



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:46 PM UTC

PDB ID : 6TGF / pdb_00006tgf
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

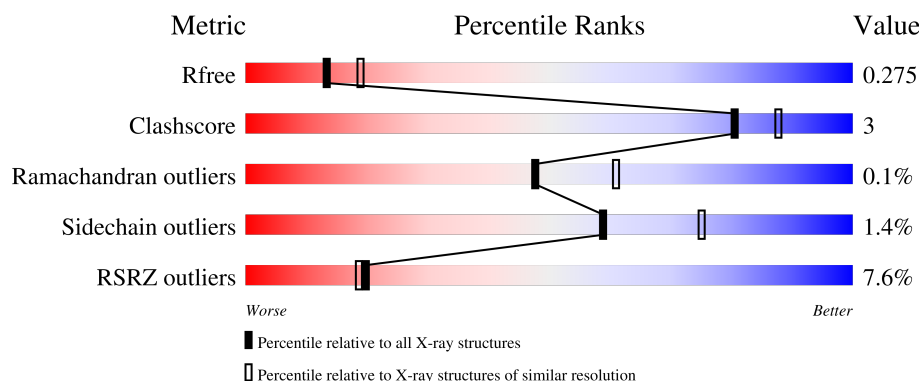
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	D	736	
1	E	736	
1	F	736	

2 Entry composition [i](#)

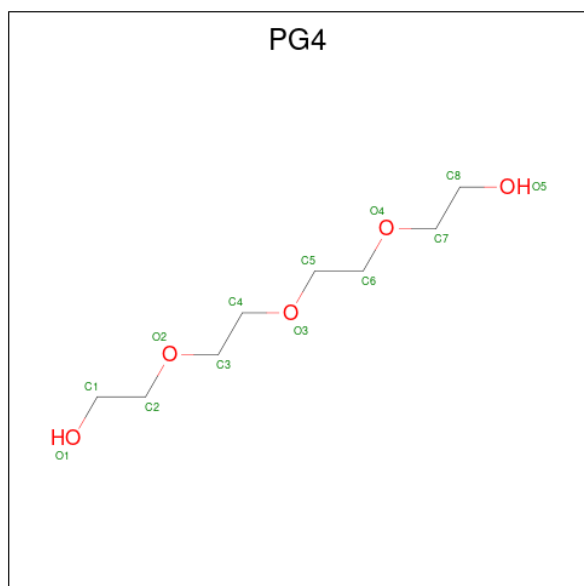
There are 4 unique types of molecules in this entry. The entry contains 16651 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

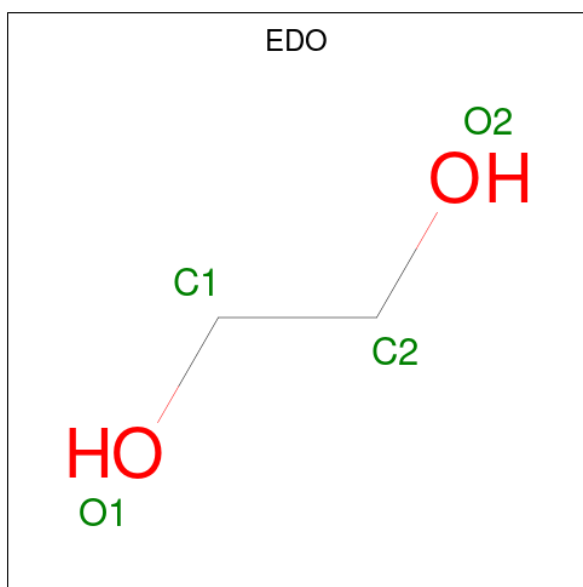
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	682	Total	C	N	O	S	0	2	0
			5295	3329	939	1008	19			
1	D	687	Total	C	N	O	S	0	0	0
			5318	3345	941	1013	19			
1	E	673	Total	C	N	O	S	0	1	0
			5226	3286	926	995	19			

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

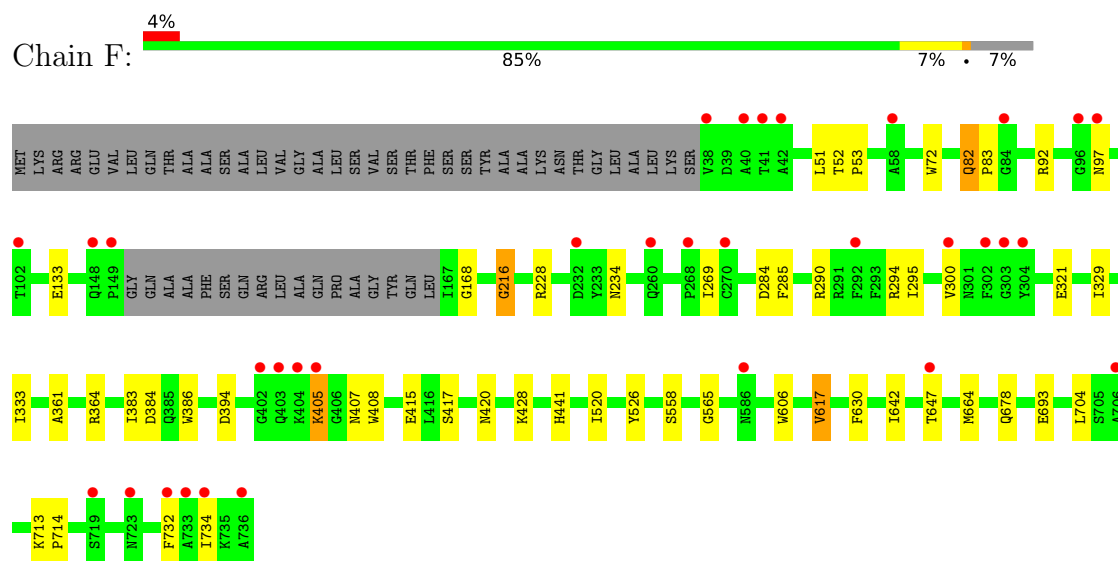
- Molecule 4 is water.

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

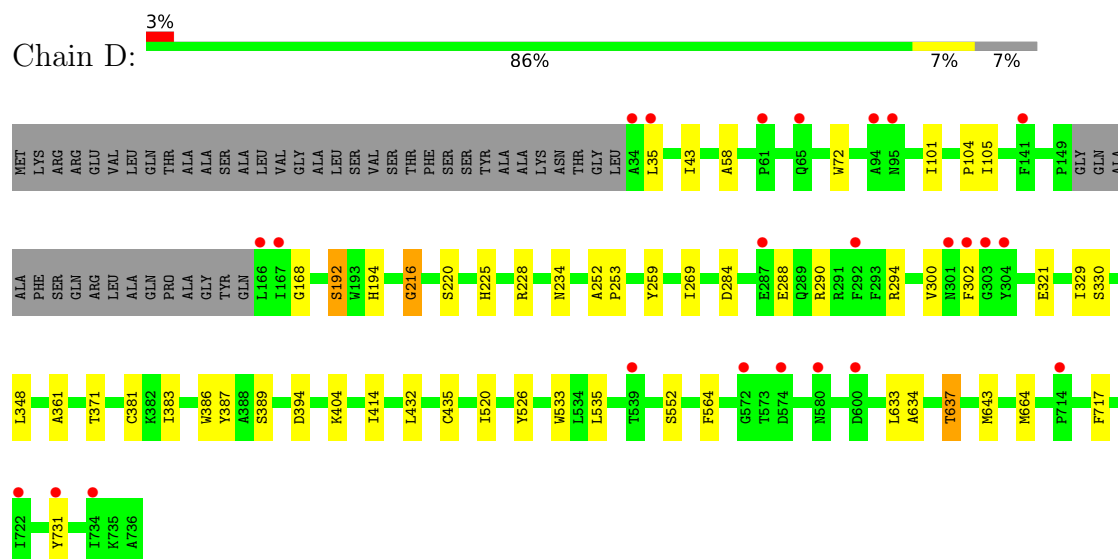
3 Residue-property plots [i](#)

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.

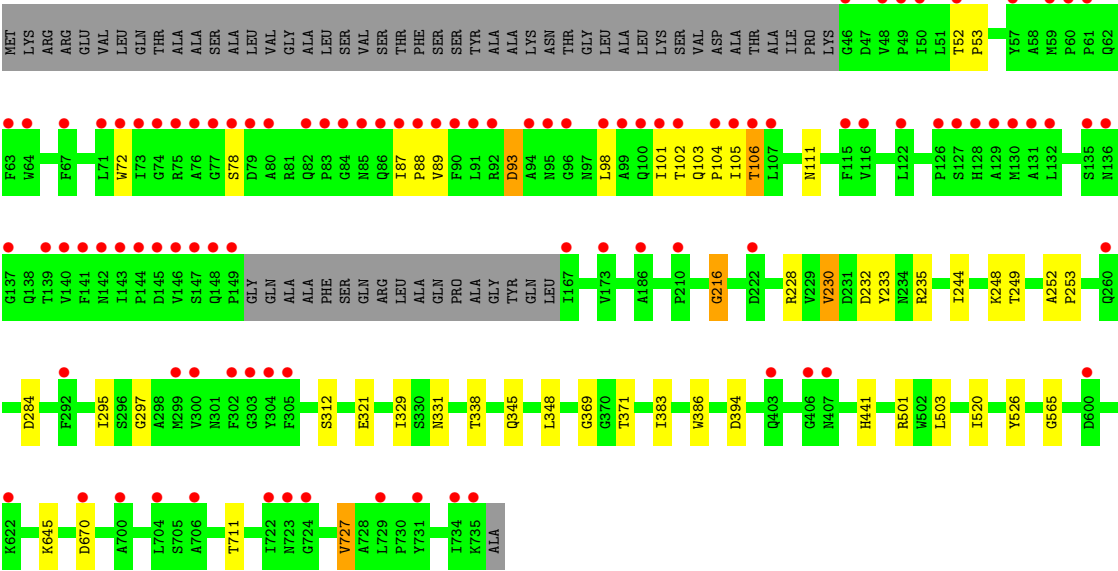
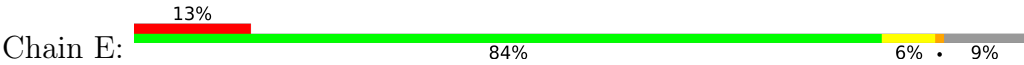
- Molecule 1: Exopolysaccharide biosynthesis protein



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.227 , 0.273 0.229 , 0.275	Depositor DCC
R_{free} test set	2101 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16651	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PG4

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	1.01	0/5449	1.29	1/7403 (0.0%)
1	E	1.01	0/5359	1.29	1/7281 (0.0%)
1	F	1.01	0/5432	1.30	2/7380 (0.0%)
All	All	1.01	0/16240	1.29	4/22064 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	565	GLY	CA-C-O	-5.88	118.21	122.45
1	D	637	THR	CB-CA-C	5.49	115.38	110.44
1	F	565	GLY	CA-C-O	-5.37	117.98	122.33
1	F	168	GLY	CA-C-O	-5.08	118.18	122.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5318	0	5118	33	0
1	E	5226	0	5015	26	0
1	F	5295	0	5092	31	0
2	D	13	0	18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
4	F	216	0	0	0	0
All	All	16651	0	15510	83	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 (83) 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:F:642:ILE:HG13	1:F:664:MET:HE1	1.91	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:405:LYS:C	1:F:407:ASN:H	2.19	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:713:LYS:C	1:F:732:PHE:CE2	2.93	0.47
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
1:E:103:GLN:HA	1:E:104:PRO:C	2.40	0.46
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:D:259:TYR:OH	1:D:290:ARG:HD2	2.16	0.45
1:F:333:ILE:HG12	1:F:364:ARG:HB2	2.00	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: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:D:643:MET:HE1	1:E:645:LYS:HD3	1.99	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:F:714:PRO:N	1:F:732:PHE:CE2	2.87	0.43
1:E:252:ALA:N	1:E:253:PRO:CD	2.81	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:D:533:TRP:CG	1:D:664:MET:HE3	2.53	0.43
1:D:564:PHE:HB2	1:D:643:MET:HE2	2.01	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: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:E:93:ASP:OD1	1:E:93:ASP:N	2.52	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:F:405:LYS:C	1:F:407:ASN:N	2.78	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:405:LYS:O	1:F:408:TRP:CD1	2.74	0.41
1:F:420:ASN:HD21	3:F:809:EDO:H11	1.86	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:E:284:ASP:HA	1:E:321:GLU:HB2	2.03	0.41
1:F:51:LEU:HD13	2:F:801:PG4:H41	2.03	0.40
1:E:371:THR:HA	1:E:394:ASP:O	2.21	0.40
1:F:285:PHE:O	1:F:290:ARG:NH1	2.51	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:D:414:ILE:HG13	1:D:435:CYS:SG	2.61	0.40
1:F:284:ASP:HA	1:F:321:GLU:HB2	2.04	0.40
1:E:312:SER:HB3	1:E:345:GLN:OE1	2.21	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	D	683/736 (93%)	648 (95%)	34 (5%)	1 (0%)	48	61
1	E	670/736 (91%)	629 (94%)	40 (6%)	1 (0%)	48	61
1	F	680/736 (92%)	647 (95%)	32 (5%)	1 (0%)	48	61
All	All	2033/2208 (92%)	1924 (95%)	106 (5%)	3 (0%)	48	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	216	GLY

Continued on next page...

Continued from previous page...

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

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	D	565/600 (94%)	559 (99%)	6 (1%)	65	79
1	E	556/600 (93%)	544 (98%)	12 (2%)	45	64
1	F	563/600 (94%)	557 (99%)	6 (1%)	65	79
All	All	1684/1800 (94%)	1660 (99%)	24 (1%)	59	75

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	82	GLN
1	F	300	VAL
1	F	405	LYS
1	F	617	VAL
1	F	678	GLN
1	F	693	GLU
1	D	35	LEU
1	D	43	ILE
1	D	192	SER
1	D	288	GLU
1	D	404	LYS
1	D	552	SER
1	E	78	SER
1	E	89	VAL
1	E	93	ASP
1	E	98	LEU
1	E	102	THR
1	E	106	THR
1	E	230	VAL
1	E	248	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	295	ILE
1	E	670	ASP
1	E	711	THR
1	E	727	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	62	GLN
1	F	331	ASN
1	F	367	ASN
1	F	385	GLN
1	F	437	GLN
1	F	471	ASN
1	F	538	ASN
1	F	568	GLN
1	F	628	GLN
1	D	85	ASN
1	D	264	GLN
1	D	301	ASN
1	D	331	ASN
1	D	335	ASN
1	D	337	ASN
1	D	367	ASN
1	D	422	GLN
1	D	484	GLN
1	D	488	GLN
1	D	495	ASN
1	D	538	ASN
1	E	138	GLN
1	E	263	GLN
1	E	264	GLN
1	E	289	GLN
1	E	366	ASN
1	E	385	GLN
1	E	418	ASN
1	E	471	ASN
1	E	495	ASN
1	E	538	ASN
1	E	628	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 ⓘ

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	D	808	-	3,3,3	0.08	0	2,2,2	0.23	0
3	EDO	D	817	-	3,3,3	0.07	0	2,2,2	0.13	0
3	EDO	F	802	-	3,3,3	0.07	0	2,2,2	0.15	0
3	EDO	F	812	-	3,3,3	0.07	0	2,2,2	0.15	0
3	EDO	D	806	-	3,3,3	0.07	0	2,2,2	0.16	0
3	EDO	F	806	-	3,3,3	0.07	0	2,2,2	0.12	0
3	EDO	D	804	-	3,3,3	0.09	0	2,2,2	0.23	0
3	EDO	E	805	-	3,3,3	0.07	0	2,2,2	0.12	0
3	EDO	E	808	-	3,3,3	0.05	0	2,2,2	0.09	0
3	EDO	F	816	-	3,3,3	0.07	0	2,2,2	0.20	0
3	EDO	F	813	-	3,3,3	0.08	0	2,2,2	0.19	0
3	EDO	F	809	-	3,3,3	0.05	0	2,2,2	0.12	0
3	EDO	E	807	-	3,3,3	0.06	0	2,2,2	0.14	0
3	EDO	F	808	-	3,3,3	0.07	0	2,2,2	0.15	0
3	EDO	D	816	-	3,3,3	0.07	0	2,2,2	0.13	0
3	EDO	F	810	-	3,3,3	0.06	0	2,2,2	0.16	0
3	EDO	F	817	-	3,3,3	0.07	0	2,2,2	0.15	0
3	EDO	E	801	-	3,3,3	0.06	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	F	814	-	3,3,3	0.06	0	2,2,2	0.14	0
3	EDO	F	815	-	3,3,3	0.07	0	2,2,2	0.15	0
3	EDO	D	811	-	3,3,3	0.07	0	2,2,2	0.14	0
3	EDO	E	802	-	3,3,3	0.06	0	2,2,2	0.15	0
3	EDO	E	806	-	3,3,3	0.08	0	2,2,2	0.17	0
3	EDO	F	819	-	3,3,3	0.07	0	2,2,2	0.15	0
3	EDO	D	814	-	3,3,3	0.06	0	2,2,2	0.13	0
3	EDO	F	803	3	3,3,3	0.17	0	2,2,2	0.10	0
3	EDO	D	807	-	3,3,3	0.06	0	2,2,2	0.15	0
2	PG4	F	801	-	12,12,12	0.18	0	11,11,11	0.12	0
3	EDO	E	804	-	3,3,3	0.05	0	2,2,2	0.14	0
2	PG4	D	801	-	12,12,12	0.18	0	11,11,11	0.11	0
3	EDO	F	811	-	3,3,3	0.06	0	2,2,2	0.18	0
3	EDO	D	805	-	3,3,3	0.08	0	2,2,2	0.21	0
3	EDO	D	809	-	3,3,3	0.08	0	2,2,2	0.23	0
3	EDO	D	813	-	3,3,3	0.07	0	2,2,2	0.16	0
3	EDO	D	802	-	3,3,3	0.06	0	2,2,2	0.17	0
3	EDO	D	803	-	3,3,3	0.07	0	2,2,2	0.15	0
3	EDO	D	812	-	3,3,3	0.05	0	2,2,2	0.09	0
3	EDO	D	810	-	3,3,3	0.06	0	2,2,2	0.17	0
3	EDO	F	804	3	3,3,3	0.15	0	2,2,2	0.07	0
3	EDO	E	803	-	3,3,3	0.09	0	2,2,2	0.23	0
3	EDO	F	805	-	3,3,3	0.06	0	2,2,2	0.15	0
3	EDO	F	818	-	3,3,3	0.07	0	2,2,2	0.11	0
3	EDO	D	815	-	3,3,3	0.05	0	2,2,2	0.13	0
3	EDO	F	807	-	3,3,3	0.07	0	2,2,2	0.16	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	808	-	-	1/1/1/1	-
3	EDO	D	817	-	-	0/1/1/1	-
3	EDO	F	802	-	-	0/1/1/1	-
3	EDO	F	812	-	-	0/1/1/1	-
3	EDO	D	806	-	-	1/1/1/1	-
3	EDO	F	806	-	-	0/1/1/1	-
3	EDO	D	804	-	-	1/1/1/1	-
3	EDO	E	805	-	-	0/1/1/1	-
3	EDO	E	808	-	-	1/1/1/1	-
3	EDO	F	816	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) 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
2	F	801	PG4	O1-C1-C2-O2
3	D	804	EDO	O1-C1-C2-O2
3	D	805	EDO	O1-C1-C2-O2
3	D	808	EDO	O1-C1-C2-O2
3	E	803	EDO	O1-C1-C2-O2
3	D	809	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
2	D	801	PG4	C8-C7-O4-C6
3	F	803	EDO	O1-C1-C2-O2
2	F	801	PG4	C5-C6-O4-C7
2	D	801	PG4	O4-C7-C8-O5
2	F	801	PG4	C3-C4-O3-C5
3	F	813	EDO	O1-C1-C2-O2
3	F	816	EDO	O1-C1-C2-O2
2	D	801	PG4	C4-C3-O2-C2
3	F	811	EDO	O1-C1-C2-O2
3	F	818	EDO	O1-C1-C2-O2
3	D	802	EDO	O1-C1-C2-O2
3	F	815	EDO	O1-C1-C2-O2
3	D	810	EDO	O1-C1-C2-O2
3	E	808	EDO	O1-C1-C2-O2
3	F	807	EDO	O1-C1-C2-O2
3	D	806	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
3	F	809	EDO	1	0
2	F	801	PG4	1	0
3	D	815	EDO	2	0

5.7 Other polymers [i](#)

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, 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	D	687/736 (93%)	0.40	24 (3%) 47 48	23, 41, 71, 92	0
1	E	673/736 (91%)	0.83	98 (14%) 6 5	20, 49, 120, 143	1 (0%)
1	F	682/736 (92%)	0.40	33 (4%) 35 35	20, 42, 73, 95	2 (0%)
All	All	2042/2208 (92%)	0.54	155 (7%) 20 19	20, 43, 92, 143	3 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	98	LEU	7.6
1	E	84	GLY	5.0
1	D	304	TYR	4.9
1	D	35	LEU	4.8
1	E	80	ALA	4.6
1	E	71	LEU	4.5
1	E	94	ALA	4.4
1	E	75	ARG	4.4
1	E	304	TYR	4.4
1	E	76	ALA	4.4
1	E	90	PHE	4.3
1	E	141	PHE	4.3
1	E	77	GLY	4.2
1	F	41	THR	4.2
1	E	105	ILE	4.2
1	E	101	ILE	4.1
1	E	89	VAL	4.1
1	E	87	ILE	4.1
1	E	88	PRO	4.0
1	D	34	ALA	4.0
1	F	38	VAL	3.9
1	D	141	PHE	3.9
1	E	99	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	46	GLY	3.9
1	E	131	ALA	3.8
1	F	404	LYS	3.8
1	E	73	ILE	3.7
1	E	167	ILE	3.7
1	E	140	VAL	3.6
1	E	83	PRO	3.5
1	E	59	MET	3.4
1	E	132	LEU	3.4
1	E	107	LEU	3.4
1	F	733	ALA	3.4
1	E	147	SER	3.4
1	F	40	ALA	3.3
1	D	303	GLY	3.3
1	E	303	GLY	3.3
1	E	144	PRO	3.3
1	E	143	ILE	3.2
1	E	723	ASN	3.2
1	F	96	GLY	3.2
1	D	166	LEU	3.2
1	F	300	VAL	3.2
1	D	292	PHE	3.1
1	E	146	VAL	3.1
1	E	139	THR	3.1
1	D	302	PHE	3.1
1	F	304	TYR	3.1
1	E	122	LEU	3.1
1	F	97	ASN	3.1
1	F	405	LYS	3.1
1	F	736	ALA	3.1
1	E	403	GLN	3.0
1	E	130	MET	3.0
1	E	149	PRO	3.0
1	F	734	ILE	2.9
1	E	100	GLN	2.9
1	E	91	LEU	2.9
1	E	302	PHE	2.9
1	D	65	GLN	2.9
1	E	86	GLN	2.9
1	F	403	GLN	2.9
1	E	50	ILE	2.9
1	E	129	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	128	HIS	2.8
1	F	292	PHE	2.8
1	F	723	ASN	2.8
1	E	145	ASP	2.8
1	E	72	TRP	2.7
1	F	42	ALA	2.7
1	D	301	ASN	2.7
1	E	57	TYR	2.7
1	D	95	ASN	2.7
1	E	78	SER	2.7
1	E	127	SER	2.7
1	E	74	GLY	2.7
1	E	137	GLY	2.7
1	E	734	ILE	2.7
1	F	148	GLN	2.7
1	E	260[A]	GLN	2.6
1	F	303	GLY	2.6
1	E	67	PHE	2.6
1	E	722	ILE	2.6
1	E	82	GLN	2.6
1	E	64	TRP	2.6
1	F	402	GLY	2.6
1	E	210	PRO	2.6
1	E	735	LYS	2.6
1	E	48	VAL	2.6
1	E	106	THR	2.6
1	E	186	ALA	2.6
1	E	406	GLY	2.5
1	F	706	ALA	2.5
1	E	49	PRO	2.5
1	E	60	PRO	2.5
1	E	63	PHE	2.5
1	E	704	LEU	2.5
1	E	135	SER	2.5
1	E	79	ASP	2.5
1	E	600	ASP	2.5
1	D	734	ILE	2.5
1	E	136	ASN	2.5
1	E	142	ASN	2.5
1	D	287	GLU	2.5
1	E	95	ASN	2.5
1	E	300	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	149	PRO	2.4
1	E	724	GLY	2.4
1	F	270	CYS	2.4
1	E	731	TYR	2.4
1	F	58	ALA	2.4
1	F	719	SER	2.4
1	E	222	ASP	2.4
1	F	647	THR	2.3
1	F	260	GLN	2.3
1	E	292	PHE	2.3
1	E	115	PHE	2.3
1	E	706	ALA	2.3
1	D	539	THR	2.3
1	D	574	ASP	2.3
1	D	600	ASP	2.3
1	F	102	THR	2.2
1	E	299	MET	2.2
1	E	61	PRO	2.2
1	F	586	ASN	2.2
1	F	232	ASP	2.2
1	E	305	PHE	2.2
1	E	700	ALA	2.2
1	D	572	GLY	2.2
1	D	722	ILE	2.2
1	E	670	ASP	2.2
1	E	92	ARG	2.2
1	D	714	PRO	2.1
1	F	732	PHE	2.1
1	E	116	VAL	2.1
1	E	148	GLN	2.1
1	D	94	ALA	2.1
1	F	84	GLY	2.1
1	E	52	THR	2.1
1	E	96	GLY	2.1
1	E	102	THR	2.1
1	D	61	PRO	2.1
1	E	104	PRO	2.1
1	E	126	PRO	2.1
1	D	580	ASN	2.0
1	E	407	ASN	2.0
1	E	729	LEU	2.0
1	D	167	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	622	LYS	2.0
1	F	268	PRO	2.0
1	D	731	TYR	2.0
1	F	302	PHE	2.0
1	E	173	VAL	2.0
1	E	85	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	D	814	4/4	0.55	0.38	88,89,89,89	0
3	EDO	F	804	4/4	0.58	0.35	107,108,108,108	0
3	EDO	D	811	4/4	0.64	0.27	82,82,83,83	0
3	EDO	F	810	4/4	0.67	0.34	100,100,100,101	0
3	EDO	D	808	4/4	0.70	0.27	69,69,69,69	0
3	EDO	F	816	4/4	0.71	0.28	86,86,86,87	0
3	EDO	F	803	4/4	0.71	0.28	105,105,105,106	0
3	EDO	F	814	4/4	0.72	0.29	84,84,84,84	0
3	EDO	D	810	4/4	0.72	0.22	71,72,72,72	0
3	EDO	D	815	4/4	0.72	0.23	66,66,66,66	0
3	EDO	D	807	4/4	0.75	0.23	82,83,83,83	0
3	EDO	F	812	4/4	0.75	0.21	78,78,78,78	0
3	EDO	D	805	4/4	0.75	0.26	84,84,84,84	0
3	EDO	E	807	4/4	0.75	0.25	76,76,77,77	0
3	EDO	F	808	4/4	0.76	0.27	83,84,84,84	0
3	EDO	F	818	4/4	0.76	0.27	73,73,73,73	0
3	EDO	E	801	4/4	0.78	0.22	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	F	807	4/4	0.78	0.23	79,79,80,80	0
3	EDO	E	808	4/4	0.78	0.25	67,67,67,67	0
3	EDO	D	817	4/4	0.79	0.23	79,79,79,80	0
3	EDO	F	819	4/4	0.79	0.25	71,71,72,72	0
3	EDO	D	816	4/4	0.80	0.27	78,79,79,79	0
3	EDO	F	813	4/4	0.80	0.30	78,79,79,79	0
3	EDO	D	813	4/4	0.80	0.25	72,72,73,73	0
3	EDO	F	802	4/4	0.80	0.26	68,68,68,68	0
3	EDO	D	806	4/4	0.80	0.22	73,73,73,74	0
3	EDO	E	803	4/4	0.81	0.20	67,68,68,68	0
3	EDO	F	815	4/4	0.82	0.18	71,71,72,72	0
3	EDO	E	806	4/4	0.83	0.29	85,86,86,86	0
3	EDO	D	812	4/4	0.83	0.25	80,80,80,81	0
3	EDO	F	806	4/4	0.83	0.21	83,83,83,83	0
3	EDO	D	809	4/4	0.84	0.23	82,83,83,83	0
3	EDO	E	802	4/4	0.84	0.25	92,93,93,93	0
3	EDO	D	804	4/4	0.85	0.23	69,70,70,70	0
3	EDO	F	817	4/4	0.85	0.23	76,76,76,76	0
3	EDO	F	805	4/4	0.86	0.19	88,88,88,88	0
3	EDO	F	809	4/4	0.87	0.27	72,72,73,73	0
3	EDO	E	805	4/4	0.88	0.21	67,68,68,68	0
3	EDO	D	803	4/4	0.88	0.29	71,71,71,71	0
3	EDO	F	811	4/4	0.90	0.20	64,65,65,65	0
3	EDO	E	804	4/4	0.90	0.19	75,75,75,75	0
3	EDO	D	802	4/4	0.92	0.16	57,58,58,58	0
2	PG4	F	801	13/13	0.93	0.26	88,89,90,90	0
2	PG4	D	801	13/13	0.95	0.24	77,78,80,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.