Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:01 pm BST

PDB ID	:	2QMX
Title	:	The crystal structure of L-Phe inhibited prephenate dehydratase from Chlorobium tepidum TLS
Authors	:	Tan, K.; Li, H.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2007-07-17
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

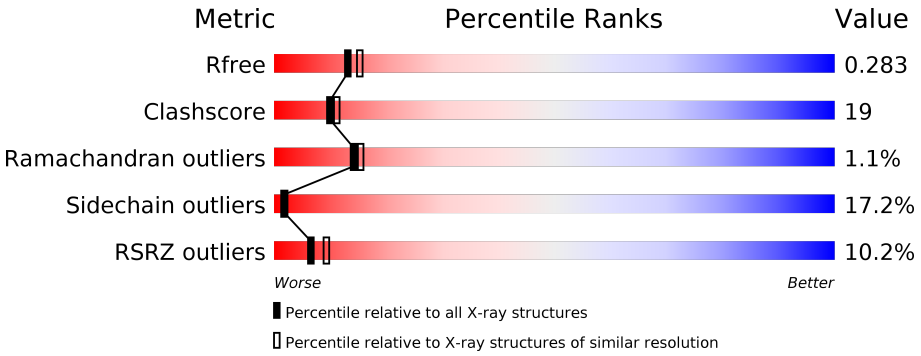
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 >=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 <=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	283	10% 57% 34% 6%
1	B	283	10% 58% 28% 10%

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	ACT	A	301	-	-	X	-
4	EDO	B	282	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4478 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.

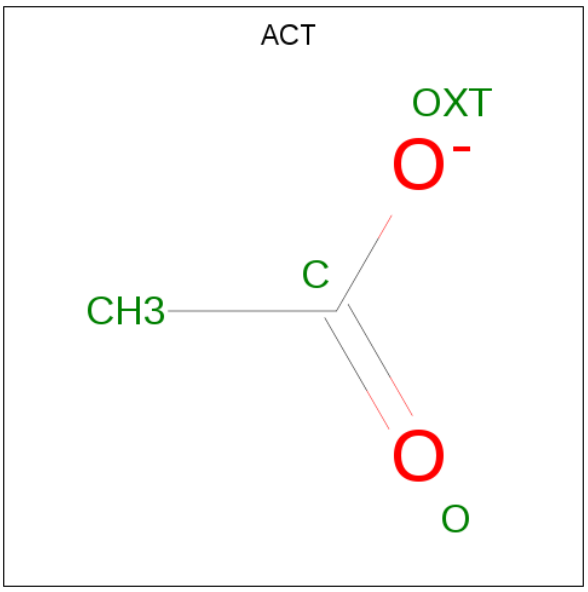
- Molecule 1 is a protein called Prephenate dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	Se	0	1	0
			2185	1391	379	408	4	3			
1	B	278	Total	C	N	O	S	Se	0	0	0
			2179	1386	378	408	4	3			

There are 6 discrepancies between the modelled and reference sequences:

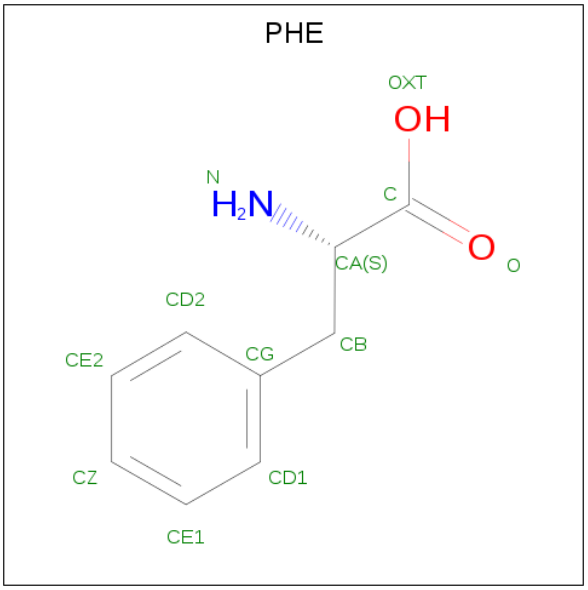
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	CLONING ARTIFACT	UNP Q8KBW6
A	-1	ASN	-	CLONING ARTIFACT	UNP Q8KBW6
A	0	ALA	-	CLONING ARTIFACT	UNP Q8KBW6
B	-2	SER	-	CLONING ARTIFACT	UNP Q8KBW6
B	-1	ASN	-	CLONING ARTIFACT	UNP Q8KBW6
B	0	ALA	-	CLONING ARTIFACT	UNP Q8KBW6

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



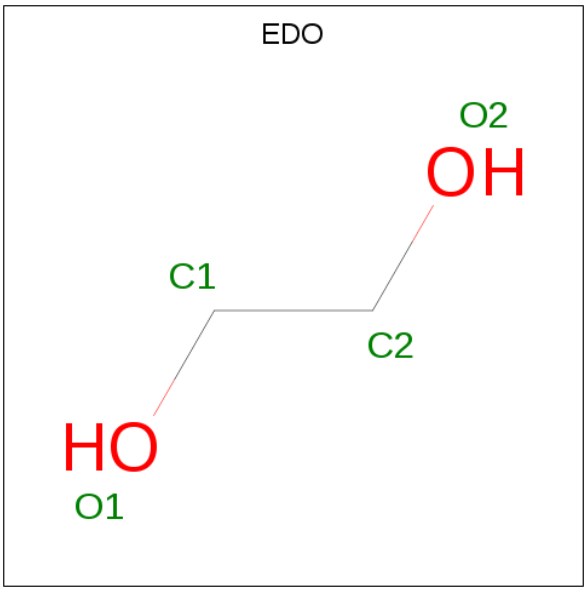
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 12 9 1 2	0	0
3	A	1	Total C N O 12 9 1 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	24	Total O 24 24	0	0

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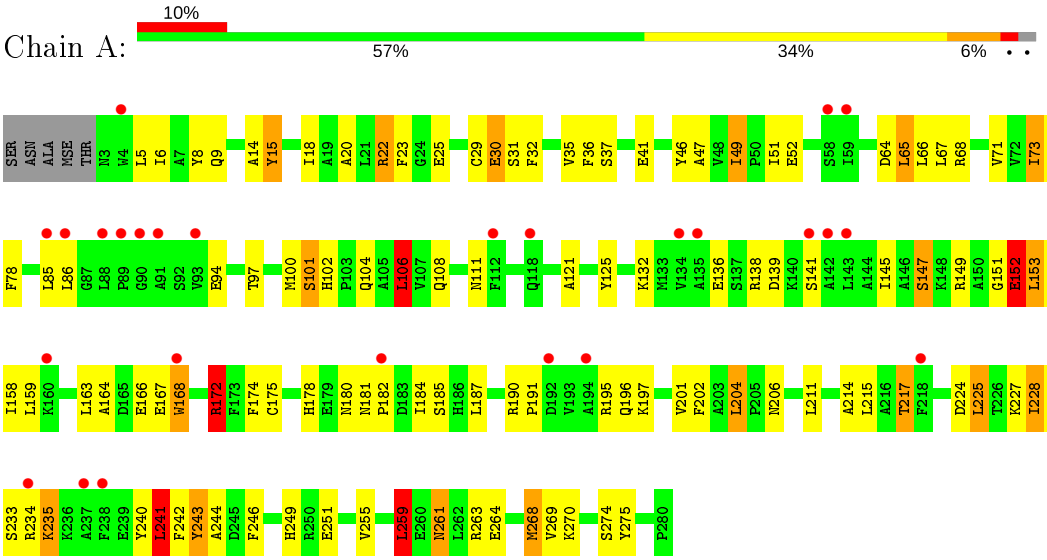
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	14	Total	O	0	0
			14	14		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

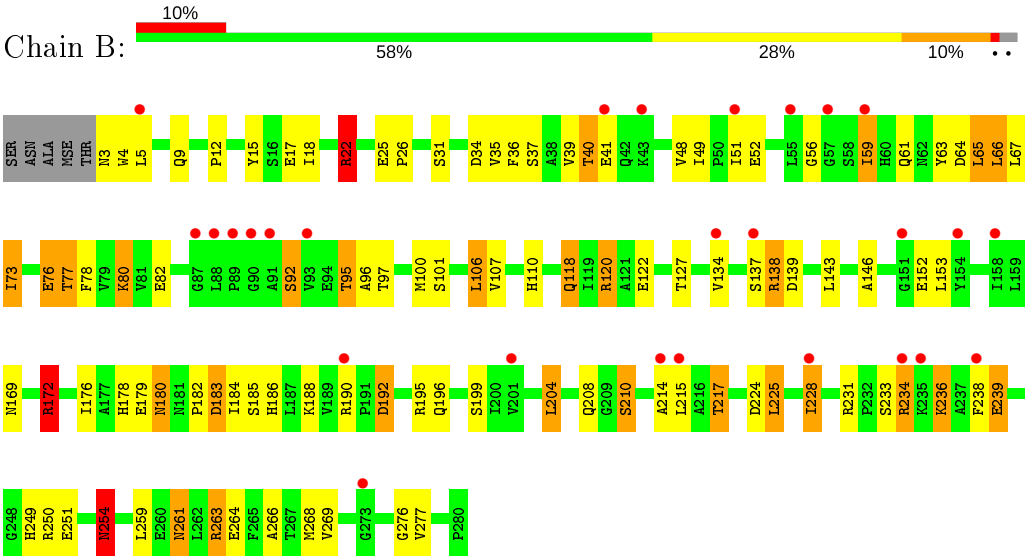
- Molecule 1: Prephenate dehydratase

Chain A:



- Molecule 1: Prephenate dehydratase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	86.87Å 127.89Å 56.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.13 – 2.30 41.13 – 2.30	Depositor EDS
% Data completeness (in resolution range)	82.6 (41.13-2.30) 82.6 (41.13-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.72 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.289 0.219 , 0.283	Depositor DCC
R_{free} test set	1347 reflections (5.67%)	wwPDB-VP
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4478	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, ACT

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	1.18	8/2233 (0.4%)	1.16	10/3020 (0.3%)
1	B	1.10	1/2225 (0.0%)	1.19	16/3012 (0.5%)
All	All	1.14	9/4458 (0.2%)	1.18	26/6032 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	GLU	CD-OE2	8.89	1.35	1.25
1	A	243	TYR	CE1-CZ	6.30	1.46	1.38
1	A	240	TYR	CE1-CZ	6.10	1.46	1.38
1	A	125	TYR	CE2-CZ	5.92	1.46	1.38
1	A	185	SER	CB-OG	5.85	1.49	1.42
1	A	32	PHE	CE2-CZ	5.84	1.48	1.37
1	A	15	TYR	CE1-CZ	5.33	1.45	1.38
1	A	147	SER	CB-OG	5.16	1.49	1.42
1	B	210	SER	CB-OG	-5.05	1.35	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	22	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	A	22	ARG	NE-CZ-NH1	9.88	125.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	172	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	A	172	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	22	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	B	172	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	B	67	LEU	CA-CB-CG	7.89	133.45	115.30
1	A	106	LEU	CA-CB-CG	6.70	130.71	115.30
1	A	241	LEU	CA-CB-CG	-6.47	100.41	115.30
1	B	263	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	76	GLU	O-C-N	-6.21	112.77	122.70
1	B	65	LEU	CA-CB-CG	6.16	129.48	115.30
1	A	263	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	245	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	22	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	56	GLY	N-CA-C	-5.96	98.19	113.10
1	B	172	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	259	LEU	CB-CG-CD2	5.93	121.09	111.00
1	B	5	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	86	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	153	LEU	CA-CB-CG	5.27	127.41	115.30
1	B	66	LEU	CA-CB-CG	5.26	127.40	115.30
1	B	69	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	B	68	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	69	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	B	269	VAL	CG1-CB-CG2	-5.11	102.73	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	3	ASN	Peptide
1	B	77	THR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2185	0	2159	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2179	0	2146	85	0
2	A	8	0	6	2	0
3	A	24	0	16	2	0
4	A	32	0	48	2	0
4	B	12	0	18	6	0
5	A	24	0	0	1	0
5	B	14	0	0	1	0
All	All	4478	0	4393	169	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 19.

All (169) 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:92:SER:HB3	1:B:95:THR:HB	1.45	0.98
1:B:69:ARG:HH21	1:B:69:ARG:HG2	1.36	0.91
1:A:73:ILE:HD13	1:A:174:PHE:CD1	2.09	0.87
1:B:100:MSE:HE3	1:B:134:VAL:HG23	1.60	0.82
1:B:71:VAL:HG21	1:B:176:ILE:HD12	1.62	0.81
1:A:202:PHE:HA	1:A:268:MSE:HE2	1.60	0.81
1:A:78:PHE:CZ	1:A:172:ARG:HD3	2.17	0.80
1:B:261:ASN:O	1:B:264:GLU:HB2	1.82	0.80
1:A:78:PHE:CE1	1:A:172:ARG:HB2	2.18	0.79
1:A:234:ARG:NH1	1:B:168:TRP:HB2	1.97	0.79
1:A:64:ASP:HB3	1:A:68:ARG:CZ	2.13	0.79
1:B:69:ARG:CG	1:B:69:ARG:HH21	1.96	0.78
1:B:92:SER:CB	1:B:95:THR:HB	2.12	0.78
1:A:73:ILE:HG12	1:A:275:TYR:CD1	2.18	0.78
1:B:36:PHE:O	1:B:40:THR:HG23	1.85	0.76
1:A:178:HIS:HD2	1:A:180:ASN:H	1.34	0.75
1:B:100:MSE:CE	1:B:134:VAL:HG23	2.17	0.74
1:B:73:ILE:HD13	1:B:73:ILE:H	1.52	0.73
1:B:214:ALA:O	1:B:217:THR:HB	1.88	0.73
1:B:73:ILE:N	1:B:73:ILE:HD13	2.02	0.73
1:B:96:ALA:CB	1:B:143:LEU:HD11	2.19	0.72
1:A:268:MSE:HE3	1:A:270:LYS:N	2.04	0.71
1:A:268:MSE:HE3	1:A:270:LYS:H	1.56	0.69
1:B:118:GLN:HB2	5:B:291:HOH:O	1.90	0.69
1:B:120:ARG:NH1	1:B:122:GLU:OE2	2.26	0.69
1:A:158:ILE:HD12	1:A:158:ILE:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LYS:HB3	1:B:239:GLU:HG3	1.76	0.67
1:B:195:ARG:HH21	1:B:247:ILE:HD13	1.59	0.67
1:B:137:SER:O	1:B:138:ARG:HG2	1.96	0.66
1:B:76:GLU:OE1	1:B:172:ARG:NH1	2.26	0.64
1:B:39:VAL:O	1:B:41:GLU:N	2.31	0.64
1:A:64:ASP:HB3	1:A:68:ARG:NH2	2.13	0.64
1:B:100:MSE:CE	1:B:134:VAL:CG2	2.75	0.64
1:A:31:SER:O	1:A:35:VAL:HG23	1.98	0.64
1:A:51:ILE:HG23	1:A:52:GLU:HG3	1.80	0.63
1:B:76:GLU:HG3	1:B:277:VAL:HG23	1.79	0.63
1:B:78:PHE:CE1	1:B:172:ARG:HD3	2.32	0.62
1:B:71:VAL:CG2	1:B:176:ILE:HD12	2.27	0.62
1:A:215:LEU:HD12	1:B:215:LEU:HD12	1.82	0.62
1:B:78:PHE:CZ	1:B:172:ARG:HD3	2.34	0.61
1:B:22:ARG:NH2	1:B:77:THR:OG1	2.32	0.61
1:A:225:LEU:O	3:A:303:PHE:N	2.34	0.60
1:B:178:HIS:HD2	1:B:180:ASN:H	1.47	0.60
1:A:268:MSE:HG2	1:A:269:VAL:N	2.17	0.59
1:B:40:THR:HG21	1:B:69:ARG:HD3	1.84	0.59
1:B:69:ARG:CG	1:B:69:ARG:NH2	2.62	0.58
1:A:102:HIS:HD2	1:A:104:GLN:H	1.50	0.58
1:A:224:ASP:OD2	4:A:306:EDO:H22	2.03	0.57
1:A:73:ILE:CD1	1:A:75:ALA:O	2.52	0.57
1:B:238:PHE:C	1:B:239:GLU:HG2	2.23	0.57
1:B:61:GLN:O	1:B:64:ASP:HB2	2.04	0.57
1:A:233:SER:HB2	1:A:241:LEU:HD12	1.87	0.57
1:A:73:ILE:HD12	1:A:75:ALA:O	2.05	0.57
1:A:97:THR:HG22	1:A:97:THR:O	2.04	0.56
1:A:85:LEU:HB2	1:A:163:LEU:HD22	1.86	0.56
1:B:204:LEU:HD12	1:B:266:ALA:HA	1.88	0.56
1:A:201:VAL:O	1:A:268:MSE:CE	2.55	0.55
1:B:160:LYS:HG3	1:B:163:LEU:CD1	2.36	0.55
1:A:145:ILE:HD12	1:A:163:LEU:HD23	1.89	0.55
1:B:160:LYS:HG3	1:B:163:LEU:HD13	1.89	0.54
1:B:184:ILE:HD12	1:B:190:ARG:HD2	1.88	0.54
1:B:80:LYS:HD3	1:B:169:ASN:O	2.07	0.54
1:A:132[B]:LYS:HG3	1:A:154:TYR:CE1	2.43	0.54
1:B:224:ASP:HB3	4:B:282:EDO:H22	1.89	0.54
1:A:225:LEU:HD22	1:A:246:PHE:HB3	1.88	0.54
1:A:149:ARG:O	1:A:153:LEU:HB2	2.07	0.54
1:B:247:ILE:HB	4:B:282:EDO:H21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ARG:NH2	1:B:69:ARG:HG2	2.12	0.54
1:B:96:ALA:HB2	1:B:143:LEU:HD11	1.88	0.53
1:A:166:GLU:HG3	1:A:167:GLU:O	2.08	0.53
1:B:80:LYS:HD2	1:B:82:GLU:HG3	1.90	0.53
1:A:214:ALA:O	1:A:217:THR:HB	2.09	0.53
1:A:75:ALA:HB2	1:A:191:PRO:HG3	1.92	0.52
1:A:100:MSE:O	1:A:101:SER:HB2	2.09	0.52
1:A:14:ALA:O	1:A:18:ILE:HD13	2.09	0.52
1:B:15:TYR:HA	1:B:18:ILE:HD12	1.92	0.52
1:A:229:GLU:O	1:A:242:PHE:HA	2.09	0.52
1:A:49:ILE:H	1:A:49:ILE:HD13	1.75	0.51
1:B:31:SER:HB2	1:B:34:ASP:H	1.75	0.51
1:A:227:LYS:O	1:A:244:ALA:HA	2.10	0.51
1:B:39:VAL:C	1:B:41:GLU:H	2.14	0.51
1:B:73:ILE:N	1:B:73:ILE:CD1	2.71	0.51
1:A:196:GLN:NE2	1:A:249:HIS:CD2	2.80	0.50
1:B:101:SER:HB3	1:B:106:LEU:HD13	1.93	0.50
1:A:15:TYR:HB2	2:A:301:ACT:OXT	2.12	0.50
1:B:247:ILE:HB	4:B:282:EDO:C2	2.41	0.50
1:A:101:SER:HB3	1:A:106:LEU:HD13	1.93	0.50
1:A:215:LEU:CD1	1:B:215:LEU:HD12	2.41	0.50
1:A:6:ILE:HB	1:A:20:ALA:HB1	1.93	0.50
1:A:15:TYR:O	1:A:18:ILE:HB	2.12	0.50
1:B:183:ASP:OD1	1:B:186:HIS:HB2	2.12	0.49
1:A:78:PHE:CD1	1:A:172:ARG:HB2	2.47	0.49
1:A:224:ASP:OD2	4:A:306:EDO:C2	2.60	0.49
1:B:225:LEU:HD22	1:B:246:PHE:HB3	1.94	0.49
1:A:73:ILE:HG12	1:A:275:TYR:CE1	2.48	0.49
1:B:192:ASP:O	1:B:276:GLY:HA3	2.13	0.49
1:B:36:PHE:CE1	1:B:65:LEU:HD23	2.48	0.49
1:A:51:ILE:HG22	1:A:172:ARG:HG2	1.94	0.49
1:A:106:LEU:HG	1:A:121:ALA:HB1	1.94	0.48
1:A:102:HIS:CD2	1:A:104:GLN:H	2.29	0.48
1:A:49:ILE:HD13	1:A:174:PHE:O	2.13	0.48
1:A:73:ILE:CG1	1:A:275:TYR:CD1	2.93	0.48
1:A:97:THR:CG2	1:A:97:THR:O	2.62	0.48
1:A:168:TRP:CE3	1:B:234:ARG:NH2	2.82	0.48
1:A:261:ASN:O	1:A:264:GLU:HB2	2.14	0.47
1:A:180:ASN:O	1:A:181:ASN:HB2	2.14	0.47
1:A:211:LEU:HD11	1:A:228:ILE:HD11	1.95	0.47
1:B:225:LEU:HD23	1:B:225:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:HA	1:A:235:LYS:HD3	1.54	0.47
1:B:101:SER:OG	1:B:127:THR:HG22	2.14	0.47
1:A:234:ARG:HD2	1:B:168:TRP:CG	2.49	0.47
1:A:149:ARG:O	1:A:152:GLU:HB2	2.15	0.47
1:A:30:GLU:HG2	1:B:110:HIS:CE1	2.50	0.47
1:B:31:SER:O	1:B:35:VAL:HG23	2.15	0.47
1:B:231:ARG:HD3	1:B:243:TYR:CZ	2.49	0.46
1:A:74:LEU:HD21	1:A:182:PRO:HA	1.98	0.46
1:A:47:ALA:O	1:A:175:CYS:HA	2.15	0.46
1:A:168:TRP:HE3	1:B:234:ARG:HH22	1.62	0.46
1:B:100:MSE:HE3	1:B:134:VAL:CG2	2.36	0.46
1:B:100:MSE:HA	1:B:122:GLU:O	2.16	0.46
1:B:228:ILE:O	1:B:228:ILE:CG2	2.64	0.46
1:B:263:ARG:HG2	4:B:283:EDO:H22	1.98	0.45
1:A:64:ASP:HB3	1:A:68:ARG:NH1	2.31	0.45
1:A:151:GLY:O	1:A:152:GLU:C	2.55	0.45
1:A:231:ARG:NH1	1:A:243:TYR:OH	2.50	0.45
1:A:51:ILE:HG12	1:A:174:PHE:CE2	2.51	0.45
1:A:206:ASN:OD1	3:A:304:PHE:N	2.50	0.45
1:A:6:ILE:HD13	1:A:46:TYR:HB2	1.99	0.44
1:B:96:ALA:CB	1:B:143:LEU:CD1	2.94	0.44
1:A:197:LYS:O	1:A:274:SER:HA	2.17	0.44
1:A:132[B]:LYS:HE2	1:A:136:GLU:OE2	2.16	0.44
1:A:139:ASP:OD2	1:A:141:SER:HB3	2.17	0.44
1:A:49:ILE:N	1:A:49:ILE:HD13	2.33	0.44
1:B:195:ARG:HH21	1:B:247:ILE:CD1	2.29	0.44
1:B:195:ARG:NH2	1:B:247:ILE:HD13	2.29	0.44
1:B:59:ILE:O	1:B:59:ILE:HG13	2.17	0.44
1:A:178:HIS:CD2	1:A:180:ASN:H	2.25	0.43
1:A:23:PHE:CE2	1:A:77:THR:HG22	2.54	0.43
1:B:247:ILE:HG22	4:B:282:EDO:H21	2.01	0.43
1:A:145:ILE:CD1	1:A:163:LEU:CD2	2.96	0.43
1:B:78:PHE:CZ	1:B:172:ARG:CD	3.01	0.43
1:A:108:GLN:O	1:A:164:ALA:CB	2.67	0.42
1:A:36:PHE:CZ	1:A:65:LEU:HB3	2.54	0.42
1:B:190:ARG:HH11	1:B:190:ARG:HG3	1.84	0.42
1:A:78:PHE:CE1	1:A:172:ARG:HD3	2.53	0.42
1:A:36:PHE:CE2	1:A:65:LEU:HB3	2.55	0.42
1:A:8:TYR:O	1:A:29:CYS:N	2.52	0.42
1:B:234:ARG:H	1:B:234:ARG:HG2	1.65	0.42
1:A:104:GLN:O	1:A:108:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:HG12	1:A:259:LEU:HD22	2.02	0.42
1:A:202:PHE:HD2	1:A:204:LEU:HD13	1.85	0.42
1:B:231:ARG:HD3	1:B:243:TYR:OH	2.20	0.42
1:B:179:GLU:O	1:B:182:PRO:HG3	2.20	0.41
1:B:204:LEU:O	1:B:239:GLU:HB3	2.20	0.41
1:A:18:ILE:HD11	1:A:149:ARG:HG2	2.01	0.41
1:A:202:PHE:HA	1:A:268:MSE:CE	2.41	0.41
1:B:127:THR:HB	1:B:146:ALA:HA	2.01	0.41
1:B:51:ILE:HG13	1:B:63:TYR:CE2	2.55	0.41
1:B:254:ASN:HA	1:B:254:ASN:HD22	1.60	0.41
1:B:25:GLU:HA	1:B:26:PRO:HD3	1.97	0.41
1:A:228:ILE:HA	1:A:243:TYR:O	2.20	0.41
2:A:301:ACT:H2	5:A:315:HOH:O	2.21	0.41
1:A:37:SER:O	1:A:41:GLU:HG2	2.21	0.41
1:A:201:VAL:O	1:A:268:MSE:HE3	2.21	0.41
1:B:247:ILE:CG2	4:B:282:EDO:H21	2.51	0.41
1:A:108:GLN:O	1:A:164:ALA:HB1	2.20	0.40
1:B:12:PRO:HA	1:B:17:GLU:CD	2.42	0.40
1:B:249:HIS:CD2	1:B:251:GLU:H	2.40	0.40
1:B:49:ILE:HD12	1:B:49:ILE:HG23	1.76	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	277/283 (98%)	254 (92%)	22 (8%)	1 (0%)	34 42
1	B	276/283 (98%)	255 (92%)	16 (6%)	5 (2%)	8 7
All	All	553/566 (98%)	509 (92%)	38 (7%)	6 (1%)	14 15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	THR
1	B	196	GLN
1	B	250	ARG
1	B	254	ASN
1	A	152	GLU
1	B	233	SER

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	230/229 (100%)	195 (85%)	35 (15%)	3 2
1	B	229/229 (100%)	185 (81%)	44 (19%)	1 1
All	All	459/458 (100%)	380 (83%)	79 (17%)	2 2

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	GLN
1	A	22	ARG
1	A	25	GLU
1	A	30	GLU
1	A	49	ILE
1	A	65	LEU
1	A	66	LEU
1	A	67	LEU
1	A	71	VAL
1	A	73	ILE
1	A	101	SER
1	A	106	LEU
1	A	111	ASN
1	A	138	ARG
1	A	147	SER
1	A	152	GLU
1	A	156	LEU

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Mol	Chain	Res	Type
1	A	159	LEU
1	A	168	TRP
1	A	172	ARG
1	A	184	ILE
1	A	187	LEU
1	A	190	ARG
1	A	195	ARG
1	A	204	LEU
1	A	217	THR
1	A	225	LEU
1	A	228	ILE
1	A	235	LYS
1	A	241	LEU
1	A	251	GLU
1	A	259	LEU
1	A	261	ASN
1	A	268	MSE
1	B	4	TRP
1	B	9	GLN
1	B	22	ARG
1	B	37	SER
1	B	48	VAL
1	B	52	GLU
1	B	59	ILE
1	B	66	LEU
1	B	69	ARG
1	B	71	VAL
1	B	73	ILE
1	B	80	LYS
1	B	92	SER
1	B	95	THR
1	B	97	THR
1	B	106	LEU
1	B	107	VAL
1	B	118	GLN
1	B	120	ARG
1	B	138	ARG
1	B	139	ASP
1	B	152	GLU
1	B	153	LEU
1	B	160	LYS
1	B	172	ARG

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Mol	Chain	Res	Type
1	B	180	ASN
1	B	183	ASP
1	B	185	SER
1	B	188	LYS
1	B	192	ASP
1	B	199	SER
1	B	204	LEU
1	B	208	GLN
1	B	210	SER
1	B	217	THR
1	B	225	LEU
1	B	228	ILE
1	B	234	ARG
1	B	236	LYS
1	B	239	GLU
1	B	254	ASN
1	B	259	LEU
1	B	261	ASN
1	B	268	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	178	HIS
1	A	180	ASN
1	A	196	GLN
1	B	9	GLN
1	B	60	HIS
1	B	102	HIS
1	B	110	HIS
1	B	178	HIS
1	B	249	HIS
1	B	254	ASN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

15 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	$\#\|Z\| > 2$
4	EDO	B	281	-	3,3,3	0.81	0	2,2,2	0.34	0
4	EDO	A	310	-	3,3,3	0.74	0	2,2,2	0.32	0
4	EDO	B	282	-	3,3,3	0.61	0	2,2,2	0.57	0
4	EDO	A	311	-	3,3,3	0.52	0	2,2,2	0.28	0
4	EDO	A	307	-	3,3,3	0.59	0	2,2,2	0.26	0
4	EDO	A	309	-	3,3,3	0.69	0	2,2,2	0.29	0
4	EDO	A	306	-	3,3,3	0.57	0	2,2,2	0.07	0
2	ACT	A	301	-	1,3,3	1.22	0	0,3,3	0.00	-
2	ACT	A	302	-	1,3,3	1.80	0	0,3,3	0.00	-
4	EDO	A	312	-	3,3,3	0.63	0	2,2,2	0.31	0
4	EDO	A	308	-	3,3,3	0.59	0	2,2,2	0.20	0
4	EDO	A	305	-	3,3,3	0.50	0	2,2,2	0.30	0
4	EDO	B	283	-	3,3,3	0.81	0	2,2,2	0.31	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	EDO	A	310	-	-	1/1/1/1	-
4	EDO	B	282	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	311	-	-	1/1/1/1	-
4	EDO	A	307	-	-	1/1/1/1	-
4	EDO	A	309	-	-	0/1/1/1	-
4	EDO	A	306	-	-	1/1/1/1	-
4	EDO	B	281	-	-	1/1/1/1	-
4	EDO	A	312	-	-	0/1/1/1	-
4	EDO	A	308	-	-	0/1/1/1	-
4	EDO	A	305	-	-	0/1/1/1	-
4	EDO	B	283	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	310	EDO	O1-C1-C2-O2
4	B	281	EDO	O1-C1-C2-O2
4	B	282	EDO	O1-C1-C2-O2
4	A	307	EDO	O1-C1-C2-O2
4	B	283	EDO	O1-C1-C2-O2
4	A	306	EDO	O1-C1-C2-O2
4	A	311	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	282	EDO	5	0
4	A	306	EDO	2	0
2	A	301	ACT	2	0
4	B	283	EDO	1	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, 95^{th} 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	275/283 (97%)	0.66	27 (9%)	7	10	51, 59, 71, 79	0
1	B	275/283 (97%)	0.70	29 (10%)	6	8	49, 58, 73, 83	0
All	All	550/566 (97%)	0.68	56 (10%)	6	9	49, 59, 72, 83	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	PHE	7.3
1	B	168	TRP	7.3
1	B	88	LEU	6.6
1	A	237	ALA	6.3
1	A	160	LYS	5.5
1	B	238	PHE	4.6
1	A	135	ALA	4.5
1	A	141	SER	4.3
1	B	91	ALA	4.1
1	A	142	ALA	4.1
1	B	87	GLY	4.1
1	B	59	ILE	3.9
1	A	168	TRP	3.9
1	A	89	PRO	3.8
1	B	5	LEU	3.7
1	B	190	ARG	3.6
1	B	134	VAL	3.6
1	B	90	GLY	3.5
1	A	88	LEU	3.5
1	A	90	GLY	3.5
1	A	156	LEU	3.4
1	B	89	PRO	3.3
1	A	234	ARG	3.2
1	A	112	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	91	ALA	3.1
1	A	118	GLN	3.0
1	A	134	VAL	3.0
1	A	182	PRO	2.9
1	B	43	LYS	2.8
1	B	57	GLY	2.8
1	B	41	GLU	2.8
1	B	93	VAL	2.7
1	B	158	ILE	2.7
1	B	228	ILE	2.6
1	B	51	ILE	2.6
1	A	192	ASP	2.6
1	B	234	ARG	2.5
1	B	151	GLY	2.5
1	A	93	VAL	2.4
1	A	86	LEU	2.4
1	A	58	SER	2.3
1	A	194	ALA	2.3
1	B	215	LEU	2.3
1	A	4	TRP	2.3
1	B	273	GLY	2.3
1	A	143	LEU	2.2
1	B	243	TYR	2.2
1	B	154	TYR	2.2
1	B	201	VAL	2.2
1	A	218	PHE	2.2
1	B	235	LYS	2.1
1	A	59	ILE	2.1
1	A	85	LEU	2.1
1	B	214	ALA	2.1
1	B	137	SER	2.1
1	B	55	LEU	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 carbohydrates 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^{th} 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
4	EDO	B	281	4/4	0.60	0.23	69,70,72,74	0
4	EDO	A	307	4/4	0.66	0.23	89,92,93,94	0
4	EDO	A	310	4/4	0.73	0.28	70,75,77,79	0
4	EDO	A	309	4/4	0.77	0.17	78,79,79,80	0
4	EDO	B	283	4/4	0.80	0.18	73,74,76,77	0
4	EDO	A	312	4/4	0.83	0.30	64,69,70,70	0
4	EDO	B	282	4/4	0.85	0.43	44,56,59,64	0
4	EDO	A	308	4/4	0.86	0.44	74,78,80,84	0
4	EDO	A	311	4/4	0.86	0.12	76,78,78,79	0
2	ACT	A	301	4/4	0.89	0.18	74,74,75,76	0
3	PHE	A	304	12/12	0.90	0.15	45,49,51,52	0
4	EDO	A	305	4/4	0.91	0.11	84,86,87,87	0
3	PHE	A	303	12/12	0.92	0.17	47,48,51,52	0
4	EDO	A	306	4/4	0.93	0.38	63,64,65,65	0
2	ACT	A	302	4/4	0.94	0.25	75,75,75,76	0

6.5 Other polymers (i)

There are no such residues in this entry.