



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:05 AM UTC

PDB ID : 9EYG / pdb_00009eyg
Title : Structure of Tannerella forsythia endopeptidase O (TfPepO)
Authors : Zak, K.M.; Grudnik, P.; Waligorska, I.; Ksiazek, M.
Deposited on : 2024-04-09
Resolution : 1.80 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

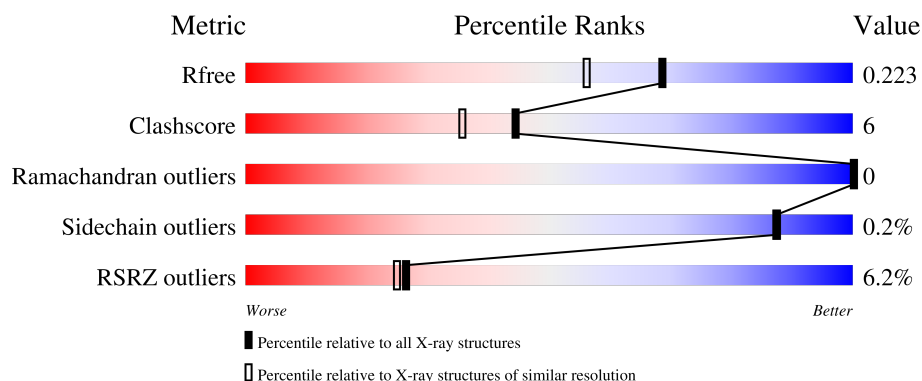
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	652	5% 89% 10%
1	B	652	7% 88% 11%

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
2	EDO	B	704	-	-	X	-
4	IMD	A	713	-	-	X	-
4	IMD	A	714	-	-	X	-

2 Entry composition [i](#)

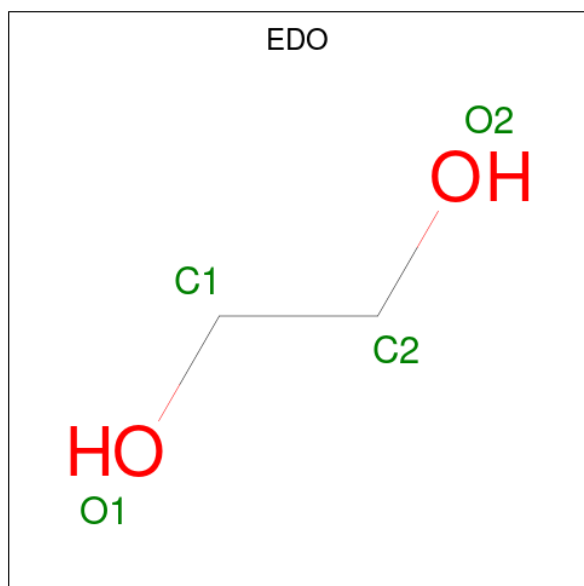
There are 7 unique types of molecules in this entry. The entry contains 11540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peptidase family M13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	8	0
			5298	3381	888	1004	25			
1	B	649	Total	C	N	O	S	0	8	0
			5285	3370	884	1005	26			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



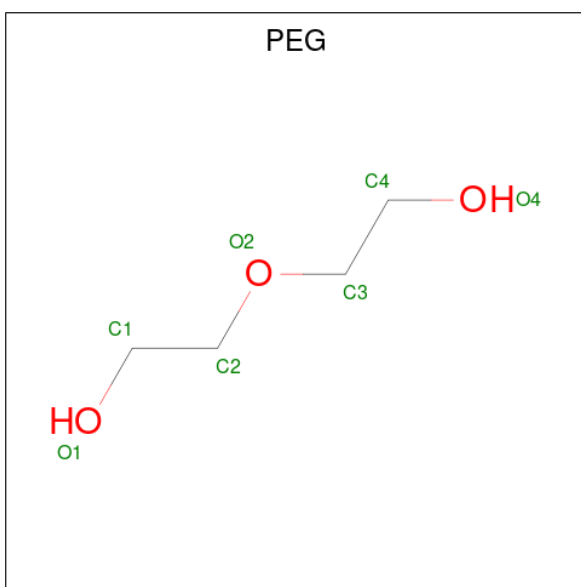
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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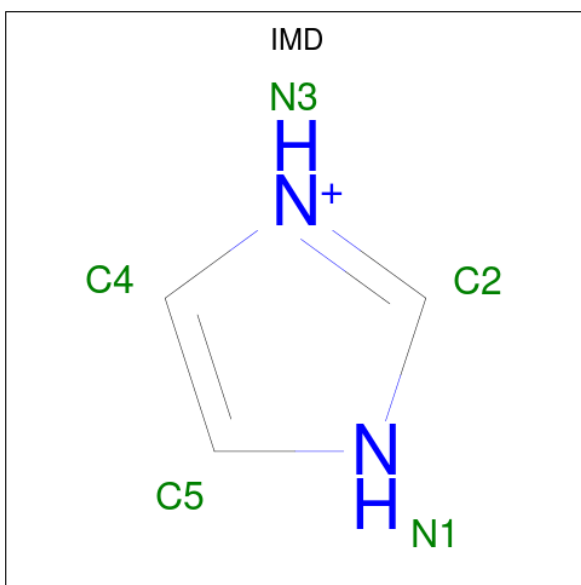
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



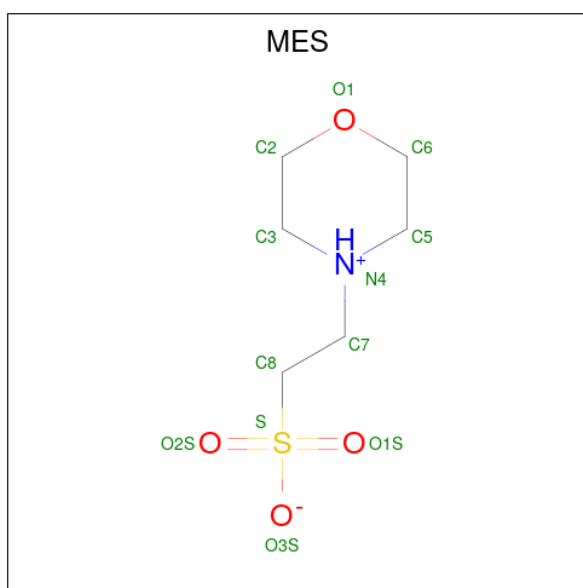
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 5 3 2	0	0
4	A	1	Total C N 5 3 2	0	0
4	A	1	Total C N 5 3 2	0	0
4	A	1	Total C N 5 3 2	0	0
4	B	1	Total C N 5 3 2	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O S 12 6 1 4 1	0	0
5	A	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Zn 2 2	0	0
6	B	2	Total Zn 2 2	0	0

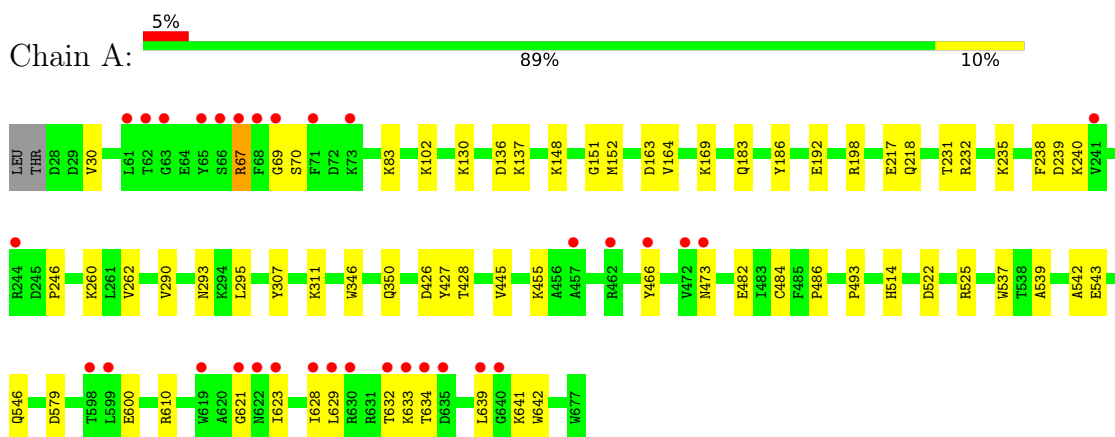
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	401	Total 404	O 404	0	3
7	B	398	Total 400	O 400	0	2

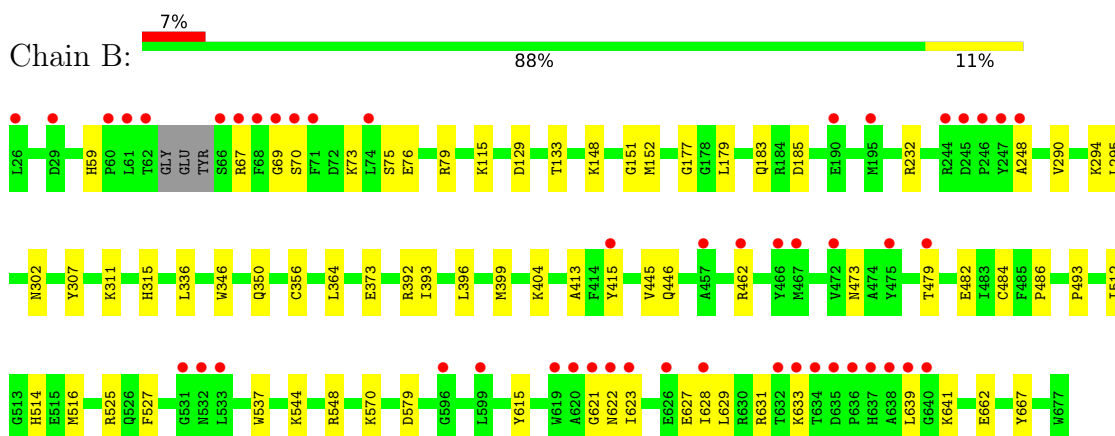
3 Residue-property plots [i](#)

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: Peptidase family M13



- Molecule 1: Peptidase family M13



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.41Å 95.41Å 301.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.75 – 1.80 48.75 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.75-1.80) 100.0 (48.75-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.194 , 0.223 0.194 , 0.223	Depositor DCC
R_{free} test set	7430 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11540	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: ZN, IMD, EDO, MES, PEG

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	0.40	0/5448	0.56	0/7365
1	B	0.39	0/5427	0.56	0/7337
All	All	0.40	0/10875	0.56	0/14702

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5298	0	5138	59	0
1	B	5285	0	5118	58	0
2	A	44	0	66	11	0
2	B	28	0	42	9	0
3	A	14	0	20	0	0
3	B	14	0	20	1	0
4	A	20	0	20	16	0
4	B	5	0	5	0	0
5	A	24	0	26	2	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	404	0	0	14	0
7	B	400	0	0	14	0
All	All	11540	0	10455	127	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 6.

All (127) 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:B:76:GLU:HG2	1:B:79:ARG:HH21	1.29	0.96
1:B:396:LEU:HD12	1:B:399:MET:HE2	1.49	0.92
1:B:393:ILE:HG23	1:B:399:MET:HE1	1.63	0.81
1:B:70:SER:HB2	1:B:493:PRO:HG3	1.63	0.80
1:B:399:MET:SD	7:B:1173:HOH:O	2.41	0.78
1:B:179:LEU:HB2	2:B:704:EDO:H12	1.69	0.75
1:A:137:LYS:HB2	2:A:701:EDO:H12	1.68	0.74
1:A:484[B]:CYS:SG	2:A:712:EDO:O2	2.45	0.74
1:B:302:ASN:ND2	7:B:806:HOH:O	2.21	0.73
1:B:623:ILE:HB	2:B:703:EDO:H12	1.72	0.72
1:B:59:HIS:O	1:B:622:ASN:ND2	2.24	0.71
1:B:356[B]:CYS:SG	7:B:1161:HOH:O	2.49	0.70
1:B:446[B]:GLN:OE1	7:B:802:HOH:O	2.09	0.70
2:B:703:EDO:H11	7:B:1088:HOH:O	1.92	0.70
1:A:183:GLN:HG2	7:A:1089:HOH:O	1.92	0.70
1:A:543:GLU:OE1	4:A:714:IMD:H4	1.91	0.70
1:B:248:ALA:O	7:B:803:HOH:O	2.09	0.70
1:B:579[B]:ASP:OD2	1:B:615:TYR:OH	2.10	0.69
1:A:70:SER:HB2	1:A:493:PRO:HG3	1.74	0.69
1:A:543:GLU:CD	4:A:714:IMD:H4	2.17	0.68
1:A:30:VAL:HG23	1:A:610:ARG:HD3	1.77	0.67
1:B:76:GLU:HG2	1:B:79:ARG:NH2	2.08	0.66
4:A:713:IMD:N1	7:A:806:HOH:O	2.28	0.65
1:B:307:TYR:CE1	1:B:311:LYS:HE2	2.35	0.62
1:B:346:TRP:O	1:B:350:GLN:HG3	2.01	0.61
1:B:641:LYS:N	7:B:805:HOH:O	2.16	0.61
1:B:396:LEU:HD12	1:B:399:MET:CE	2.26	0.61
1:A:600:GLU:O	1:A:610:ARG:NH2	2.35	0.60
1:A:426:ASP:OD1	1:A:428:THR:HG23	2.01	0.60
1:A:67[A]:ARG:HH21	1:A:621:GLY:HA3	1.66	0.60
1:A:466:TYR:CD2	2:A:712:EDO:H22	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LEU:H	2:B:704:EDO:C1	2.15	0.59
1:A:239:ASP:OD1	1:A:240:LYS:N	2.36	0.59
4:A:716:IMD:H2	7:A:858:HOH:O	2.03	0.58
4:A:714:IMD:H2	7:A:1065:HOH:O	2.03	0.56
1:A:610:ARG:HD2	7:A:855:HOH:O	2.06	0.56
1:A:83:LYS:HA	1:A:350:GLN:HE22	1.72	0.55
1:B:315:HIS:HD2	7:B:1121:HOH:O	1.90	0.55
1:B:415:TYR:CE2	1:B:462:ARG:HD2	2.42	0.55
1:B:639:LEU:H	1:B:639:LEU:HD12	1.71	0.55
1:B:639:LEU:HB3	7:B:805:HOH:O	2.05	0.55
1:B:183:GLN:HG2	7:B:1073:HOH:O	2.06	0.55
1:B:514:HIS:ND1	1:B:579[A]:ASP:OD1	2.38	0.54
1:B:75:SER:O	1:B:79:ARG:HG3	2.08	0.54
1:A:307:TYR:CE1	1:A:311:LYS:HE2	2.42	0.53
1:A:240:LYS:NZ	4:A:715:IMD:H5	2.24	0.53
1:A:525:ARG:HD3	1:A:537:TRP:CD2	2.43	0.53
1:A:69:GLY:HA2	1:A:621:GLY:HA2	1.91	0.52
1:B:641:LYS:HB3	7:B:805:HOH:O	2.10	0.52
1:B:399:MET:HE3	1:B:404:LYS:HG2	1.90	0.52
1:A:231:THR:O	1:A:235:LYS:HG3	2.10	0.52
1:A:455:LYS:HG2	2:A:706:EDO:H21	1.92	0.52
1:A:628:ILE:HG23	1:A:639[B]:LEU:HD11	1.93	0.51
1:B:179:LEU:CB	2:B:704:EDO:H12	2.38	0.51
1:B:129:ASP:O	1:B:133:THR:HG23	2.11	0.51
1:A:629:LEU:HD22	7:A:803:HOH:O	2.10	0.50
1:B:151:GLY:HA3	1:B:445:VAL:HG11	1.93	0.50
1:B:392:ARG:NH2	3:B:702:PEG:H31	2.27	0.50
1:B:628:ILE:HG23	1:B:639:LEU:HD21	1.94	0.50
1:A:482:GLU:HG3	1:A:484[B]:CYS:SG	2.52	0.49
1:B:413:ALA:HA	2:B:707:EDO:H12	1.93	0.49
1:A:136:ASP:OD1	2:A:701:EDO:O1	2.21	0.49
1:B:232:ARG:HD3	1:B:295:LEU:HD21	1.94	0.49
1:A:522:ASP:OD2	4:A:713:IMD:N1	2.41	0.49
1:B:482:GLU:HG3	1:B:484[B]:CYS:SG	2.52	0.49
2:A:703:EDO:H21	7:A:1031:HOH:O	2.13	0.48
2:A:709:EDO:O2	7:A:801:HOH:O	2.19	0.48
1:B:177:GLY:HA2	2:B:704:EDO:H11	1.96	0.47
4:A:714:IMD:C2	7:A:1065:HOH:O	2.62	0.47
1:A:546:GLN:HG3	4:A:713:IMD:C2	2.44	0.47
1:A:192:GLU:OE1	7:A:802:HOH:O	2.20	0.47
1:A:639[A]:LEU:HD12	1:A:641:LYS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:LYS:NZ	7:A:803:HOH:O	2.24	0.47
1:A:473:ASN:O	1:A:486:PRO:HD2	2.16	0.46
1:B:479:THR:HG22	1:B:527:PHE:CE2	2.51	0.46
1:A:238:PHE:CE1	5:A:717:MES:H72	2.52	0.45
1:A:639[A]:LEU:CD1	1:A:641:LYS:HB3	2.46	0.45
1:A:623:ILE:HG21	2:A:709:EDO:H22	1.96	0.45
1:A:633:LYS:HB2	1:A:634:THR:HG23	1.98	0.45
1:A:67[B]:ARG:HD2	7:A:867:HOH:O	2.15	0.45
1:A:346:TRP:O	1:A:350:GLN:HG3	2.17	0.45
1:A:543:GLU:CD	4:A:714:IMD:C4	2.87	0.45
2:A:708:EDO:H22	7:A:1148:HOH:O	2.17	0.45
1:A:163:ASP:OD2	1:A:169:LYS:HE3	2.17	0.45
1:A:639[A]:LEU:HD12	1:A:641:LYS:N	2.32	0.45
1:A:240:LYS:HZ1	4:A:715:IMD:H5	1.83	0.44
1:A:514:HIS:ND1	1:A:579:ASP:OD1	2.43	0.44
1:A:164:VAL:HG11	1:A:246:PRO:HB2	1.99	0.44
1:A:539:ALA:CB	4:A:714:IMD:HN3	2.31	0.44
1:A:542:ALA:HB1	4:A:713:IMD:N3	2.32	0.44
5:A:718:MES:H51	5:A:718:MES:H81	1.82	0.43
1:B:473:ASN:O	1:B:486:PRO:HD2	2.18	0.43
1:A:102:LYS:NZ	1:A:427:TYR:O	2.51	0.43
1:A:639[A]:LEU:HD11	1:A:641:LYS:HB3	2.01	0.43
1:B:67:ARG:NH2	2:B:703:EDO:H21	2.33	0.43
1:B:290:VAL:HG12	1:B:294:LYS:HE2	1.99	0.43
1:B:627:GLU:OE2	1:B:631:ARG:NE	2.51	0.43
1:B:629:LEU:HA	7:B:1114:HOH:O	2.18	0.43
1:A:67[A]:ARG:HH21	1:A:621:GLY:CA	2.31	0.43
1:B:570:LYS:HB2	1:B:570:LYS:HE2	1.90	0.43
1:A:260:LYS:HA	1:A:260:LYS:HD3	1.80	0.42
1:B:662:GLU:HA	1:B:667:TYR:CG	2.54	0.42
1:B:185:ASP:HB3	2:B:706:EDO:H12	2.01	0.42
1:A:262:VAL:HG13	1:A:293:ASN:HB2	2.02	0.42
4:A:716:IMD:C2	7:A:858:HOH:O	2.66	0.42
1:A:151:GLY:HA3	1:A:445:VAL:HG11	2.01	0.42
1:B:336:LEU:HD23	1:B:336:LEU:HA	1.88	0.42
1:A:130:LYS:HD2	2:A:708:EDO:O2	2.19	0.41
1:B:364:LEU:HD23	1:B:364:LEU:HA	1.88	0.41
1:B:544:LYS:O	1:B:548:ARG:HG2	2.19	0.41
1:A:186:TYR:O	1:A:198:ARG:HG3	2.20	0.41
1:B:639:LEU:HD12	1:B:639:LEU:N	2.35	0.41
1:B:67:ARG:HH12	1:B:69:GLY:HA3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:LYS:HD3	7:B:1011:HOH:O	2.19	0.41
1:A:148:LYS:HA	1:A:152:MET:O	2.21	0.41
1:B:148:LYS:HA	1:B:152:MET:O	2.21	0.41
1:B:525:ARG:HD3	1:B:537:TRP:CD2	2.56	0.41
1:A:217:GLU:OE2	1:A:218[B]:GLN:HG2	2.20	0.41
1:A:525:ARG:NH2	4:A:713:IMD:C5	2.84	0.41
1:B:512:ILE:O	1:B:516:MET:HG3	2.21	0.41
1:A:232:ARG:HD3	1:A:295:LEU:HD21	2.03	0.41
1:A:639[A]:LEU:HD11	1:A:642:TRP:CD1	2.56	0.41
1:A:290:VAL:HG11	4:A:716:IMD:C5	2.51	0.40
1:A:632:THR:HG22	2:A:705:EDO:O2	2.22	0.40
1:B:115:LYS:HE3	7:B:1077:HOH:O	2.21	0.40
1:B:373:GLU:H	1:B:373:GLU:CD	2.29	0.40
1:B:69:GLY:HA2	1:B:621:GLY:HA2	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	A	655/652 (100%)	645 (98%)	10 (2%)	0	100	100
1	B	652/652 (100%)	641 (98%)	11 (2%)	0	100	100
All	All	1307/1304 (100%)	1286 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	560/554 (101%)	558 (100%)	2 (0%)	84	83
1	B	560/554 (101%)	559 (100%)	1 (0%)	87	87
All	All	1120/1108 (101%)	1117 (100%)	3 (0%)	87	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67[A]	ARG
1	A	67[B]	ARG
1	B	73	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	81	GLN
1	A	328	ASN
1	A	343	GLN
1	A	350	GLN
1	A	387	ASN
1	A	491	GLN
1	B	78	ASN
1	B	315	HIS
1	B	327	GLN
1	B	523	GLN
1	B	566	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 4 are monoatomic - leaving 29 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	IMD	A	713	-	5,5,5	0.34	0	5,5,5	0.92	0
2	EDO	A	712	-	3,3,3	0.23	0	2,2,2	0.45	0
4	IMD	A	714	-	5,5,5	0.25	0	5,5,5	0.37	0
5	MES	A	717	-	12,12,12	1.15	1 (8%)	15,16,16	1.29	1 (6%)
3	PEG	A	704	-	6,6,6	0.21	0	5,5,5	0.28	0
2	EDO	A	701	-	3,3,3	0.23	0	2,2,2	0.14	0
2	EDO	A	707	-	3,3,3	0.27	0	2,2,2	0.18	0
3	PEG	B	701	-	6,6,6	0.30	0	5,5,5	0.22	0
3	PEG	B	702	-	6,6,6	0.26	0	5,5,5	0.50	0
2	EDO	B	706	-	3,3,3	0.28	0	2,2,2	0.12	0
2	EDO	A	711	-	3,3,3	0.24	0	2,2,2	0.41	0
3	PEG	A	702	-	6,6,6	0.21	0	5,5,5	0.38	0
2	EDO	A	710	-	3,3,3	0.24	0	2,2,2	0.37	0
4	IMD	B	710	-	5,5,5	0.31	0	5,5,5	0.83	0
2	EDO	B	704	-	3,3,3	0.23	0	2,2,2	0.35	0
5	MES	A	718	-	12,12,12	1.14	1 (8%)	15,16,16	1.10	2 (13%)
4	IMD	A	715	-	5,5,5	0.65	0	5,5,5	0.90	0
2	EDO	A	721	-	3,3,3	0.27	0	2,2,2	0.19	0
2	EDO	B	709	-	3,3,3	0.26	0	2,2,2	0.18	0
2	EDO	A	703	-	3,3,3	0.31	0	2,2,2	0.26	0
2	EDO	B	708	-	3,3,3	0.24	0	2,2,2	0.31	0
2	EDO	A	709	-	3,3,3	0.32	0	2,2,2	0.22	0
2	EDO	B	703	-	3,3,3	0.33	0	2,2,2	0.79	0
4	IMD	A	716	-	5,5,5	0.35	0	5,5,5	0.80	0
2	EDO	A	705	-	3,3,3	0.25	0	2,2,2	0.62	0
2	EDO	B	707	-	3,3,3	0.25	0	2,2,2	0.43	0
2	EDO	A	708	-	3,3,3	0.18	0	2,2,2	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	706	-	3,3,3	0.21	0	2,2,2	0.39	0
2	EDO	B	705	-	3,3,3	0.25	0	2,2,2	0.30	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	IMD	A	713	-	-	-	0/1/1/1
2	EDO	A	712	-	-	1/1/1/1	-
5	MES	A	717	-	-	2/6/14/14	0/1/1/1
4	IMD	A	714	-	-	-	0/1/1/1
3	PEG	A	704	-	-	2/4/4/4	-
2	EDO	A	701	-	-	1/1/1/1	-
2	EDO	A	707	-	-	0/1/1/1	-
3	PEG	B	701	-	-	2/4/4/4	-
3	PEG	B	702	-	-	1/4/4/4	-
2	EDO	B	706	-	-	0/1/1/1	-
2	EDO	A	711	-	-	0/1/1/1	-
3	PEG	A	702	-	-	2/4/4/4	-
2	EDO	A	710	-	-	0/1/1/1	-
4	IMD	B	710	-	-	-	0/1/1/1
2	EDO	B	704	-	-	0/1/1/1	-
5	MES	A	718	-	-	3/6/14/14	0/1/1/1
4	IMD	A	715	-	-	-	0/1/1/1
2	EDO	A	721	-	-	1/1/1/1	-
2	EDO	B	709	-	-	1/1/1/1	-
2	EDO	A	703	-	-	1/1/1/1	-
2	EDO	B	708	-	-	1/1/1/1	-
2	EDO	A	709	-	-	1/1/1/1	-
2	EDO	B	703	-	-	1/1/1/1	-
4	IMD	A	716	-	-	-	0/1/1/1
2	EDO	A	705	-	-	0/1/1/1	-
2	EDO	B	707	-	-	0/1/1/1	-
2	EDO	A	708	-	-	1/1/1/1	-
2	EDO	A	706	-	-	1/1/1/1	-
2	EDO	B	705	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	718	MES	C8-S	2.74	1.81	1.77
5	A	717	MES	C8-S	2.71	1.81	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	717	MES	O2S-S-C8	-2.58	102.83	106.73
5	A	718	MES	O1S-S-C8	-2.38	103.14	106.73
5	A	718	MES	O2S-S-C8	-2.17	103.45	106.73

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	717	MES	C8-C7-N4-C5
5	A	718	MES	C7-C8-S-O1S
5	A	718	MES	C7-C8-S-O3S
3	A	702	PEG	C4-C3-O2-C2
3	A	702	PEG	O1-C1-C2-O2
3	B	701	PEG	O1-C1-C2-O2
3	A	704	PEG	O2-C3-C4-O4
3	B	702	PEG	O1-C1-C2-O2
2	A	701	EDO	O1-C1-C2-O2
2	B	703	EDO	O1-C1-C2-O2
5	A	717	MES	C8-C7-N4-C3
2	A	721	EDO	O1-C1-C2-O2
5	A	718	MES	C7-C8-S-O2S
2	A	703	EDO	O1-C1-C2-O2
2	A	712	EDO	O1-C1-C2-O2
2	B	709	EDO	O1-C1-C2-O2
2	A	706	EDO	O1-C1-C2-O2
2	A	708	EDO	O1-C1-C2-O2
2	A	709	EDO	O1-C1-C2-O2
2	B	708	EDO	O1-C1-C2-O2
3	B	701	PEG	O2-C3-C4-O4
3	A	704	PEG	C4-C3-O2-C2

There are no ring outliers.

18 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	713	IMD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	712	EDO	2	0
4	A	714	IMD	6	0
5	A	717	MES	1	0
2	A	701	EDO	2	0
3	B	702	PEG	1	0
2	B	706	EDO	1	0
2	B	704	EDO	4	0
5	A	718	MES	1	0
4	A	715	IMD	2	0
2	A	703	EDO	1	0
2	A	709	EDO	2	0
2	B	703	EDO	3	0
4	A	716	IMD	3	0
2	A	705	EDO	1	0
2	B	707	EDO	1	0
2	A	708	EDO	2	0
2	A	706	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	650/652 (99%)	0.16	32 (4%)	35 33	11, 31, 54, 104	8 (1%)
1	B	649/652 (99%)	0.31	48 (7%)	20 19	12, 33, 62, 90	8 (1%)
All	All	1299/1304 (99%)	0.24	80 (6%)	26 25	11, 32, 59, 104	16 (1%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	639	LEU	6.5
1	A	639[A]	LEU	5.9
1	A	599	LEU	5.7
1	B	26	LEU	5.6
1	B	623	ILE	5.6
1	B	457	ALA	5.2
1	B	466	TYR	4.9
1	B	247	TYR	4.8
1	A	466	TYR	4.8
1	B	61	LEU	4.1
1	B	599	LEU	4.1
1	B	246	PRO	4.1
1	B	71	PHE	4.1
1	A	628	ILE	4.0
1	B	619	TRP	4.0
1	B	640	GLY	3.9
1	A	619	TRP	3.9
1	B	248	ALA	3.8
1	B	638	ALA	3.8
1	B	70	SER	3.7
1	A	68	PHE	3.7
1	B	69	GLY	3.6
1	A	457	ALA	3.6
1	A	640	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	621	GLY	3.6
1	B	632	THR	3.6
1	A	65	TYR	3.5
1	A	241	VAL	3.5
1	A	623	ILE	3.4
1	B	462	ARG	3.4
1	B	68	PHE	3.3
1	A	244	ARG	3.2
1	B	67	ARG	3.2
1	B	636	PRO	3.2
1	B	245	ASP	3.1
1	B	60	PRO	3.1
1	B	628	ILE	3.1
1	B	533	LEU	3.1
1	A	633	LYS	3.1
1	A	473	ASN	3.0
1	B	633	LYS	3.0
1	B	62	THR	2.9
1	B	634	THR	2.9
1	A	62	THR	2.9
1	B	620	ALA	2.8
1	B	531	GLY	2.8
1	A	630	ARG	2.8
1	B	244	ARG	2.8
1	B	622	ASN	2.7
1	A	629	LEU	2.7
1	B	635	ASP	2.7
1	B	637	HIS	2.7
1	B	195	MET	2.6
1	A	634	THR	2.6
1	A	66	SER	2.6
1	B	415	TYR	2.6
1	B	66	SER	2.6
1	A	67[A]	ARG	2.6
1	B	475	TYR	2.6
1	A	71	PHE	2.5
1	A	462	ARG	2.5
1	B	74	LEU	2.4
1	A	61	LEU	2.3
1	A	621	GLY	2.3
1	A	73	LYS	2.3
1	B	472	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	63	GLY	2.3
1	B	626	GLU	2.3
1	A	472	VAL	2.3
1	B	596	GLY	2.2
1	A	622	ASN	2.2
1	A	632	THR	2.2
1	B	479	THR	2.2
1	A	69	GLY	2.2
1	B	190	GLU	2.1
1	B	29	ASP	2.1
1	B	467	MET	2.1
1	B	532	ASN	2.0
1	A	635	ASP	2.0
1	A	598	THR	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($\text{\AA}^2$)	Q<0.9
4	IMD	A	714	5/5	0.50	0.24	49,54,61,61	0
4	IMD	A	716	5/5	0.50	0.26	57,61,61,64	0
2	EDO	B	707	4/4	0.66	0.19	53,54,57,63	0
2	EDO	A	709	4/4	0.66	0.21	54,55,56,67	0
2	EDO	A	712	4/4	0.66	0.22	51,59,60,66	0
4	IMD	A	713	5/5	0.67	0.20	56,59,63,63	0
4	IMD	B	710	5/5	0.76	0.16	46,52,55,56	0
2	EDO	A	711	4/4	0.77	0.14	51,55,56,59	0
2	EDO	A	710	4/4	0.79	0.15	48,50,51,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	B	708	4/4	0.81	0.13	52,55,55,66	0
3	PEG	B	701	7/7	0.81	0.14	47,49,50,54	0
2	EDO	B	709	4/4	0.82	0.13	54,55,57,58	0
2	EDO	A	703	4/4	0.83	0.19	37,46,50,50	0
2	EDO	B	706	4/4	0.83	0.16	53,55,56,57	0
3	PEG	B	702	7/7	0.84	0.14	35,39,48,52	0
2	EDO	B	704	4/4	0.85	0.15	27,30,39,40	0
3	PEG	A	702	7/7	0.85	0.13	38,44,50,50	0
2	EDO	A	706	4/4	0.87	0.13	41,48,51,59	0
2	EDO	A	707	4/4	0.88	0.12	49,50,50,56	0
2	EDO	A	708	4/4	0.88	0.13	40,45,55,55	0
2	EDO	A	721	4/4	0.88	0.13	44,47,48,49	0
2	EDO	B	703	4/4	0.88	0.16	33,47,50,56	0
5	MES	A	718	12/12	0.88	0.11	40,44,65,65	0
3	PEG	A	704	7/7	0.89	0.12	45,51,52,54	0
2	EDO	B	705	4/4	0.90	0.11	36,38,44,53	0
2	EDO	A	701	4/4	0.91	0.14	30,34,40,55	0
4	IMD	A	715	5/5	0.92	0.18	16,32,49,58	0
2	EDO	A	705	4/4	0.92	0.12	42,53,53,54	0
5	MES	A	717	12/12	0.97	0.09	26,33,40,43	0
6	ZN	B	712	1/1	0.97	0.05	34,34,34,34	0
6	ZN	A	720	1/1	0.99	0.03	34,34,34,34	0
6	ZN	B	711	1/1	0.99	0.12	38,38,38,38	0
6	ZN	A	719	1/1	0.99	0.09	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.