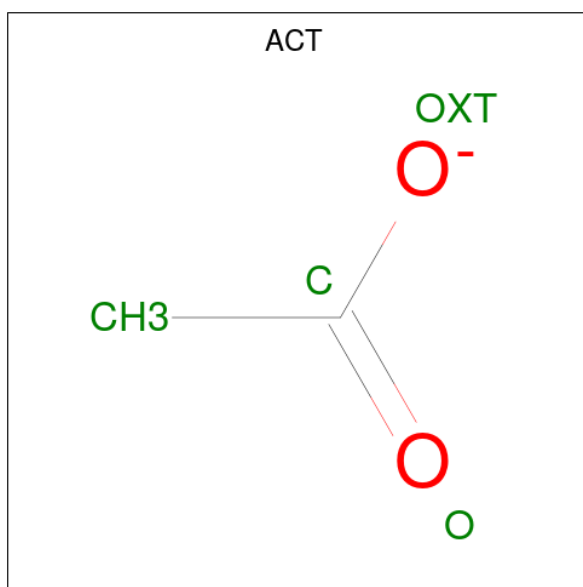
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			7	2	3	2		

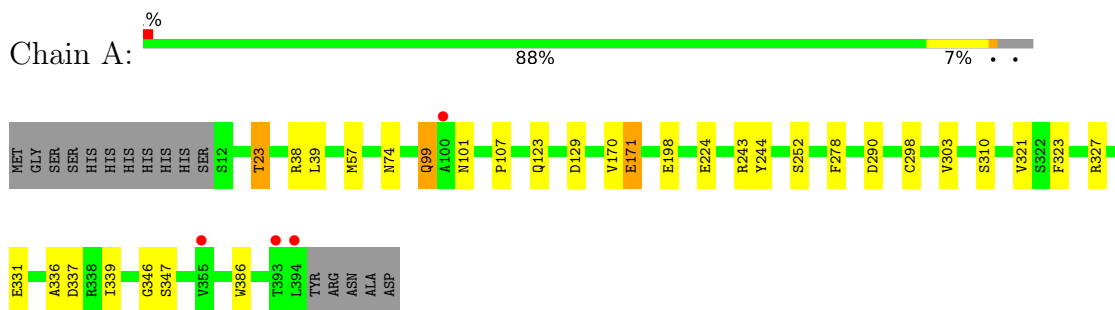
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	310	Total	O	0	0
			310	310		
6	B	252	Total	O	0	0
			252	252		
6	C	264	Total	O	0	0
			264	264		
6	D	312	Total	O	0	0
			312	312		

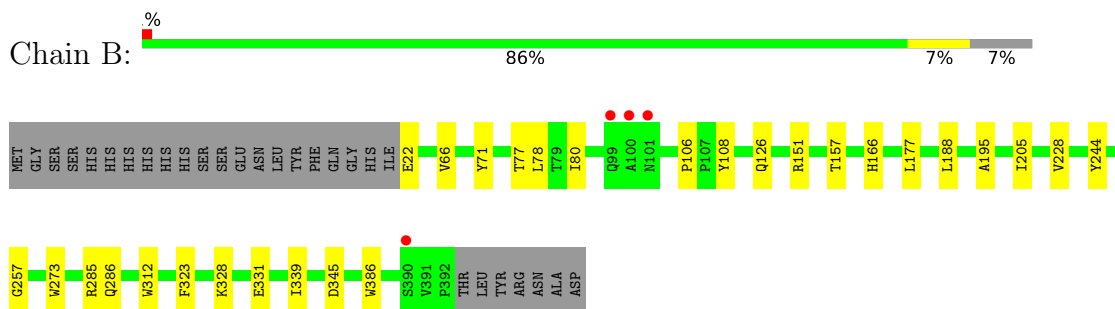
3 Residue-property plots [i](#)

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.

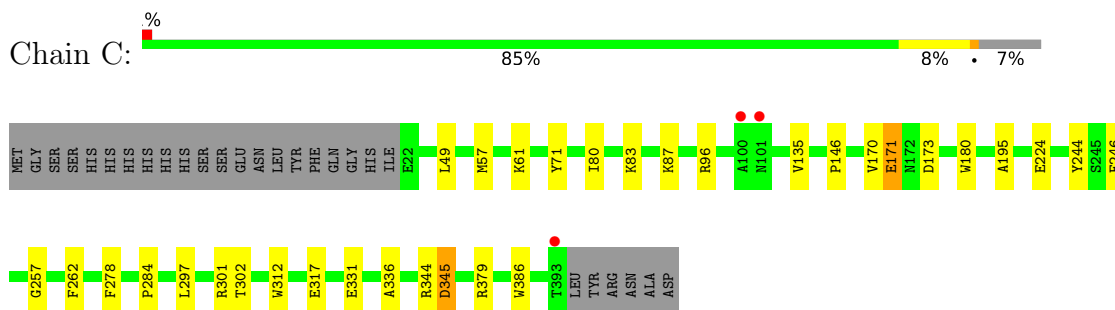
- Molecule 1: Beta-xylanase



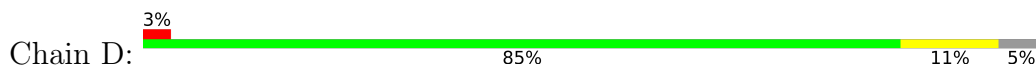
- Molecule 1: Beta-xylanase

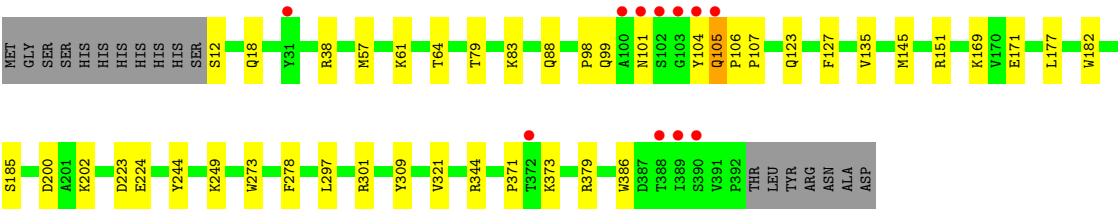


- Molecule 1: Beta-xylanase



- Molecule 1: Beta-xylanase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.06Å 116.90Å 160.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.62 – 1.89 48.62 – 1.89	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.62-1.89) 97.3 (48.62-1.89)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.167 , 0.207 0.168 , 0.207	Depositor DCC
R_{free} test set	2000 reflections (1.34%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13567	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.31	0/3148	0.49	0/4289
1	B	0.28	0/3032	0.47	0/4132
1	C	0.30	0/3040	0.46	0/4143
1	D	0.31	0/3150	0.50	0/4292
All	All	0.30	0/12370	0.48	0/16856

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3058	0	2891	31	0
1	B	2945	0	2780	22	0
1	C	2953	0	2789	24	0
1	D	3059	0	2881	40	0
2	A	10	14	14	2	0
2	C	10	14	14	0	0
3	A	24	36	36	7	0
3	B	12	18	18	0	0
3	C	32	48	48	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	28	42	42	7	0
4	A	7	10	10	0	0
4	B	21	30	30	3	0
4	D	21	30	30	8	0
5	B	4	3	3	0	0
6	A	310	0	0	7	0
6	B	252	0	0	5	0
6	C	264	0	0	7	0
6	D	312	0	0	6	0
All	All	13322	245	11586	116	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 5.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243[B]:ARG:NH1	6:A:501:HOH:O	1.92	1.03
1:D:105:GLN:HG3	1:D:106:PRO:HD2	1.55	0.89
1:A:346:GLY:H	3:A:405:EDO:C1	1.90	0.85
1:A:327:ARG:O	1:A:331[B]:GLU:HG3	1.79	0.82
1:D:61:LYS:HD2	4:D:409:PEG:O2	1.82	0.79
1:A:346:GLY:H	3:A:405:EDO:H12	1.51	0.76
1:B:151:ARG:HD3	1:B:157:THR:OG1	1.88	0.73
1:B:166:HIS:ND1	6:B:501:HOH:O	2.25	0.70
1:A:347:SER:HB3	6:A:750:HOH:O	1.92	0.68
1:A:252:SER:HA	2:A:401:PGE:H52	1.75	0.67
1:D:151:ARG:HD2	3:D:401:EDO:C2	2.25	0.67
1:C:224:GLU:HG3	6:C:673:HOH:O	1.93	0.67
1:D:223:ASP:HB2	4:D:409:PEG:H42	1.76	0.66
1:B:66:VAL:HG12	6:B:583:HOH:O	1.95	0.66
1:C:345:ASP:H	3:C:407:EDO:H11	1.61	0.66
1:D:64[A]:THR:HG22	6:D:589:HOH:O	1.96	0.65
1:B:331:GLU:HG2	4:B:402:PEG:H41	1.77	0.65
1:D:185:SER:HB2	4:D:409:PEG:H21	1.79	0.64
1:C:379:ARG:HE	3:C:406:EDO:H21	1.63	0.64
1:C:173:ASP:HB3	6:C:655:HOH:O	1.97	0.64
1:C:87:LYS:HD3	6:C:730:HOH:O	1.98	0.63
1:A:252:SER:H	3:A:402:EDO:C1	2.13	0.62
1:A:346:GLY:H	3:A:405:EDO:H11	1.65	0.62
1:D:244:TYR:CZ	1:D:386:TRP:HB3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:GLU:HB2	6:C:592:HOH:O	1.99	0.61
1:A:23:THR:HG22	6:B:587:HOH:O	1.99	0.61
1:B:66:VAL:HG12	6:B:612:HOH:O	2.02	0.59
1:D:61:LYS:HE3	4:D:409:PEG:H11	1.85	0.59
6:A:681:HOH:O	1:B:126:GLN:HG2	2.03	0.58
1:A:224:GLU:HG3	6:A:740:HOH:O	2.04	0.57
1:D:83:LYS:HE2	1:D:88:GLN:OE1	2.04	0.57
1:D:151:ARG:HD2	3:D:401:EDO:H11	1.85	0.57
1:C:345:ASP:H	3:C:407:EDO:C1	2.17	0.57
1:D:151:ARG:HD2	3:D:401:EDO:C1	2.35	0.56
1:D:64[A]:THR:HG23	6:D:740:HOH:O	2.03	0.56
1:A:23:THR:HG23	1:B:77:THR:HG21	1.87	0.56
1:C:61:LYS:HE3	6:C:558:HOH:O	2.06	0.56
1:B:71:TYR:CE1	1:B:195:ALA:HA	2.40	0.55
1:D:309:TYR:CE2	1:D:379:ARG:HD3	2.41	0.55
1:A:23:THR:HG23	1:B:77:THR:CG2	2.37	0.55
1:C:344:ARG:HB2	3:C:407:EDO:H11	1.88	0.55
1:D:18[B]:GLN:NE2	1:D:249:LYS:HE3	2.21	0.54
1:C:331[B]:GLU:HG3	1:C:336:ALA:HB2	1.90	0.54
1:D:309:TYR:CZ	1:D:379:ARG:HD3	2.42	0.54
1:D:12:SER:N	6:D:506:HOH:O	2.41	0.54
1:B:106:PRO:HD3	1:B:108:TYR:OH	2.08	0.53
1:B:244:TYR:CE1	1:B:386:TRP:HB3	2.46	0.51
1:A:129:ASP:HB2	3:A:403:EDO:H22	1.94	0.50
1:A:23:THR:O	1:A:243[B]:ARG:NH1	2.45	0.50
1:A:252:SER:H	3:A:402:EDO:H11	1.76	0.50
1:A:99:GLN:HB2	1:A:101:ASN:OD1	2.11	0.50
1:C:244:TYR:CE1	1:C:386:TRP:HB3	2.47	0.50
1:D:57:MET:HA	1:D:278:PHE:HB2	1.94	0.49
1:A:321:VAL:HG22	1:A:386:TRP:CD2	2.48	0.49
1:D:185:SER:CB	4:D:409:PEG:H21	2.44	0.48
1:C:49:LEU:HB2	1:C:297:LEU:HD21	1.95	0.48
1:C:302:THR:HG23	3:C:403:EDO:H12	1.95	0.47
1:A:331[B]:GLU:HG2	1:A:336:ALA:HB2	1.95	0.47
1:D:107:PRO:HB2	1:D:200:ASP:HB2	1.95	0.47
1:D:185:SER:CB	4:D:409:PEG:C2	2.93	0.47
1:A:252:SER:HA	2:A:401:PGE:C5	2.45	0.47
1:D:202:LYS:NZ	6:D:512:HOH:O	2.46	0.47
1:A:74:ASN:HB2	6:A:713:HOH:O	2.14	0.47
1:A:337:ASP:HB2	6:A:739:HOH:O	2.15	0.47
1:D:123:GLN:HG2	6:D:501:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:LYS:HE2	1:D:171:GLU:OE2	2.14	0.47
3:C:406:EDO:O2	6:C:501:HOH:O	2.21	0.46
1:D:177:LEU:HG	1:D:273:TRP:HB3	1.98	0.46
1:C:257:GLY:H	1:C:312:TRP:CG	2.33	0.46
1:C:71:TYR:CE1	1:C:195:ALA:HA	2.51	0.45
1:C:379:ARG:HE	3:C:406:EDO:C2	2.29	0.45
1:A:57:MET:HA	1:A:278:PHE:HB2	1.98	0.45
1:D:185:SER:OG	4:D:409:PEG:H42	2.17	0.45
1:D:224:GLU:HA	1:D:301:ARG:CZ	2.47	0.45
1:A:323:PHE:CE1	1:A:339:ILE:HG12	2.51	0.45
1:D:83:LYS:HE3	1:D:83:LYS:HB2	1.67	0.45
1:A:123:GLN:HG2	6:A:502:HOH:O	2.17	0.45
1:A:243[B]:ARG:HD2	1:A:290:ASP:OD2	2.17	0.45
1:D:127:PHE:HB2	3:D:404:EDO:H21	1.99	0.44
1:B:66:VAL:HG22	1:B:66:VAL:O	2.18	0.44
1:A:23:THR:HG21	6:B:534:HOH:O	2.16	0.44
1:B:188:LEU:HD23	1:B:188:LEU:HA	1.86	0.44
1:C:83:LYS:HE2	1:C:83:LYS:HB3	1.67	0.44
1:D:79:THR:HG21	3:D:402:EDO:H21	1.99	0.44
1:B:177:LEU:HG	1:B:273:TRP:HB3	2.00	0.44
1:C:57:MET:HA	1:C:278:PHE:HB2	2.01	0.43
1:A:171:GLU:H	1:A:171:GLU:CD	2.25	0.43
1:B:71:TYR:CZ	1:B:195:ALA:HA	2.54	0.43
1:A:244:TYR:CZ	1:A:386:TRP:HB3	2.52	0.43
1:D:98:PRO:HB3	1:D:135:VAL:O	2.18	0.43
1:D:344:ARG:C	1:D:344:ARG:HD2	2.45	0.42
1:A:107:PRO:HA	1:A:198:GLU:O	2.20	0.42
1:B:257:GLY:H	1:B:312:TRP:CG	2.38	0.42
1:C:246:PHE:CD1	1:C:317:GLU:HB3	2.55	0.42
1:B:323:PHE:CE1	1:B:339:ILE:HG12	2.55	0.42
1:B:22:GLU:OE2	1:B:285:ARG:NH1	2.51	0.42
1:C:96:ARG:HD2	6:C:523:HOH:O	2.19	0.42
1:D:145[B]:MET:SD	6:D:797:HOH:O	2.61	0.41
1:A:310:SER:OG	3:A:405:EDO:C1	2.68	0.41
1:B:78:LEU:HD21	1:B:80:ILE:HD11	2.02	0.41
1:C:96:ARG:HG2	1:C:135:VAL:HG11	2.01	0.41
1:D:371:PRO:C	1:D:373:LYS:H	2.27	0.41
1:D:18[B]:GLN:HE21	1:D:249:LYS:HE3	1.86	0.41
1:D:182:TRP:HA	4:D:409:PEG:H32	2.02	0.41
1:C:262:PHE:CG	1:C:284:PRO:HG3	2.56	0.41
1:A:298:CYS:HB2	1:A:303:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:PRO:O	1:D:373:LYS:N	2.48	0.40
1:B:205:ILE:HG23	1:B:228:VAL:HB	2.03	0.40
1:B:286:GLN:HG2	4:B:406:PEG:H41	2.03	0.40
1:B:328:LYS:HD3	4:B:402:PEG:H31	2.02	0.40
1:D:151:ARG:HD2	3:D:401:EDO:O2	2.21	0.40
1:D:151:ARG:HG3	3:D:401:EDO:O2	2.21	0.40
1:D:321:VAL:HG22	1:D:386:TRP:CE2	2.56	0.40
1:C:146:PRO:HB3	1:C:180:TRP:CD1	2.55	0.40
1:C:224:GLU:HA	1:C:301:ARG:CZ	2.52	0.40
1:D:297:LEU:HA	1:D:297:LEU:HD23	1.90	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	385/399 (96%)	375 (97%)	10 (3%)	0	100	100
1	B	372/399 (93%)	361 (97%)	10 (3%)	1 (0%)	36	26
1	C	373/399 (94%)	361 (97%)	11 (3%)	1 (0%)	36	26
1	D	385/399 (96%)	372 (97%)	13 (3%)	0	100	100
All	All	1515/1596 (95%)	1469 (97%)	44 (3%)	2 (0%)	48	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	345	ASP
1	C	345	ASP

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	317/327 (97%)	311 (98%)	6 (2%)	50	36
1	B	305/327 (93%)	305 (100%)	0	100	100
1	C	306/327 (94%)	303 (99%)	3 (1%)	68	60
1	D	317/327 (97%)	312 (98%)	5 (2%)	55	43
All	All	1245/1308 (95%)	1231 (99%)	14 (1%)	65	56

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	38	ARG
1	A	39	LEU
1	A	99	GLN
1	A	170	VAL
1	A	171	GLU
1	C	80	ILE
1	C	170	VAL
1	C	171	GLU
1	D	38	ARG
1	D	99	GLN
1	D	101	ASN
1	D	104	TYR
1	D	105	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	76	ASN
1	A	99	GLN
1	A	230	ASN
1	A	268	ASN

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Mol	Chain	Res	Type
1	B	168	ASN
1	B	258	ASN
1	B	291	GLN
1	C	250	GLN
1	D	126	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

34 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	D	403	-	3,3,3	0.55	0	2,2,2	0.27	0
3	EDO	C	408	-	3,3,3	0.48	0	2,2,2	0.31	0
3	EDO	A	402	-	3,3,3	0.49	0	2,2,2	0.65	0
4	PEG	D	406	-	6,6,6	0.54	0	5,5,5	0.32	0
3	EDO	A	407	-	3,3,3	0.47	0	2,2,2	0.29	0
3	EDO	A	403	-	3,3,3	0.48	0	2,2,2	0.28	0
3	EDO	D	402	-	3,3,3	0.55	0	2,2,2	0.03	0
3	EDO	D	407	-	3,3,3	0.52	0	2,2,2	0.27	0
4	PEG	B	402	-	6,6,6	0.53	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	404	-	3,3,3	0.46	0	2,2,2	0.38	0
2	PGE	A	401	-	9,9,9	0.35	0	8,8,8	0.42	0
4	PEG	B	406	-	6,6,6	0.51	0	5,5,5	0.32	0
2	PGE	C	405	-	9,9,9	0.33	0	8,8,8	0.39	0
3	EDO	A	406	-	3,3,3	0.51	0	2,2,2	0.36	0
3	EDO	C	406	-	3,3,3	0.44	0	2,2,2	0.24	0
3	EDO	B	401	-	3,3,3	0.49	0	2,2,2	0.69	0
3	EDO	A	405	-	3,3,3	0.32	0	2,2,2	0.68	0
3	EDO	C	407	-	3,3,3	0.49	0	2,2,2	0.16	0
3	EDO	C	404	-	3,3,3	0.50	0	2,2,2	0.19	0
3	EDO	C	402	-	3,3,3	0.40	0	2,2,2	1.06	0
3	EDO	C	409	-	3,3,3	0.47	0	2,2,2	0.31	0
4	PEG	A	404	-	6,6,6	0.53	0	5,5,5	0.40	0
4	PEG	B	403	-	6,6,6	0.52	0	5,5,5	0.39	0
3	EDO	B	405	-	3,3,3	0.49	0	2,2,2	0.33	0
4	PEG	D	405	-	6,6,6	0.51	0	5,5,5	0.53	0
5	ACT	B	407	-	3,3,3	1.97	1 (33%)	3,3,3	1.32	0
3	EDO	C	403	-	3,3,3	0.55	0	2,2,2	0.07	0
3	EDO	D	408	-	3,3,3	0.58	0	2,2,2	0.03	0
3	EDO	C	401	-	3,3,3	0.53	0	2,2,2	0.26	0
3	EDO	D	404	-	3,3,3	0.51	0	2,2,2	0.33	0
3	EDO	D	410	-	3,3,3	0.47	0	2,2,2	0.34	0
4	PEG	D	409	-	6,6,6	0.51	0	5,5,5	0.39	0
3	EDO	D	401	-	3,3,3	0.49	0	2,2,2	0.40	0
3	EDO	A	408	-	3,3,3	0.45	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
3	EDO	D	403	-	-	0/1/1/1	-
3	EDO	C	408	-	-	0/1/1/1	-
3	EDO	A	402	-	-	1/1/1/1	-
4	PEG	D	406	-	-	2/4/4/4	-
3	EDO	A	407	-	-	1/1/1/1	-
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	D	402	-	-	1/1/1/1	-
3	EDO	D	407	-	-	0/1/1/1	-
4	PEG	B	402	-	-	3/4/4/4	-
3	EDO	B	404	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	A	401	-	-	2/7/7/7	-
4	PEG	B	406	-	-	3/4/4/4	-
2	PGE	C	405	-	-	3/7/7/7	-
3	EDO	A	406	-	-	0/1/1/1	-
3	EDO	C	406	-	-	1/1/1/1	-
3	EDO	B	401	-	-	1/1/1/1	-
3	EDO	A	405	-	-	1/1/1/1	-
3	EDO	C	407	-	-	1/1/1/1	-
3	EDO	C	404	-	-	1/1/1/1	-
3	EDO	C	402	-	-	1/1/1/1	-
3	EDO	C	409	-	-	0/1/1/1	-
4	PEG	A	404	-	-	2/4/4/4	-
4	PEG	B	403	-	-	1/4/4/4	-
3	EDO	B	405	-	-	0/1/1/1	-
4	PEG	D	405	-	-	3/4/4/4	-
3	EDO	C	403	-	-	0/1/1/1	-
3	EDO	D	408	-	-	1/1/1/1	-
3	EDO	C	401	-	-	1/1/1/1	-
3	EDO	D	404	-	-	0/1/1/1	-
3	EDO	D	410	-	-	0/1/1/1	-
4	PEG	D	409	-	-	2/4/4/4	-
3	EDO	D	401	-	-	1/1/1/1	-
3	EDO	A	408	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	407	ACT	CH3-C	3.02	1.61	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	402	PEG	O2-C3-C4-O4
4	D	405	PEG	O2-C3-C4-O4
2	C	405	PGE	C4-C3-O2-C2
2	A	401	PGE	O2-C3-C4-O3
4	A	404	PEG	O1-C1-C2-O2
3	A	407	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	405	PGE	O2-C3-C4-O3
4	D	406	PEG	O1-C1-C2-O2
4	D	409	PEG	O2-C3-C4-O4
4	B	402	PEG	O1-C1-C2-O2
3	A	405	EDO	O1-C1-C2-O2
3	C	401	EDO	O1-C1-C2-O2
4	B	406	PEG	O2-C3-C4-O4
4	D	409	PEG	O1-C1-C2-O2
2	C	405	PGE	O1-C1-C2-O2
4	D	405	PEG	C1-C2-O2-C3
4	B	402	PEG	C4-C3-O2-C2
3	C	407	EDO	O1-C1-C2-O2
2	A	401	PGE	O1-C1-C2-O2
4	B	406	PEG	C1-C2-O2-C3
4	B	406	PEG	O1-C1-C2-O2
3	C	402	EDO	O1-C1-C2-O2
3	C	406	EDO	O1-C1-C2-O2
3	D	402	EDO	O1-C1-C2-O2
3	B	401	EDO	O1-C1-C2-O2
3	D	401	EDO	O1-C1-C2-O2
4	A	404	PEG	C4-C3-O2-C2
4	D	406	PEG	C1-C2-O2-C3
4	B	403	PEG	C1-C2-O2-C3
4	D	405	PEG	C4-C3-O2-C2
3	D	408	EDO	O1-C1-C2-O2
3	A	402	EDO	O1-C1-C2-O2
3	C	404	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	EDO	2	0
3	A	403	EDO	1	0
3	D	402	EDO	1	0
4	B	402	PEG	2	0
2	A	401	PGE	2	0
4	B	406	PEG	1	0
3	C	406	EDO	3	0
3	A	405	EDO	4	0
3	C	407	EDO	3	0
3	C	403	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	404	EDO	1	0
4	D	409	PEG	8	0
3	D	401	EDO	5	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	383/399 (95%)	-0.40	4 (1%)	79 83	11, 26, 45, 75	4 (1%)
1	B	371/399 (92%)	-0.23	4 (1%)	78 82	14, 29, 52, 76	3 (0%)
1	C	372/399 (93%)	-0.25	3 (0%)	82 86	12, 29, 48, 78	3 (0%)
1	D	381/399 (95%)	-0.28	11 (2%)	53 58	14, 27, 47, 82	6 (1%)
All	All	1507/1596 (94%)	-0.29	22 (1%)	72 77	11, 28, 49, 82	16 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	100	ALA	5.0
1	D	104	TYR	4.7
1	A	394	LEU	4.5
1	D	102	SER	3.9
1	D	389	ILE	3.6
1	A	393	THR	3.5
1	D	103	GLY	3.3
1	B	100	ALA	3.2
1	A	355[A]	VAL	3.2
1	D	388	THR	3.2
1	C	100	ALA	2.8
1	D	105	GLN	2.6
1	A	100	ALA	2.6
1	B	101	ASN	2.4
1	D	101	ASN	2.4
1	D	372	THR	2.3
1	D	390	SER	2.2
1	C	393	THR	2.2
1	B	390	SER	2.1
1	C	101	ASN	2.1
1	D	31	TYR	2.0
1	B	99	GLN	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
5	ACT	B	407	4/4	0.50	0.19	50,60,65,66	0
4	PEG	B	406	7/7	0.66	0.13	68,82,96,96	0
3	EDO	D	401	4/4	0.71	0.20	45,54,63,70	0
3	EDO	B	404	4/4	0.73	0.14	52,64,67,77	0
4	PEG	D	406	7/7	0.74	0.14	43,67,84,84	0
3	EDO	C	404	4/4	0.74	0.12	66,80,80,81	0
3	EDO	A	406	4/4	0.75	0.14	51,63,67,76	0
4	PEG	B	402	7/7	0.76	0.14	45,58,71,71	0
3	EDO	A	408	4/4	0.76	0.13	53,63,67,78	0
3	EDO	C	409	4/4	0.77	0.11	57,69,70,84	0
2	PGE	A	401	10/10	0.79	0.16	40,57,69,70	0
3	EDO	D	403	4/4	0.80	0.12	44,53,64,77	0
3	EDO	D	410	4/4	0.80	0.12	54,65,71,75	0
3	EDO	D	404	4/4	0.81	0.13	47,57,65,66	0
4	PEG	A	404	7/7	0.81	0.13	52,62,71,74	0
3	EDO	C	407	4/4	0.82	0.26	39,47,66,80	0
3	EDO	D	402	4/4	0.82	0.22	41,54,64,65	0
4	PEG	D	409	7/7	0.83	0.13	37,48,60,66	0
3	EDO	D	407	4/4	0.83	0.12	50,60,64,75	0
4	PEG	D	405	7/7	0.84	0.12	42,59,72,79	0
4	PEG	B	403	7/7	0.84	0.12	55,66,78,80	0
3	EDO	D	408	4/4	0.85	0.19	37,53,64,75	0
2	PGE	C	405	10/10	0.85	0.10	41,56,70,71	0
3	EDO	C	408	4/4	0.86	0.13	44,56,68,68	0
3	EDO	C	401	4/4	0.87	0.19	35,42,69,75	0
3	EDO	C	406	4/4	0.87	0.19	23,39,53,63	0
3	EDO	B	405	4/4	0.88	0.21	36,57,66,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	405	4/4	0.88	0.16	22,29,37,45	10
3	EDO	A	402	4/4	0.89	0.16	24,38,59,59	0
3	EDO	A	407	4/4	0.91	0.08	49,61,62,73	0
3	EDO	A	403	4/4	0.92	0.10	42,51,57,66	0
3	EDO	C	402	4/4	0.92	0.12	28,47,61,61	0
3	EDO	C	403	4/4	0.93	0.12	40,49,58,59	0
3	EDO	B	401	4/4	0.94	0.14	31,45,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.