



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:37 PM GMT

PDB ID : 3RBH  
Title : Structure of alginate export protein AlgE from *Pseudomonas aeruginosa*  
Authors : Whitney, J.C.; Hay, I.D.; Li, C.; Eckford, P.D.; Robinson, H.; Amaya, M.F.;  
Wood, L.F.; Ohman, D.E.; Bear, C.E.; Rehm, B.H.; Howell, P.L.  
Deposited on : 2011-03-29  
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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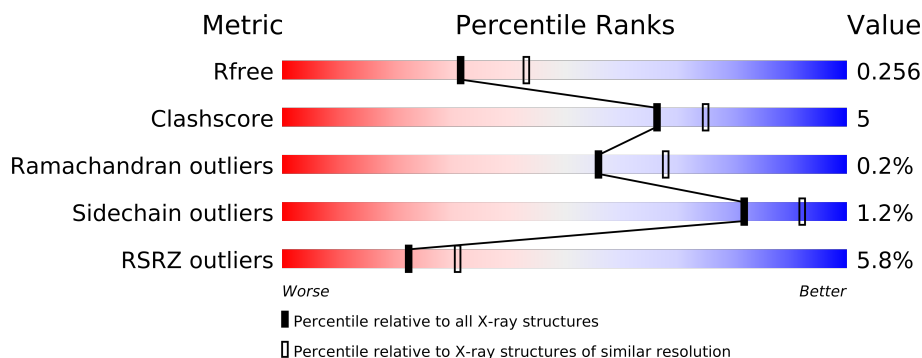
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	479	
1	B	479	
1	C	479	
1	D	479	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	A	492	-	X
3	EDO	A	493	-	X
3	EDO	A	8	-	X
3	EDO	B	494	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	B	495	-	X
3	EDO	C	491	-	X
3	EDO	C	492	-	X
3	EDO	C	493	-	X
3	EDO	D	491	-	X
3	EDO	D	492	-	X
4	C8E	A	10	-	X
4	C8E	B	496	-	X
4	C8E	B	501	-	X
4	C8E	B	502	-	X
4	C8E	B	8	-	X
4	C8E	C	498	-	X
4	C8E	D	494	-	X
4	C8E	D	496	-	X
4	C8E	D	497	-	X
4	C8E	D	498	-	X
4	C8E	D	499	-	X
4	C8E	D	5	-	X
4	C8E	D	501	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14038 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Alginate production protein AlgE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	Se	0	2	0
			3305	2073	585	643	4			
1	B	429	Total	C	N	O	Se	0	5	0
			3328	2084	588	652	4			
1	C	409	Total	C	N	O	Se	0	1	0
			3165	1987	564	610	4			
1	D	410	Total	C	N	O	Se	0	1	0
			3165	1992	560	609	4			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MSE	-	EXPRESSION TAG	UNP P18895
A	13	GLY	-	EXPRESSION TAG	UNP P18895
A	14	SER	-	EXPRESSION TAG	UNP P18895
A	15	SER	-	EXPRESSION TAG	UNP P18895
A	16	HIS	-	EXPRESSION TAG	UNP P18895
A	17	HIS	-	EXPRESSION TAG	UNP P18895
A	18	HIS	-	EXPRESSION TAG	UNP P18895
A	19	HIS	-	EXPRESSION TAG	UNP P18895
A	20	HIS	-	EXPRESSION TAG	UNP P18895
A	21	HIS	-	EXPRESSION TAG	UNP P18895
A	22	SER	-	EXPRESSION TAG	UNP P18895
A	23	SER	-	EXPRESSION TAG	UNP P18895
A	24	GLY	-	EXPRESSION TAG	UNP P18895
A	25	LEU	-	EXPRESSION TAG	UNP P18895
A	26	VAL	-	EXPRESSION TAG	UNP P18895
A	27	PRO	-	EXPRESSION TAG	UNP P18895
A	28	ARG	-	EXPRESSION TAG	UNP P18895
A	29	GLY	-	EXPRESSION TAG	UNP P18895
A	30	SER	-	EXPRESSION TAG	UNP P18895
A	31	HIS	-	EXPRESSION TAG	UNP P18895
A	32	MSE	-	EXPRESSION TAG	UNP P18895

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Chain	Residue	Modelled	Actual	Comment	Reference
B	12	MSE	-	EXPRESSION TAG	UNP P18895
B	13	GLY	-	EXPRESSION TAG	UNP P18895
B	14	SER	-	EXPRESSION TAG	UNP P18895
B	15	SER	-	EXPRESSION TAG	UNP P18895
B	16	HIS	-	EXPRESSION TAG	UNP P18895
B	17	HIS	-	EXPRESSION TAG	UNP P18895
B	18	HIS	-	EXPRESSION TAG	UNP P18895
B	19	HIS	-	EXPRESSION TAG	UNP P18895
B	20	HIS	-	EXPRESSION TAG	UNP P18895
B	21	HIS	-	EXPRESSION TAG	UNP P18895
B	22	SER	-	EXPRESSION TAG	UNP P18895
B	23	SER	-	EXPRESSION TAG	UNP P18895
B	24	GLY	-	EXPRESSION TAG	UNP P18895
B	25	LEU	-	EXPRESSION TAG	UNP P18895
B	26	VAL	-	EXPRESSION TAG	UNP P18895
B	27	PRO	-	EXPRESSION TAG	UNP P18895
B	28	ARG	-	EXPRESSION TAG	UNP P18895
B	29	GLY	-	EXPRESSION TAG	UNP P18895
B	30	SER	-	EXPRESSION TAG	UNP P18895
B	31	HIS	-	EXPRESSION TAG	UNP P18895
B	32	MSE	-	EXPRESSION TAG	UNP P18895
C	12	MSE	-	EXPRESSION TAG	UNP P18895
C	13	GLY	-	EXPRESSION TAG	UNP P18895
C	14	SER	-	EXPRESSION TAG	UNP P18895
C	15	SER	-	EXPRESSION TAG	UNP P18895
C	16	HIS	-	EXPRESSION TAG	UNP P18895
C	17	HIS	-	EXPRESSION TAG	UNP P18895
C	18	HIS	-	EXPRESSION TAG	UNP P18895
C	19	HIS	-	EXPRESSION TAG	UNP P18895
C	20	HIS	-	EXPRESSION TAG	UNP P18895
C	21	HIS	-	EXPRESSION TAG	UNP P18895
C	22	SER	-	EXPRESSION TAG	UNP P18895
C	23	SER	-	EXPRESSION TAG	UNP P18895
C	24	GLY	-	EXPRESSION TAG	UNP P18895
C	25	LEU	-	EXPRESSION TAG	UNP P18895
C	26	VAL	-	EXPRESSION TAG	UNP P18895
C	27	PRO	-	EXPRESSION TAG	UNP P18895
C	28	ARG	-	EXPRESSION TAG	UNP P18895
C	29	GLY	-	EXPRESSION TAG	UNP P18895
C	30	SER	-	EXPRESSION TAG	UNP P18895
C	31	HIS	-	EXPRESSION TAG	UNP P18895
C	32	MSE	-	EXPRESSION TAG	UNP P18895

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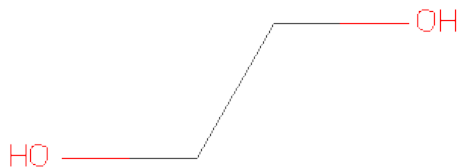
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Chain	Residue	Modelled	Actual	Comment	Reference
D	12	MSE	-	EXPRESSION TAG	UNP P18895
D	13	GLY	-	EXPRESSION TAG	UNP P18895
D	14	SER	-	EXPRESSION TAG	UNP P18895
D	15	SER	-	EXPRESSION TAG	UNP P18895
D	16	HIS	-	EXPRESSION TAG	UNP P18895
D	17	HIS	-	EXPRESSION TAG	UNP P18895
D	18	HIS	-	EXPRESSION TAG	UNP P18895
D	19	HIS	-	EXPRESSION TAG	UNP P18895
D	20	HIS	-	EXPRESSION TAG	UNP P18895
D	21	HIS	-	EXPRESSION TAG	UNP P18895
D	22	SER	-	EXPRESSION TAG	UNP P18895
D	23	SER	-	EXPRESSION TAG	UNP P18895
D	24	GLY	-	EXPRESSION TAG	UNP P18895
D	25	LEU	-	EXPRESSION TAG	UNP P18895
D	26	VAL	-	EXPRESSION TAG	UNP P18895
D	27	PRO	-	EXPRESSION TAG	UNP P18895
D	28	ARG	-	EXPRESSION TAG	UNP P18895
D	29	GLY	-	EXPRESSION TAG	UNP P18895
D	30	SER	-	EXPRESSION TAG	UNP P18895
D	31	HIS	-	EXPRESSION TAG	UNP P18895
D	32	MSE	-	EXPRESSION TAG	UNP P18895

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



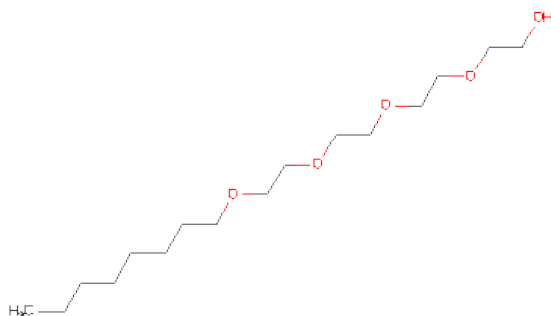
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total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

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

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	11	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	10	1		
4	A	1	Total	C	O	0	0
			10	9	1		
4	A	1	Total	C	O	0	0
			10	9	1		
4	B	1	Total	C	O	0	0
			9	8	1		
4	B	1	Total	C	O	0	0
			12	10	2		
4	B	1	Total	C	O	0	0
			21	16	5		
4	B	1	Total	C	O	0	0
			9	8	1		
4	B	1	Total	C	O	0	0
			9	8	1		
4	B	1	Total	C	O	0	0
			13	11	2		
4	B	1	Total	C	O	0	0
			10	9	1		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			21	16	5		
4	C	1	Total	C	O	0	0
			12	10	2		
4	C	1	Total	C	O	0	0
			12	10	2		
4	C	1	Total	C	O	0	0
			10	8	2		
4	C	1	Total	C	O	0	0
			9	8	1		
4	C	1	Total	C	O	0	0
			18	14	4		
4	D	1	Total	C	O	0	0
			11	10	1		
4	D	1	Total	C	O	0	0
			21	16	5		
4	D	1	Total	C	O	0	0
			19	15	4		
4	D	1	Total	C	O	0	0
			16	13	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 9 8 1	0	0
4	D	1	Total C 8 8	0	0
4	D	1	Total C O 12 10 2	0	0
4	D	1	Total C O 13 11 2	0	0
4	D	1	Total C O 15 12 3	0	0
4	D	1	Total C O 13 11 2	0	0
4	D	1	Total C O 9 8 1	0	0

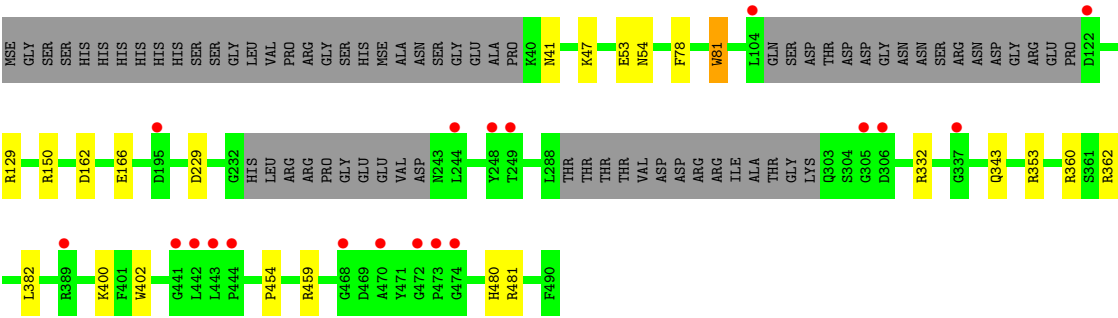
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	166	Total O 166 166	0	0
5	B	155	Total O 155 155	0	0
5	C	142	Total O 142 142	0	0
5	D	149	Total O 149 149	0	0



● Molecule 1: Alginate production protein AlgE

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.02Å 90.70Å 160.28Å 90.00° 107.65° 90.00°	Depositor
Resolution (Å)	44.76 – 2.30 44.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.0 (44.76-2.30) 99.7 (44.76-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.221 , 0.259 0.218 , 0.256	Depositor DCC
$R_{free}$ test set	4886 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.5	EDS
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 98006 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14038	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.60 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.0790e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, C8E, EDO

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	0.41	0/3387	0.55	0/4598
1	B	0.42	0/3410	0.55	0/4633
1	C	0.42	0/3244	0.55	0/4401
1	D	0.42	0/3244	0.56	0/4403
All	All	0.42	0/13285	0.56	0/18035

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3305	0	0	12	0
1	B	3328	0	0	23	0
1	C	3165	0	0	21	0
1	D	3165	0	0	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	0	36	1	0
3	B	32	0	48	3	0
3	C	28	0	42	2	0
3	D	12	0	18	1	0
4	A	44	0	74	1	0
4	B	91	0	142	8	0
4	C	82	0	129	3	0
4	D	146	0	244	3	0
5	A	166	0	0	0	0
5	B	155	0	0	10	0
5	C	142	0	0	6	0
5	D	149	0	0	5	0
All	All	14038	0	733	72	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (72) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:366:PHE:O	5:B:603:HOH:O	1.84	0.95
1:D:480:HIS:ND1	4:D:498:C8E:H102	1.97	0.79
1:B:370:PHE:CB	5:B:603:HOH:O	2.31	0.79
1:B:347:THR:N	3:B:6:EDO:HO2	1.81	0.78
1:B:370:PHE:CD2	5:B:603:HOH:O	2.37	0.77
1:A:347:THR:N	3:A:3:EDO:HO2	1.84	0.74
1:B:141:TYR:OH	4:B:500:C8E:H102	1.93	0.69
1:B:461:ARG:NH1	5:B:609:HOH:O	2.26	0.67
1:C:160:TRP:CD1	5:C:552:HOH:O	2.48	0.67
1:C:134:ASP:O	5:C:592:HOH:O	2.12	0.67
1:B:141:TYR:CZ	4:B:500:C8E:H102	2.30	0.66
1:D:343:GLN:O	5:D:624:HOH:O	2.14	0.65
1:B:483:PHE:CE2	5:B:609:HOH:O	2.49	0.65
1:D:332:ARG:NH2	5:D:561:HOH:O	2.30	0.64
1:A:81:TRP:CH2	1:C:148:PHE:CZ	2.85	0.64
1:B:387:GLN:NE2	5:B:592:HOH:O	2.31	0.63
1:D:162:ASP:OD2	1:D:362:ARG:NH2	2.32	0.61
1:B:69:ILE:CD1	4:B:8:C8E:H72	2.32	0.60
1:A:81:TRP:N	1:A:81:TRP:CE3	2.70	0.59
1:B:371:ARG:NH2	5:B:609:HOH:O	2.36	0.58
1:C:280:TRP:CE3	4:C:498:C8E:H32	2.39	0.58
1:B:223:VAL:CG1	3:B:495:EDO:H22	2.34	0.57
1:B:381[B]:THR:CG2	1:B:399:HIS:ND1	2.69	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:347:THR:N	3:C:1:EDO:HO2	2.06	0.54
1:A:81:TRP:CZ2	1:C:148:PHE:CZ	2.98	0.52
1:C:461:ARG:NH2	5:C:638:HOH:O	2.41	0.52
1:C:280:TRP:NE1	4:C:498:C8E:H112	2.24	0.52
1:C:162:ASP:OD2	1:C:362:ARG:NH2	2.42	0.52
1:B:141:TYR:CE1	4:B:500:C8E:H102	2.45	0.51
1:D:41:ASN:O	1:D:78:PHE:N	2.43	0.51
4:C:498:C8E:H52	4:C:498:C8E:O9	2.11	0.50
1:B:162:ASP:OD2	1:B:362:ARG:NH2	2.45	0.50
1:C:185:GLN:NE2	5:C:579:HOH:O	2.44	0.50
1:D:459:ARG:NH1	5:D:563:HOH:O	2.45	0.50
1:B:161:GLN:NE2	5:B:632:HOH:O	2.45	0.50
1:B:353:ARG:NH2	5:B:509:HOH:O	2.44	0.49
1:A:166:GLU:N	1:A:166:GLU:OE1	2.46	0.49
1:B:360:ARG:NH2	1:B:454:PRO:CG	2.76	0.48
1:A:360:ARG:NH2	1:A:454:PRO:CG	2.76	0.48
1:D:360:ARG:NH2	1:D:454:PRO:CG	2.77	0.47
1:C:360:ARG:NH2	1:C:454:PRO:CG	2.77	0.47
1:B:486:PHE:CD1	4:B:8:C8E:H142	2.51	0.46
4:D:5:C8E:H201	5:D:643:HOH:O	2.15	0.46
1:B:166:GLU:OE1	1:B:166:GLU:N	2.49	0.46
1:D:81:TRP:CZ2	4:D:5:C8E:H171	2.51	0.46
4:A:495:C8E:H42	4:A:495:C8E:H12	1.65	0.46
1:C:227:HIS:NE2	1:C:229:ASP:OD2	2.49	0.45
1:C:160:TRP:NE1	5:C:552:HOH:O	2.50	0.45
4:B:8:C8E:H141	4:B:8:C8E:H171	1.59	0.44
1:D:166:GLU:N	1:D:166:GLU:OE1	2.50	0.44
4:B:497:C8E:H112	3:D:492:EDO:H11	1.98	0.44
1:C:53:GLU:OE2	1:C:481:ARG:NE	2.51	0.44
1:C:413[A]:SER:OG	1:C:414:GLY:N	2.50	0.44
1:A:162:ASP:OD2	1:A:362:ARG:NH2	2.50	0.43
4:B:501:C8E:H13	4:B:501:C8E:H41	1.78	0.43
1:A:266:TYR:CZ	1:A:360:ARG:CG	3.01	0.43
1:B:159:GLN:OE1	3:B:4:EDO:H21	2.19	0.43
1:C:345:GLN:NE2	5:C:561:HOH:O	2.51	0.43
1:C:41:ASN:O	1:C:78:PHE:N	2.52	0.42
1:C:400:LYS:CD	1:C:402:TRP:CZ2	3.03	0.42
1:A:400:LYS:CD	1:A:402:TRP:CZ2	3.02	0.42
1:D:53:GLU:OE2	1:D:481:ARG:NE	2.52	0.42
1:B:400:LYS:CD	1:B:402:TRP:CZ2	3.03	0.42
1:A:81:TRP:CZ2	1:C:148:PHE:CE1	3.08	0.41
1:B:416:ASN:ND2	5:B:578:HOH:O	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:400:LYS:CD	1:D:402:TRP:CZ2	3.04	0.41
1:A:65:THR:O	1:A:66:LEU:CD1	2.69	0.41
1:C:218:HIS:O	3:C:493:EDO:H12	2.21	0.41
1:D:353:ARG:NH2	5:D:522:HOH:O	2.54	0.41
1:C:166:GLU:N	1:C:166:GLU:OE1	2.55	0.40
1:A:81:TRP:CG	1:A:81:TRP:O	2.74	0.40
1:D:129:ARG:O	1:D:150:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	424/479 (88%)	404 (95%)	19 (4%)	1 (0%)	56 68
1	B	428/479 (89%)	411 (96%)	16 (4%)	1 (0%)	56 68
1	C	402/479 (84%)	387 (96%)	14 (4%)	1 (0%)	56 68
1	D	403/479 (84%)	386 (96%)	16 (4%)	1 (0%)	56 68
All	All	1657/1916 (86%)	1588 (96%)	65 (4%)	4 (0%)	56 68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	B	54	ASN
1	C	54	ASN
1	D	54	ASN

### 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	316/382 (83%)	311 (98%)	5 (2%)	75	88
1	B	320/382 (84%)	317 (99%)	3 (1%)	87	95
1	C	302/382 (79%)	299 (99%)	3 (1%)	85	94
1	D	301/382 (79%)	297 (99%)	4 (1%)	80	91
All	All	1239/1528 (81%)	1224 (99%)	15 (1%)	82	92

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	229	ASP
1	A	242	ASP
1	A	382	LEU
1	A	413	SER
1	B	47	LYS
1	B	229	ASP
1	B	382	LEU
1	C	47	LYS
1	C	81	TRP
1	C	229	ASP
1	D	47	LYS
1	D	81	TRP
1	D	229	ASP
1	D	382	LEU

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 57 ligands modelled in this entry, 4 are monoatomic - leaving 53 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	C8E	A	10	-	10,10,20	1.93	1 (10%)	8,9,19	0.47	0
4	C8E	A	11	-	8,9,20	0.51	0	7,8,19	0.76	0
3	EDO	A	2	-	3,3,3	0.49	0	2,2,2	0.40	0
3	EDO	A	3	-	3,3,3	0.66	0	2,2,2	0.25	0
3	EDO	A	491	-	3,3,3	0.54	0	2,2,2	0.44	0
3	EDO	A	492	-	3,3,3	0.57	0	2,2,2	0.46	0
3	EDO	A	493	-	3,3,3	0.55	0	2,2,2	0.38	0
4	C8E	A	494	-	11,12,20	0.51	0	10,11,19	0.45	0
4	C8E	A	495	-	8,9,20	0.44	0	7,8,19	0.50	0
3	EDO	A	8	-	3,3,3	0.57	0	2,2,2	0.42	0
3	EDO	B	4	-	3,3,3	0.55	0	2,2,2	0.54	0
3	EDO	B	491	-	3,3,3	0.54	0	2,2,2	0.47	0
3	EDO	B	492	-	3,3,3	0.60	0	2,2,2	0.26	0
3	EDO	B	493	-	3,3,3	0.61	0	2,2,2	0.36	0
3	EDO	B	494	-	3,3,3	0.68	0	2,2,2	0.07	0
3	EDO	B	495	-	3,3,3	0.52	0	2,2,2	0.44	0
4	C8E	B	496	-	8,8,20	2.57	2 (25%)	6,7,19	0.60	0
4	C8E	B	497	-	11,11,20	0.49	0	10,10,19	0.50	0
4	C8E	B	498	-	8,8,20	0.51	0	7,7,19	0.79	0
4	C8E	B	499	-	7,8,20	2.49	1 (14%)	6,7,19	1.09	0
4	C8E	B	500	-	11,12,20	0.49	0	10,11,19	0.37	0
4	C8E	B	501	-	8,9,20	0.48	0	7,8,19	0.80	0
4	C8E	B	502	-	6,7,20	1.74	1 (16%)	5,6,19	1.04	0
3	EDO	B	6	-	3,3,3	0.64	0	2,2,2	0.26	0
4	C8E	B	8	-	20,20,20	0.42	0	19,19,19	0.36	0
3	EDO	B	9	-	3,3,3	0.58	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	C	1	-	3,3,3	0.60	0	2,2,2	0.45	0
3	EDO	C	10	-	3,3,3	0.58	0	2,2,2	0.35	0
3	EDO	C	11	-	3,3,3	0.59	0	2,2,2	0.44	0
3	EDO	C	491	-	3,3,3	0.55	0	2,2,2	0.33	0
3	EDO	C	492	-	3,3,3	0.54	0	2,2,2	0.47	0
3	EDO	C	493	-	3,3,3	0.60	0	2,2,2	0.20	0
4	C8E	C	494	-	20,20,20	0.47	0	19,19,19	0.41	0
4	C8E	C	495	-	10,11,20	1.25	1 (10%)	9,10,19	0.40	0
4	C8E	C	496	-	8,9,20	1.76	1 (12%)	7,8,19	0.78	0
4	C8E	C	497	-	8,8,20	0.50	0	7,7,19	0.72	0
4	C8E	C	498	-	17,17,20	0.48	0	16,16,19	0.45	0
3	EDO	C	5	-	3,3,3	0.62	0	2,2,2	0.08	0
4	C8E	C	7	-	11,11,20	0.40	0	10,10,19	0.91	1 (10%)
3	EDO	D	491	-	3,3,3	0.57	0	2,2,2	0.44	0
3	EDO	D	492	-	3,3,3	0.62	0	2,2,2	0.24	0
4	C8E	D	493	-	10,10,20	1.62	1 (10%)	8,9,19	0.45	0
4	C8E	D	494	-	14,15,20	0.49	0	13,14,19	0.45	0
4	C8E	D	495	-	8,8,20	0.49	0	7,7,19	0.73	0
4	C8E	D	496	-	7,7,20	2.03	1 (14%)	6,6,19	0.52	0
4	C8E	D	497	-	11,11,20	0.46	0	10,10,19	0.56	0
4	C8E	D	498	-	11,12,20	0.47	0	10,11,19	0.35	0
4	C8E	D	499	-	14,14,20	0.50	0	13,13,19	0.54	0
4	C8E	D	5	-	20,20,20	0.43	0	19,19,19	0.35	0
4	C8E	D	500	-	11,12,20	0.49	0	10,11,19	0.42	0
4	C8E	D	501	-	8,8,20	0.48	0	7,7,19	0.95	0
3	EDO	D	7	-	3,3,3	0.64	0	2,2,2	0.64	0
4	C8E	D	9	-	17,18,20	0.51	0	16,17,19	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	C8E	A	10	-	-	0/8/8/18	0/0/0/0
4	C8E	A	11	-	-	0/7/7/18	0/0/0/0
3	EDO	A	2	-	-	0/1/1/1	0/0/0/0
3	EDO	A	3	-	-	0/1/1/1	0/0/0/0
3	EDO	A	491	-	-	0/1/1/1	0/0/0/0
3	EDO	A	492	-	-	0/1/1/1	0/0/0/0
3	EDO	A	493	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	C8E	A	494	-	-	0/10/10/18	0/0/0/0
4	C8E	A	495	-	-	0/7/7/18	0/0/0/0
3	EDO	A	8	-	-	0/1/1/1	0/0/0/0
3	EDO	B	4	-	-	0/1/1/1	0/0/0/0
3	EDO	B	491	-	-	0/1/1/1	0/0/0/0
3	EDO	B	492	-	-	0/1/1/1	0/0/0/0
3	EDO	B	493	-	-	0/1/1/1	0/0/0/0
3	EDO	B	494	-	-	0/1/1/1	0/0/0/0
3	EDO	B	495	-	-	0/1/1/1	0/0/0/0
4	C8E	B	496	-	-	0/6/6/18	0/0/0/0
4	C8E	B	497	-	-	0/9/9/18	0/0/0/0
4	C8E	B	498	-	-	0/6/6/18	0/0/0/0
4	C8E	B	499	-	-	0/6/6/18	0/0/0/0
4	C8E	B	500	-	-	0/10/10/18	0/0/0/0
4	C8E	B	501	-	-	0/7/7/18	0/0/0/0
4	C8E	B	502	-	-	0/5/5/18	0/0/0/0
3	EDO	B	6	-	-	0/1/1/1	0/0/0/0
4	C8E	B	8	-	-	0/18/18/18	0/0/0/0
3	EDO	B	9	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1	-	-	0/1/1/1	0/0/0/0
3	EDO	C	10	-	-	0/1/1/1	0/0/0/0
3	EDO	C	11	-	-	0/1/1/1	0/0/0/0
3	EDO	C	491	-	-	0/1/1/1	0/0/0/0
3	EDO	C	492	-	-	0/1/1/1	0/0/0/0
3	EDO	C	493	-	-	0/1/1/1	0/0/0/0
4	C8E	C	494	-	-	0/18/18/18	0/0/0/0
4	C8E	C	495	-	-	0/9/9/18	0/0/0/0
4	C8E	C	496	-	-	0/7/7/18	0/0/0/0
4	C8E	C	497	-	-	0/6/6/18	0/0/0/0
4	C8E	C	498	-	-	0/15/15/18	0/0/0/0
3	EDO	C	5	-	-	0/1/1/1	0/0/0/0
4	C8E	C	7	-	-	0/9/9/18	0/0/0/0
3	EDO	D	491	-	-	0/1/1/1	0/0/0/0
3	EDO	D	492	-	-	0/1/1/1	0/0/0/0
4	C8E	D	493	-	-	0/8/8/18	0/0/0/0
4	C8E	D	494	-	-	0/13/13/18	0/0/0/0
4	C8E	D	495	-	-	0/6/6/18	0/0/0/0
4	C8E	D	496	-	-	0/5/5/18	0/0/0/0
4	C8E	D	497	-	-	0/9/9/18	0/0/0/0
4	C8E	D	498	-	-	0/10/10/18	0/0/0/0
4	C8E	D	499	-	-	0/12/12/18	0/0/0/0
4	C8E	D	5	-	-	0/18/18/18	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	C8E	D	500	-	-	0/10/10/18	0/0/0/0
4	C8E	D	501	-	-	0/6/6/18	0/0/0/0
3	EDO	D	7	-	-	0/1/1/1	0/0/0/0
4	C8E	D	9	-	-	0/16/16/18	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	499	C8E	C2-C3	-6.45	1.52	1.55
4	A	10	C8E	C11-C10	-6.02	1.52	1.55
4	B	496	C8E	C11-C10	-5.45	1.53	1.55
4	D	496	C8E	C8-C7	-5.33	1.53	1.55
4	D	493	C8E	C11-C10	-5.03	1.53	1.55
4	C	496	C8E	C4-C5	-4.76	1.53	1.55
4	B	496	C8E	C3-C4	-4.74	1.53	1.55
4	B	502	C8E	C6-C7	-3.88	1.53	1.55
4	C	495	C8E	C2-C3	-3.59	1.53	1.55

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	7	C8E	O12-C11-C10	-2.25	107.00	114.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	428/479 (89%)	0.37	24 (5%)	24	33	15, 36, 78, 105	2 (0%)
1	B	429/479 (89%)	0.33	23 (5%)	25	34	17, 36, 72, 102	3 (0%)
1	C	409/479 (85%)	0.39	34 (8%)	11	18	18, 38, 73, 102	0
1	D	410/479 (85%)	0.27	19 (4%)	31	41	17, 36, 68, 101	0
All	All	1676/1916 (87%)	0.34	100 (5%)	22	30	15, 36, 74, 105	5 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	PRO	6.3
1	A	237	PRO	6.1
1	A	473	PRO	5.9
1	D	443	LEU	5.8
1	C	443	LEU	5.7
1	A	238	GLY	5.5
1	A	288	LEU	5.2
1	B	444	PRO	4.9
1	C	473	PRO	4.7
1	C	444	PRO	4.4
1	B	442	LEU	4.4
1	B	474	GLY	4.4
1	D	444	PRO	4.2
1	B	237	PRO	4.2
1	B	450	TYR	3.7
1	C	121	PRO	3.7
1	C	104	LEU	3.6
1	C	472	GLY	3.6
1	C	406	ASP	3.6
1	B	443	LEU	3.5
1	C	441	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	472	GLY	3.5
1	A	234	LEU	3.5
1	A	289	THR	3.4
1	B	244	LEU	3.4
1	C	470	ALA	3.4
1	D	122	ASP	3.4
1	C	468	GLY	3.4
1	D	470	ALA	3.4
1	A	104	LEU	3.4
1	C	307	VAL	3.4
1	C	474	GLY	3.3
1	B	289	THR	3.3
1	C	62	PRO	3.3
1	C	122	ASP	3.2
1	A	443	LEU	3.2
1	C	442	LEU	3.2
1	C	306	ASP	3.1
1	A	235	ARG	3.1
1	A	299	ALA	3.1
1	B	234	LEU	3.1
1	B	288	LEU	3.1
1	A	236	ARG	3.1
1	A	444	PRO	3.1
1	A	388	LEU	3.0
1	D	248	TYR	3.0
1	D	104	LEU	3.0
1	B	339	ASP	2.9
1	C	337	GLY	2.9
1	B	422	GLY	2.8
1	C	78	PHE	2.8
1	C	195	ASP	2.8
1	C	266	TYR	2.7
1	C	199	PRO	2.7
1	D	442	LEU	2.6
1	B	472	GLY	2.6
1	D	337	GLY	2.6
1	D	468	GLY	2.6
1	D	473	PRO	2.6
1	C	388	LEU	2.6
1	D	195	ASP	2.6
1	B	241	VAL	2.6
1	B	238	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	81	TRP	2.5
1	C	289	THR	2.5
1	C	416	ASN	2.5
1	C	81	TRP	2.5
1	A	301	GLY	2.5
1	D	244	LEU	2.5
1	B	477	SER	2.4
1	C	79	GLY	2.4
1	B	441	GLY	2.4
1	D	305	GLY	2.4
1	D	474	GLY	2.4
1	C	288	LEU	2.4
1	D	306	ASP	2.3
1	D	472	GLY	2.3
1	A	241	VAL	2.3
1	C	148	PHE	2.3
1	B	475	THR	2.3
1	D	389	ARG	2.3
1	B	447	MSE	2.3
1	B	242	ASP	2.3
1	A	297	ARG	2.2
1	A	339	ASP	2.2
1	A	475	THR	2.2
1	C	305	GLY	2.2
1	A	470	ALA	2.2
1	C	135	TYR	2.2
1	C	304	SER	2.2
1	B	175	THR	2.1
1	A	477	SER	2.1
1	A	298	ILE	2.1
1	C	42	PHE	2.1
1	C	422	GLY	2.1
1	D	441	GLY	2.1
1	D	249	THR	2.1
1	B	176	LEU	2.1
1	C	387	GLN	2.0
1	A	176	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	C8E	D	497	12/21	0.26	7.91	32,53,71,74	0
3	EDO	A	493	4/4	0.25	6.46	54,58,58,62	0
3	EDO	C	492	4/4	0.20	5.58	39,42,51,56	0
4	C8E	A	10	11/21	0.20	5.23	25,35,52,59	0
3	EDO	C	491	4/4	0.19	5.17	46,55,57,63	0
4	C8E	B	501	10/21	0.24	5.11	34,42,52,59	0
4	C8E	D	498	13/21	0.22	4.98	27,45,59,62	0
3	EDO	D	491	4/4	0.19	4.93	39,53,53,62	0
3	EDO	B	494	4/4	0.21	4.76	34,35,37,39	0
3	EDO	A	8	4/4	0.22	4.16	49,52,61,63	0
4	C8E	D	499	15/21	0.21	4.06	27,51,71,74	0
3	EDO	C	493	4/4	0.21	3.92	55,55,60,73	0
3	EDO	A	492	4/4	0.19	3.54	41,48,52,55	0
4	C8E	B	8	21/21	0.21	3.49	21,41,57,63	0
4	C8E	D	496	8/21	0.22	3.14	25,41,46,49	0
4	C8E	B	496	9/21	0.19	2.80	41,53,61,68	0
4	C8E	D	501	9/21	0.18	2.71	26,34,46,47	0
4	C8E	D	5	21/21	0.23	2.68	33,51,70,75	0
3	EDO	D	492	4/4	0.23	2.59	49,56,60,65	0
4	C8E	B	502	8/21	0.20	2.56	29,47,59,65	0
4	C8E	C	498	18/21	0.24	2.41	23,76,95,101	0
3	EDO	B	495	4/4	0.16	2.16	39,48,52,55	0
4	C8E	D	494	16/21	0.20	2.04	32,44,77,79	0
4	C8E	C	496	10/21	0.20	1.88	21,43,83,84	0
4	C8E	B	499	9/21	0.17	1.84	29,35,54,59	0
3	EDO	B	6	4/4	0.23	1.83	29,34,39,51	0
3	EDO	C	5	4/4	0.20	1.82	24,25,27,37	0
3	EDO	A	2	4/4	0.19	1.76	17,30,34,40	0
4	C8E	C	495	12/21	0.17	1.73	20,41,53,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	9	4/4	0.17	1.71	56,60,71,75	0
3	EDO	B	493	4/4	0.19	1.58	54,62,71,71	0
3	EDO	A	3	4/4	0.22	1.58	20,28,33,41	0
4	C8E	D	9	19/21	0.17	1.44	17,35,53,55	0
3	EDO	A	491	4/4	0.16	1.39	33,53,57,61	0
4	C8E	A	11	10/21	0.16	1.34	28,36,46,61	0
3	EDO	B	492	4/4	0.12	1.22	44,44,54,55	0
4	C8E	C	494	21/21	0.24	1.21	23,46,71,83	0
3	EDO	C	1	4/4	0.24	1.21	14,18,25,36	0
3	EDO	D	7	4/4	0.20	1.10	16,19,21,26	0
3	EDO	C	10	4/4	0.15	1.10	58,63,71,83	0
4	C8E	C	7	12/21	0.16	1.01	25,40,60,66	0
3	EDO	B	4	4/4	0.16	0.81	18,23,28,40	0
3	EDO	C	11	4/4	0.15	0.79	35,46,53,62	0
4	C8E	B	500	13/21	0.18	0.58	24,35,75,77	0
4	C8E	A	495	10/21	0.17	0.51	25,29,50,63	0
4	C8E	B	498	9/21	0.13	0.33	27,33,42,45	0
4	C8E	D	493	11/21	0.15	0.32	15,39,52,58	0
4	C8E	C	497	9/21	0.13	0.14	36,44,59,62	0
4	C8E	B	497	12/21	0.15	-0.07	27,45,71,72	0
4	C8E	A	494	13/21	0.19	-0.09	33,46,73,76	0
4	C8E	D	500	13/21	0.13	-0.30	20,38,65,65	0
4	C8E	D	495	9/21	0.12	-0.39	29,48,58,59	0
3	EDO	B	491	4/4	0.13	-0.56	39,49,53,58	0
2	CA	C	3	1/1	0.07	-1.22	71,71,71,71	0
2	CA	D	1	1/1	0.08	-1.87	58,58,58,58	0
2	CA	B	2	1/1	0.07	-2.17	61,61,61,61	0
2	CA	A	4	1/1	0.10	-2.55	65,65,65,65	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.