



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2020 – 01:19 PM GMT

PDB ID : 6TGF  
Title : Pantoea stewartii WceF is a glycan biofilm modifying enzyme with a bacteriophage tailspike-like parallel beta-helix fold  
Authors : Irscher, T.; Roske, Y.; Gayk, I.; Heinemann, U.; Barbirz, S.  
Deposited on : 2019-11-15  
Resolution : 2.55 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

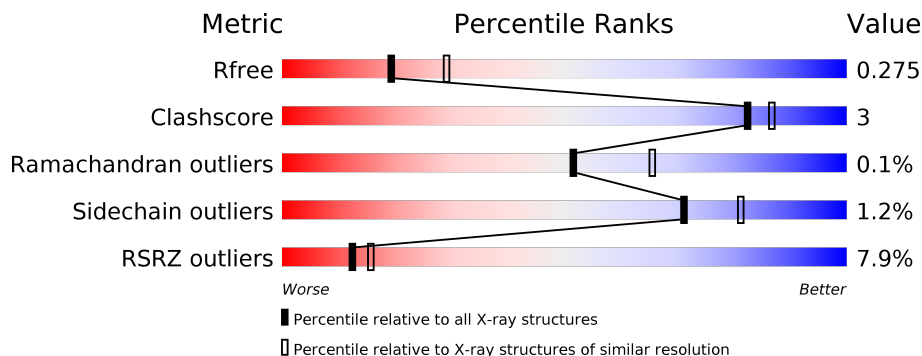
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 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	D	736	
1	E	736	
1	F	736	

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	D	805	-	-	-	X
3	EDO	D	814	-	-	-	X
3	EDO	F	805	-	-	-	X

## 2 Entry composition [i](#)

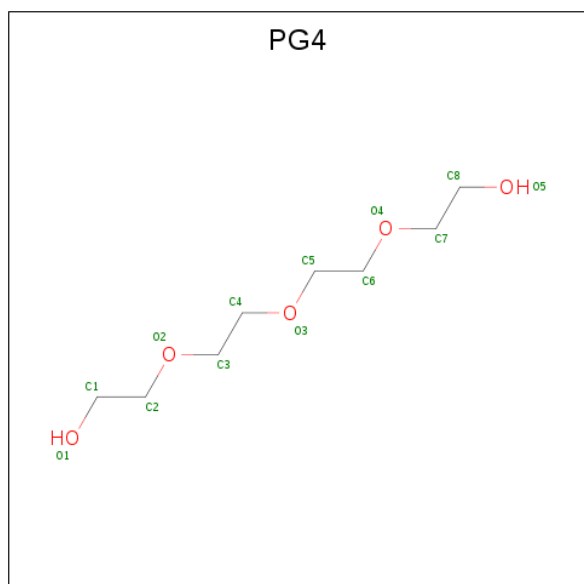
There are 4 unique types of molecules in this entry. The entry contains 16651 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Exopolysaccharide biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	F	682	Total 5295	C 3329	N 939	O 1008	S 19	0	2	0
1	D	687	Total 5318	C 3345	N 941	O 1013	S 19	0	0	0
1	E	673	Total 5226	C 3286	N 926	O 995	S 19	0	1	0

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	F	1	Total 13	C 8	O 5	0	0
2	D	1	Total 13	C 8	O 5	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	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
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
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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

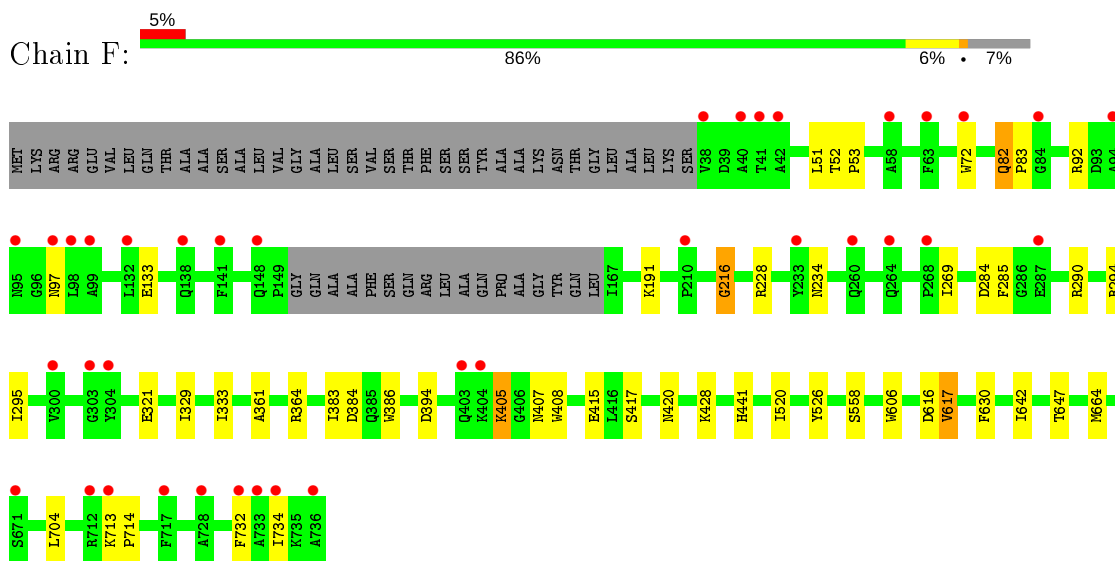
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	216	Total O 216 216	0	0
4	D	214	Total O 214 214	0	0
4	E	188	Total O 188 188	0	0

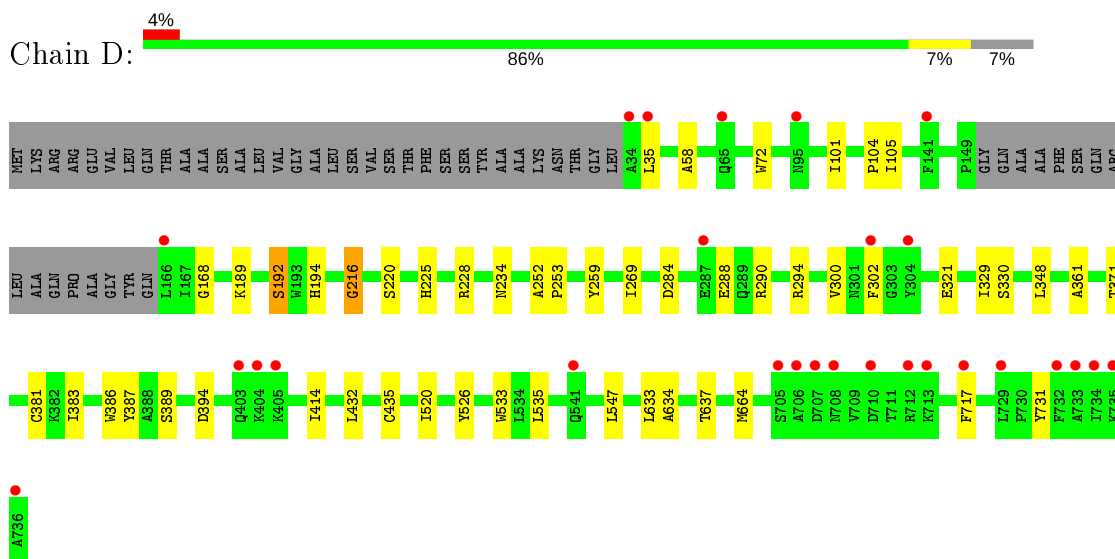
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Exopolysaccharide biosynthesis protein

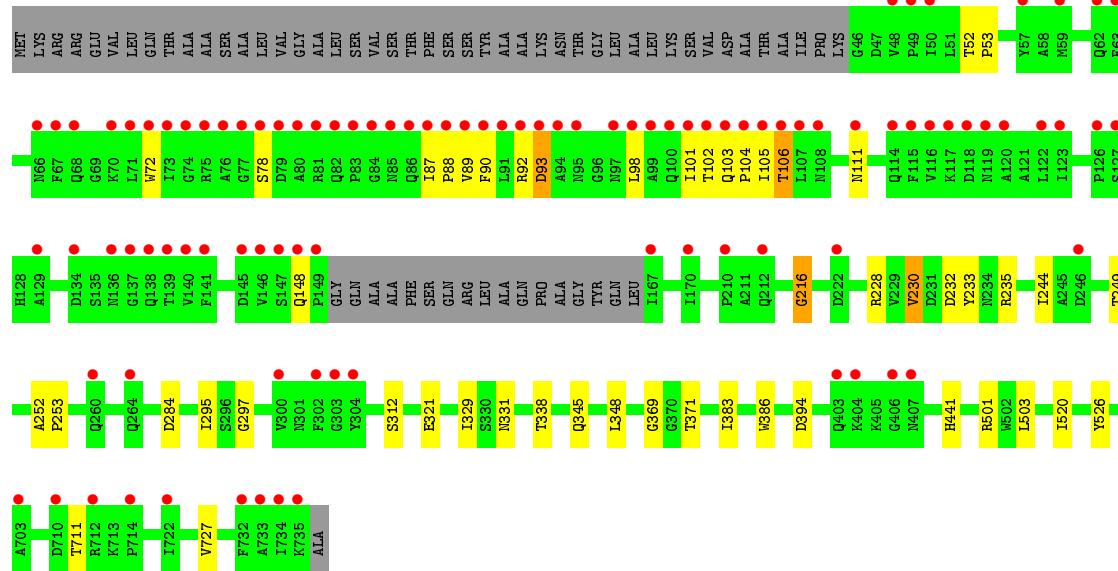
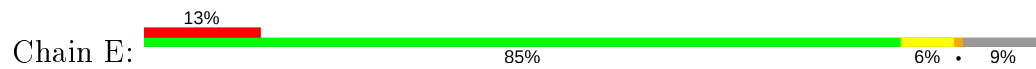


- Molecule 1: Exopolysaccharide biosynthesis protein



- Molecule 1: Exopolysaccharide biosynthesis protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.18Å 97.20Å 128.95Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	48.60 – 2.55 48.60 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.60-2.55) 96.5 (48.60-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.54Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.227 , 0.273 0.228 , 0.275	Depositor DCC
$R_{free}$ test set	2101 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtrriage
Anisotropy	0.126	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: PG4, 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	D	0.64	0/5449	0.71	0/7403
1	E	0.65	0/5359	0.71	0/7281
1	F	0.64	0/5432	0.71	0/7380
All	All	0.64	0/16240	0.71	0/22064

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	D	5318	0	5118	31	0
1	E	5226	0	5015	25	0
1	F	5295	0	5092	30	0
2	D	13	0	18	0	0
2	F	13	0	18	1	0
3	D	64	0	96	2	0
3	E	32	0	48	0	0
3	F	72	0	105	1	0
4	D	214	0	0	0	0
4	E	188	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	216	0	0	0	0
All	All	16651	0	15510	80	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 (80) 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:338:THR:HG21	1:E:369:GLY:HA3	1.69	0.75
1:F:558:SER:H	1:F:647:THR:HG22	1.52	0.74
1:D:58:ALA:O	1:D:168:GLY:HA3	1.94	0.66
1:E:338:THR:HG21	1:E:369:GLY:CA	2.28	0.63
1:E:216:GLY:O	1:E:228:ARG:NH1	2.34	0.59
1:F:732:PHE:CD1	1:D:717:PHE:HE2	2.21	0.58
1:F:269:ILE:O	1:F:294:ARG:NH1	2.37	0.58
1:D:192:SER:OG	1:D:194:HIS:O	2.22	0.57
1:F:617:VAL:HG23	1:F:630:PHE:O	2.05	0.56
1:F:216:GLY:O	1:F:228:ARG:NH1	2.38	0.55
1:D:535:LEU:HD21	1:D:664:MET:HG3	1.89	0.54
1:D:731:TYR:HB2	1:E:727:VAL:CG1	2.37	0.54
1:D:387:TYR:HB3	3:D:815:EDO:H22	1.90	0.54
1:D:234:ASN:HA	1:D:269:ILE:HD12	1.90	0.53
1:E:329:ILE:HD11	1:E:348:LEU:HD13	1.89	0.53
1:D:533:TRP:HB3	1:D:664:MET:HG2	1.90	0.53
1:E:230:VAL:HG21	1:E:233:TYR:CE1	2.45	0.51
1:F:606:TRP:CD1	1:F:617:VAL:CG1	2.94	0.51
1:D:101:ILE:HD13	1:D:105:ILE:HG12	1.93	0.51
1:D:381:CYS:HB3	1:D:414:ILE:HD13	1.93	0.50
1:D:72:TRP:CE2	1:D:104:PRO:HB3	2.46	0.50
1:D:389:SER:HB2	3:D:815:EDO:H21	1.92	0.50
1:F:92:ARG:HA	1:F:97:ASN:O	2.12	0.50
1:D:383:ILE:HG22	1:D:386:TRP:CD1	2.46	0.49
1:D:329:ILE:HD11	1:D:348:LEU:HD13	1.95	0.49
1:E:383:ILE:HG22	1:E:386:TRP:CD1	2.48	0.49
1:E:101:ILE:HD12	1:E:105:ILE:HD12	1.95	0.48
1:D:216:GLY:O	1:D:228:ARG:NH1	2.47	0.48
1:F:520:ILE:O	1:D:526:TYR:HA	2.14	0.47
1:E:501:ARG:HD2	1:E:503:LEU:O	2.13	0.47
1:F:526:TYR:HA	1:E:520:ILE:O	2.15	0.46
1:D:633:LEU:HG	1:D:637:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:VAL:HB	1:D:302:PHE:CE2	2.49	0.46
1:D:520:ILE:O	1:E:526:TYR:HA	2.16	0.46
1:E:244:ILE:HD12	1:E:249:THR:HG21	1.98	0.46
1:F:642:ILE:HG13	1:F:664:MET:HE1	1.98	0.46
1:D:259:TYR:OH	1:D:290:ARG:HD2	2.16	0.45
1:F:405:LYS:C	1:F:407:ASN:H	2.19	0.45
1:F:333:ILE:HG12	1:F:364:ARG:HB2	2.00	0.44
1:D:220:SER:HA	1:D:225:HIS:HA	1.99	0.44
1:D:633:LEU:HG	1:D:637:THR:CG2	2.48	0.44
1:F:295:ILE:O	1:F:329:ILE:HA	2.18	0.44
1:F:394:ASP:HA	1:F:428:LYS:O	2.18	0.44
1:D:330:SER:HA	1:D:361:ALA:O	2.17	0.44
1:F:234:ASN:HA	1:F:269:ILE:HD12	2.00	0.43
1:E:252:ALA:N	1:E:253:PRO:CD	2.81	0.43
1:F:714:PRO:N	1:F:732:PHE:CE2	2.87	0.43
1:D:634:ALA:O	1:D:637:THR:HG22	2.19	0.43
1:D:371:THR:HA	1:D:394:ASP:O	2.18	0.43
1:F:415:GLU:OE2	1:E:441:HIS:NE2	2.45	0.43
1:F:713:LYS:C	1:F:732:PHE:CE2	2.93	0.43
1:F:72:TRP:HZ3	1:F:133:GLU:HG2	1.83	0.43
1:E:232:ASP:HB3	1:E:235:ARG:HG3	2.00	0.42
1:E:72:TRP:CE2	1:E:104:PRO:HB3	2.55	0.42
1:E:93:ASP:OD1	1:E:93:ASP:N	2.52	0.42
1:F:52:THR:HB	1:F:53:PRO:HD2	2.01	0.42
1:F:82:GLN:HG3	1:F:83:PRO:HD2	2.01	0.42
1:D:269:ILE:O	1:D:294:ARG:NH1	2.52	0.42
1:E:87:ILE:HB	1:E:88:PRO:HD2	2.02	0.41
1:E:103:GLN:HA	1:E:104:PRO:C	2.40	0.41
1:F:361:ALA:HA	1:F:384:ASP:O	2.20	0.41
1:F:417:SER:HA	1:F:441:HIS:O	2.20	0.41
1:E:297:GLY:HA3	1:E:331:ASN:O	2.21	0.41
1:D:547:LEU:O	1:D:664:MET:HE1	2.21	0.41
1:F:383:ILE:HG22	1:F:386:TRP:CD1	2.56	0.41
1:F:704:LEU:HD21	1:F:734:ILE:CD1	2.51	0.41
1:D:252:ALA:HB3	1:D:253:PRO:HD3	2.03	0.41
1:D:284:ASP:HA	1:D:321:GLU:HB2	2.02	0.41
1:E:52:THR:HB	1:E:53:PRO:HD2	2.03	0.41
1:F:420:ASN:HD21	3:F:809:EDO:H11	1.86	0.41
1:E:284:ASP:HA	1:E:321:GLU:HB2	2.03	0.41
1:F:405:LYS:O	1:F:408:TRP:CD1	2.74	0.41
1:E:371:THR:HA	1:E:394:ASP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:LEU:HD13	2:F:801:PG4:H41	2.03	0.40
1:D:432:LEU:HB3	1:D:435:CYS:SG	2.61	0.40
1:E:106:THR:O	1:E:111:ASN:ND2	2.52	0.40
1:F:285:PHE:O	1:F:290:ARG:NH1	2.51	0.40
1:D:414:ILE:HG13	1:D:435:CYS:SG	2.61	0.40
1:E:312:SER:HB3	1:E:345:GLN:OE1	2.21	0.40
1:F:284:ASP:HA	1:F:321:GLU:HB2	2.04	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	D	683/736 (93%)	648 (95%)	34 (5%)	1 (0%)	51 65
1	E	670/736 (91%)	629 (94%)	40 (6%)	1 (0%)	51 65
1	F	680/736 (92%)	647 (95%)	32 (5%)	1 (0%)	51 65
All	All	2033/2208 (92%)	1924 (95%)	106 (5%)	3 (0%)	51 65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	216	GLY
1	E	216	GLY
1	F	216	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	565/600 (94%)	561 (99%)	4 (1%)	84	90
1	E	556/600 (93%)	544 (98%)	12 (2%)	52	66
1	F	563/600 (94%)	558 (99%)	5 (1%)	78	86
All	All	1684/1800 (94%)	1663 (99%)	21 (1%)	71	81

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	82	GLN
1	F	191	LYS
1	F	405	LYS
1	F	616	ASP
1	F	617	VAL
1	D	35	LEU
1	D	189	LYS
1	D	192	SER
1	D	288	GLU
1	E	78	SER
1	E	89	VAL
1	E	90	PHE
1	E	92	ARG
1	E	93	ASP
1	E	98	LEU
1	E	102	THR
1	E	106	THR
1	E	148	GLN
1	E	230	VAL
1	E	295	ILE
1	E	711	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	450	ASN
1	F	628	GLN
1	D	264	GLN
1	D	301	ASN
1	D	422	GLN

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Mol	Chain	Res	Type
1	E	264	GLN
1	E	337	ASN
1	E	367	ASN
1	E	450	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

44 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	E	801	-	3,3,3	0.06	0	2,2,2	0.23	0
3	EDO	E	808	-	3,3,3	0.04	0	2,2,2	0.16	0
3	EDO	F	816	-	3,3,3	0.08	0	2,2,2	0.28	0
3	EDO	D	811	-	3,3,3	0.07	0	2,2,2	0.21	0
3	EDO	D	806	-	3,3,3	0.06	0	2,2,2	0.23	0
3	EDO	D	810	-	3,3,3	0.05	0	2,2,2	0.25	0
3	EDO	E	807	-	3,3,3	0.06	0	2,2,2	0.21	0
3	EDO	D	809	-	3,3,3	0.08	0	2,2,2	0.30	0
3	EDO	E	803	-	3,3,3	0.10	0	2,2,2	0.30	0
3	EDO	F	813	-	3,3,3	0.08	0	2,2,2	0.27	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	E	802	-	3,3,3	0.06	0	2,2,2	0.23	0
3	EDO	D	813	-	3,3,3	0.07	0	2,2,2	0.24	0
3	EDO	F	817	-	3,3,3	0.07	0	2,2,2	0.22	0
3	EDO	D	804	-	3,3,3	0.09	0	2,2,2	0.31	0
3	EDO	D	816	-	3,3,3	0.07	0	2,2,2	0.20	0
3	EDO	F	818	-	3,3,3	0.07	0	2,2,2	0.17	0
3	EDO	F	811	-	3,3,3	0.06	0	2,2,2	0.26	0
3	EDO	F	810	-	3,3,3	0.06	0	2,2,2	0.23	0
3	EDO	F	815	-	3,3,3	0.07	0	2,2,2	0.23	0
3	EDO	F	814	-	3,3,3	0.06	0	2,2,2	0.21	0
3	EDO	D	808	-	3,3,3	0.09	0	2,2,2	0.31	0
2	PG4	F	801	-	12,12,12	0.19	0	11,11,11	0.12	0
3	EDO	D	814	-	3,3,3	0.06	0	2,2,2	0.20	0
3	EDO	F	819	-	3,3,3	0.07	0	2,2,2	0.22	0
3	EDO	E	805	-	3,3,3	0.07	0	2,2,2	0.20	0
3	EDO	F	805	-	3,3,3	0.06	0	2,2,2	0.22	0
3	EDO	D	802	-	3,3,3	0.06	0	2,2,2	0.24	0
3	EDO	E	804	-	3,3,3	0.05	0	2,2,2	0.21	0
3	EDO	D	815	-	3,3,3	0.05	0	2,2,2	0.21	0
3	EDO	D	803	-	3,3,3	0.07	0	2,2,2	0.22	0
3	EDO	F	809	-	3,3,3	0.05	0	2,2,2	0.19	0
3	EDO	F	804	3	3,3,3	0.15	0	2,2,2	0.10	0
3	EDO	D	812	-	3,3,3	0.05	0	2,2,2	0.16	0
3	EDO	D	817	-	3,3,3	0.07	0	2,2,2	0.21	0
3	EDO	E	806	-	3,3,3	0.08	0	2,2,2	0.24	0
3	EDO	D	805	-	3,3,3	0.08	0	2,2,2	0.28	0
3	EDO	F	812	-	3,3,3	0.07	0	2,2,2	0.22	0
3	EDO	F	802	-	3,3,3	0.07	0	2,2,2	0.22	0
3	EDO	F	803	3	3,3,3	0.18	0	2,2,2	0.17	0
3	EDO	F	806	-	3,3,3	0.06	0	2,2,2	0.19	0
3	EDO	F	808	-	3,3,3	0.07	0	2,2,2	0.23	0
3	EDO	F	807	-	3,3,3	0.07	0	2,2,2	0.23	0
3	EDO	D	807	-	3,3,3	0.06	0	2,2,2	0.22	0
2	PG4	D	801	-	12,12,12	0.18	0	11,11,11	0.12	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	E	801	-	-	0/1/1/1	-
3	EDO	E	808	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	F	816	-	-	1/1/1/1	-
3	EDO	D	811	-	-	0/1/1/1	-
3	EDO	D	806	-	-	0/1/1/1	-
3	EDO	D	810	-	-	1/1/1/1	-
3	EDO	E	807	-	-	0/1/1/1	-
3	EDO	D	809	-	-	1/1/1/1	-
3	EDO	E	803	-	-	1/1/1/1	-
3	EDO	F	813	-	-	1/1/1/1	-
3	EDO	E	802	-	-	0/1/1/1	-
3	EDO	D	813	-	-	0/1/1/1	-
3	EDO	F	817	-	-	0/1/1/1	-
3	EDO	D	804	-	-	1/1/1/1	-
3	EDO	D	816	-	-	0/1/1/1	-
3	EDO	F	818	-	-	1/1/1/1	-
3	EDO	F	811	-	-	1/1/1/1	-
3	EDO	F	810	-	-	0/1/1/1	-
3	EDO	F	815	-	-	1/1/1/1	-
3	EDO	F	814	-	-	0/1/1/1	-
3	EDO	D	808	-	-	1/1/1/1	-
2	PG4	F	801	-	-	7/10/10/10	-
3	EDO	D	814	-	-	0/1/1/1	-
3	EDO	F	819	-	-	0/1/1/1	-
3	EDO	E	805	-	-	0/1/1/1	-
3	EDO	F	805	-	-	0/1/1/1	-
3	EDO	D	802	-	-	1/1/1/1	-
3	EDO	E	804	-	-	0/1/1/1	-
3	EDO	D	815	-	-	0/1/1/1	-
3	EDO	D	803	-	-	0/1/1/1	-
3	EDO	F	809	-	-	0/1/1/1	-
3	EDO	F	804	3	-	0/1/1/1	-
3	EDO	D	812	-	-	0/1/1/1	-
3	EDO	D	817	-	-	0/1/1/1	-
3	EDO	E	806	-	-	1/1/1/1	-
3	EDO	D	805	-	-	1/1/1/1	-
3	EDO	F	812	-	-	0/1/1/1	-
3	EDO	F	802	-	-	0/1/1/1	-
3	EDO	F	803	3	-	1/1/1/1	-
3	EDO	F	806	-	-	0/1/1/1	-
3	EDO	F	808	-	-	0/1/1/1	-
3	EDO	F	807	-	-	0/1/1/1	-
3	EDO	D	807	-	-	0/1/1/1	-
2	PG4	D	801	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	801	PG4	O3-C5-C6-O4
2	F	801	PG4	O2-C3-C4-O3
2	F	801	PG4	O3-C5-C6-O4
2	D	801	PG4	O2-C3-C4-O3
3	E	803	EDO	O1-C1-C2-O2
3	D	808	EDO	O1-C1-C2-O2
3	D	805	EDO	O1-C1-C2-O2
2	F	801	PG4	O1-C1-C2-O2
3	D	809	EDO	O1-C1-C2-O2
3	D	804	EDO	O1-C1-C2-O2
3	F	813	EDO	O1-C1-C2-O2
3	F	803	EDO	O1-C1-C2-O2
2	F	801	PG4	C4-C3-O2-C2
2	D	801	PG4	C3-C4-O3-C5
2	F	801	PG4	C8-C7-O4-C6
3	F	816	EDO	O1-C1-C2-O2
2	D	801	PG4	C8-C7-O4-C6
2	F	801	PG4	C5-C6-O4-C7
2	D	801	PG4	O4-C7-C8-O5
2	D	801	PG4	C4-C3-O2-C2
2	F	801	PG4	C3-C4-O3-C5
3	F	818	EDO	O1-C1-C2-O2
3	D	810	EDO	O1-C1-C2-O2
3	F	811	EDO	O1-C1-C2-O2
3	F	815	EDO	O1-C1-C2-O2
3	E	808	EDO	O1-C1-C2-O2
3	D	802	EDO	O1-C1-C2-O2
3	E	806	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	801	PG4	1	0
3	D	815	EDO	2	0
3	F	809	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	D	687/736 (93%)	0.38	27 (3%) 39 45	23, 41, 71, 92	0
1	E	673/736 (91%)	0.85	98 (14%) 2 3	20, 49, 120, 143	0
1	F	682/736 (92%)	0.45	37 (5%) 25 30	22, 42, 73, 95	0
All	All	2042/2208 (92%)	0.56	162 (7%) 12 16	20, 43, 92, 143	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	98	LEU	11.4
1	E	77	GLY	10.5
1	E	99	ALA	7.1
1	E	97	ASN	7.0
1	E	74	GLY	6.0
1	E	48	VAL	5.9
1	E	90	PHE	5.7
1	E	115	PHE	5.3
1	E	94	ALA	5.2
1	E	101	ILE	5.2
1	D	35	LEU	5.1
1	E	403	GLN	5.0
1	E	137	GLY	4.9
1	E	92	ARG	4.8
1	E	89	VAL	4.6
1	F	732	PHE	4.4
1	E	59	MET	4.4
1	E	87	ILE	4.4
1	E	105	ILE	4.3
1	E	81	ARG	4.3
1	E	91	LEU	4.2
1	D	141	PHE	4.2
1	F	41	THR	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	139	THR	4.1
1	D	34	ALA	4.1
1	F	97	ASN	4.1
1	D	707	ASP	4.0
1	E	167	ILE	4.0
1	D	403	GLN	4.0
1	E	149	PRO	3.8
1	E	103	GLN	3.8
1	E	100	GLN	3.8
1	D	287	GLU	3.8
1	E	68	GLN	3.6
1	E	83	PRO	3.5
1	E	82	GLN	3.5
1	E	85	ASN	3.5
1	E	95	ASN	3.5
1	E	127	SER	3.5
1	E	67	PHE	3.4
1	E	222	ASP	3.4
1	E	118	ASP	3.4
1	E	732	PHE	3.3
1	F	95	ASN	3.2
1	E	136	ASN	3.2
1	E	88	PRO	3.2
1	F	40	ALA	3.1
1	F	233	TYR	3.1
1	E	119	ASN	3.1
1	E	714	PRO	3.1
1	F	42	ALA	3.1
1	E	73	ILE	3.1
1	F	148	GLN	3.1
1	E	116	VAL	3.1
1	F	404	LYS	3.0
1	E	304	TYR	3.0
1	E	122	LEU	3.0
1	E	63	PHE	3.0
1	D	706	ALA	3.0
1	E	120	ALA	3.0
1	E	50	ILE	3.0
1	E	102	THR	3.0
1	E	106	THR	3.0
1	E	703	ALA	2.9
1	E	406	GLY	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	76	ALA	2.9
1	E	404	LYS	2.9
1	E	84	GLY	2.9
1	E	210	PRO	2.9
1	E	108	ASN	2.8
1	F	733	ALA	2.8
1	E	104	PRO	2.8
1	F	734	ILE	2.7
1	E	71	LEU	2.7
1	F	99	ALA	2.7
1	E	72	TRP	2.7
1	D	736	ALA	2.7
1	E	80	ALA	2.7
1	D	733	ALA	2.7
1	F	98	LEU	2.6
1	E	141	PHE	2.6
1	D	717	PHE	2.6
1	E	145	ASP	2.6
1	F	141	PHE	2.6
1	F	58	ALA	2.6
1	E	129	ALA	2.6
1	D	735	LYS	2.6
1	E	66	ASN	2.6
1	E	75	ARG	2.6
1	F	300	VAL	2.5
1	E	111	ASN	2.5
1	D	404	LYS	2.5
1	E	93	ASP	2.5
1	D	713	LYS	2.5
1	F	671	SER	2.5
1	E	260[A]	GLN	2.5
1	F	736	ALA	2.5
1	E	117	LYS	2.5
1	E	107	LEU	2.5
1	E	114	GLN	2.5
1	E	710	ASP	2.5
1	E	303	GLY	2.4
1	E	57	TYR	2.4
1	F	138	GLN	2.4
1	D	405	LYS	2.4
1	D	734	ILE	2.4
1	E	734	ILE	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	717	PHE	2.4
1	F	84	GLY	2.4
1	D	705	SER	2.4
1	E	147	SER	2.4
1	D	304	TYR	2.4
1	D	712	ARG	2.4
1	E	78	SER	2.4
1	D	95	ASN	2.3
1	F	268	PRO	2.3
1	E	148	GLN	2.3
1	F	132	LEU	2.3
1	D	541	GLN	2.3
1	D	710	ASP	2.3
1	E	62	GLN	2.3
1	E	123	ILE	2.3
1	F	712	ARG	2.3
1	E	712	ARG	2.3
1	D	732	PHE	2.3
1	E	70	LYS	2.2
1	E	126	PRO	2.2
1	F	713	LYS	2.2
1	E	735	LYS	2.2
1	E	86	GLN	2.2
1	D	166	LEU	2.2
1	F	210	PRO	2.2
1	F	403	GLN	2.2
1	E	140	VAL	2.2
1	E	733	ALA	2.2
1	F	63	PHE	2.2
1	E	212	GLN	2.2
1	E	170	ILE	2.2
1	D	65	GLN	2.2
1	E	138	GLN	2.2
1	E	49	PRO	2.2
1	E	264	GLN	2.2
1	E	300	VAL	2.2
1	F	260	GLN	2.1
1	E	407	ASN	2.1
1	E	722	ILE	2.1
1	F	38	VAL	2.1
1	F	94	ALA	2.1
1	F	287	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	302	PHE	2.1
1	F	728	ALA	2.1
1	D	708	ASN	2.1
1	F	264	GLN	2.1
1	E	134	ASP	2.1
1	F	303	GLY	2.1
1	F	72	TRP	2.1
1	E	79	ASP	2.0
1	E	146	VAL	2.0
1	D	302	PHE	2.0
1	D	729	LEU	2.0
1	E	246	ASP	2.0
1	F	304	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	D	807	4/4	0.61	0.37	82,83,83,83	0
3	EDO	D	814	4/4	0.62	0.53	88,89,89,89	0
3	EDO	F	808	4/4	0.66	0.34	83,84,84,84	0
3	EDO	F	818	4/4	0.66	0.39	73,73,73,73	0
3	EDO	D	813	4/4	0.68	0.33	72,72,73,73	0
3	EDO	E	801	4/4	0.68	0.27	81,81,81,81	0
3	EDO	D	805	4/4	0.71	0.41	84,84,84,84	0
3	EDO	F	804	4/4	0.74	0.30	107,108,108,108	0
3	EDO	D	808	4/4	0.75	0.23	69,69,69,69	0
3	EDO	F	805	4/4	0.75	0.48	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	F	807	4/4	0.76	0.38	79,79,80,80	0
3	EDO	F	819	4/4	0.76	0.34	71,71,72,72	0
3	EDO	D	811	4/4	0.77	0.19	82,82,83,83	0
3	EDO	F	806	4/4	0.78	0.31	83,83,83,83	0
3	EDO	D	806	4/4	0.78	0.33	73,73,73,74	0
3	EDO	F	815	4/4	0.79	0.23	71,71,72,72	0
3	EDO	F	812	4/4	0.79	0.30	78,78,78,78	0
3	EDO	E	803	4/4	0.80	0.16	67,68,68,68	0
3	EDO	E	805	4/4	0.80	0.31	67,68,68,68	0
3	EDO	D	817	4/4	0.81	0.19	79,79,79,80	0
3	EDO	F	803	4/4	0.81	0.30	105,105,105,106	0
3	EDO	F	816	4/4	0.81	0.36	86,86,86,87	0
3	EDO	F	802	4/4	0.82	0.57	68,68,68,68	0
3	EDO	F	813	4/4	0.82	0.35	78,79,79,79	0
3	EDO	F	811	4/4	0.82	0.45	64,65,65,65	0
3	EDO	E	808	4/4	0.84	0.50	67,67,67,67	0
3	EDO	D	815	4/4	0.84	0.32	66,66,66,66	0
3	EDO	F	810	4/4	0.85	1.18	100,100,100,101	0
3	EDO	D	816	4/4	0.85	0.32	78,79,79,79	0
3	EDO	D	809	4/4	0.85	0.36	82,83,83,83	0
3	EDO	F	817	4/4	0.86	0.28	76,76,76,76	0
3	EDO	F	814	4/4	0.87	0.22	84,84,84,84	0
3	EDO	E	806	4/4	0.88	0.28	85,86,86,86	0
3	EDO	D	802	4/4	0.88	0.23	57,58,58,58	0
3	EDO	E	807	4/4	0.88	0.16	76,76,77,77	0
3	EDO	D	810	4/4	0.89	0.15	71,72,72,72	0
3	EDO	E	804	4/4	0.89	0.33	75,75,75,75	0
3	EDO	F	809	4/4	0.90	0.47	72,72,73,73	0
2	PG4	F	801	13/13	0.91	0.40	88,89,90,90	0
3	EDO	D	812	4/4	0.91	0.21	80,80,80,81	0
3	EDO	D	803	4/4	0.93	0.48	71,71,71,71	0
3	EDO	D	804	4/4	0.93	0.25	69,70,70,70	0
3	EDO	E	802	4/4	0.94	0.41	92,93,93,93	0
2	PG4	D	801	13/13	0.94	0.33	77,78,80,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.