



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:04 PM UTC

PDB ID : 3ETC / pdb_00003etc
Title : 2.1 Å structure of acyl-adenylate synthetase from Methanosarcina acetivorans containing a link between Lys256 and Cys298
Authors : Shah, M.B.; Gulick, A.M.; Smith, K.S.; Ingram-Smith, C.
Deposited on : 2008-10-07
Resolution : 2.10 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

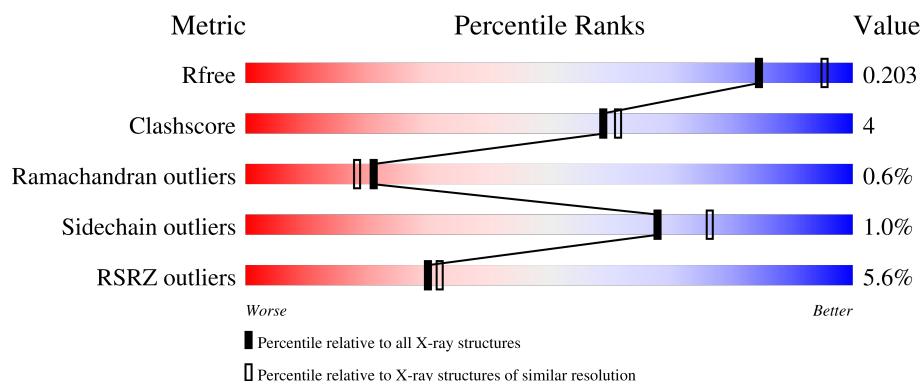
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

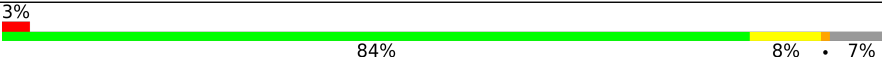
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	580	
1	B	580	

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	FOR	B	999	-	-	X	-
8	GOL	A	1005	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9016 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 AMP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	3	0
			4191	2719	663	786	23			
1	B	537	Total	C	N	O	S	0	2	0
			4233	2746	668	796	23			

There are 46 discrepancies between the modelled and reference sequences:

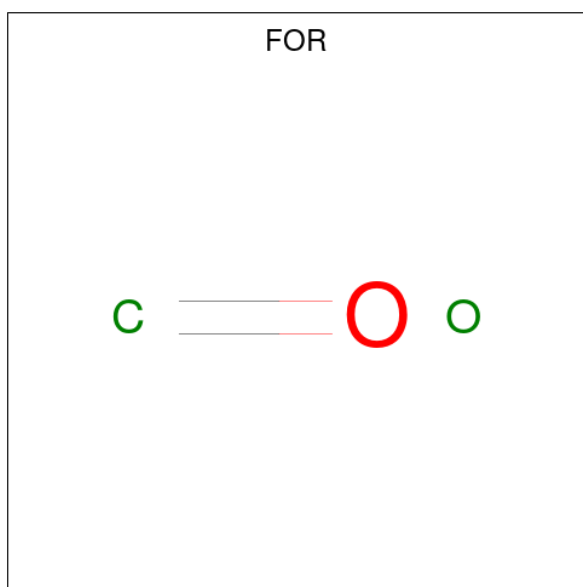
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q8TLW1
A	-21	GLY	-	expression tag	UNP Q8TLW1
A	-20	HIS	-	expression tag	UNP Q8TLW1
A	-19	HIS	-	expression tag	UNP Q8TLW1
A	-18	HIS	-	expression tag	UNP Q8TLW1
A	-17	HIS	-	expression tag	UNP Q8TLW1
A	-16	HIS	-	expression tag	UNP Q8TLW1
A	-15	HIS	-	expression tag	UNP Q8TLW1
A	-14	HIS	-	expression tag	UNP Q8TLW1
A	-13	HIS	-	expression tag	UNP Q8TLW1
A	-12	HIS	-	expression tag	UNP Q8TLW1
A	-11	HIS	-	expression tag	UNP Q8TLW1
A	-10	SER	-	expression tag	UNP Q8TLW1
A	-9	SER	-	expression tag	UNP Q8TLW1
A	-8	GLY	-	expression tag	UNP Q8TLW1
A	-7	HIS	-	expression tag	UNP Q8TLW1
A	-6	ILE	-	expression tag	UNP Q8TLW1
A	-5	ASP	-	expression tag	UNP Q8TLW1
A	-4	ASP	-	expression tag	UNP Q8TLW1
A	-3	ASP	-	expression tag	UNP Q8TLW1
A	-2	ASP	-	expression tag	UNP Q8TLW1
A	-1	LYS	-	expression tag	UNP Q8TLW1
A	0	HIS	-	expression tag	UNP Q8TLW1
B	-22	MET	-	expression tag	UNP Q8TLW1
B	-21	GLY	-	expression tag	UNP Q8TLW1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP Q8TLW1
B	-19	HIS	-	expression tag	UNP Q8TLW1
B	-18	HIS	-	expression tag	UNP Q8TLW1
B	-17	HIS	-	expression tag	UNP Q8TLW1
B	-16	HIS	-	expression tag	UNP Q8TLW1
B	-15	HIS	-	expression tag	UNP Q8TLW1
B	-14	HIS	-	expression tag	UNP Q8TLW1
B	-13	HIS	-	expression tag	UNP Q8TLW1
B	-12	HIS	-	expression tag	UNP Q8TLW1
B	-11	HIS	-	expression tag	UNP Q8TLW1
B	-10	SER	-	expression tag	UNP Q8TLW1
B	-9	SER	-	expression tag	UNP Q8TLW1
B	-8	GLY	-	expression tag	UNP Q8TLW1
B	-7	HIS	-	expression tag	UNP Q8TLW1
B	-6	ILE	-	expression tag	UNP Q8TLW1
B	-5	ASP	-	expression tag	UNP Q8TLW1
B	-4	ASP	-	expression tag	UNP Q8TLW1
B	-3	ASP	-	expression tag	UNP Q8TLW1
B	-2	ASP	-	expression tag	UNP Q8TLW1
B	-1	LYS	-	expression tag	UNP Q8TLW1
B	0	HIS	-	expression tag	UNP Q8TLW1

- Molecule 2 is FORMYL GROUP (CCD ID: FOR) (formula: CH₂O).



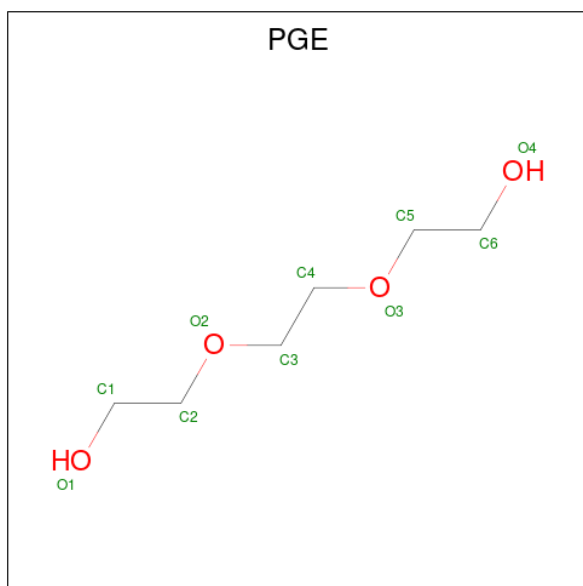
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			2	1	1		

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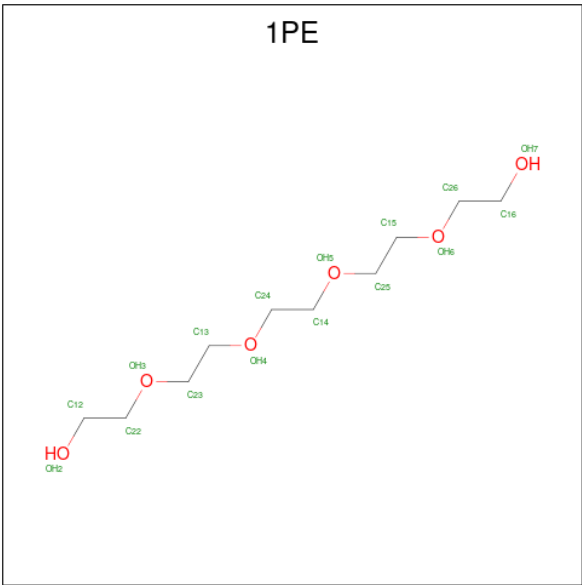
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			2	1	1		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



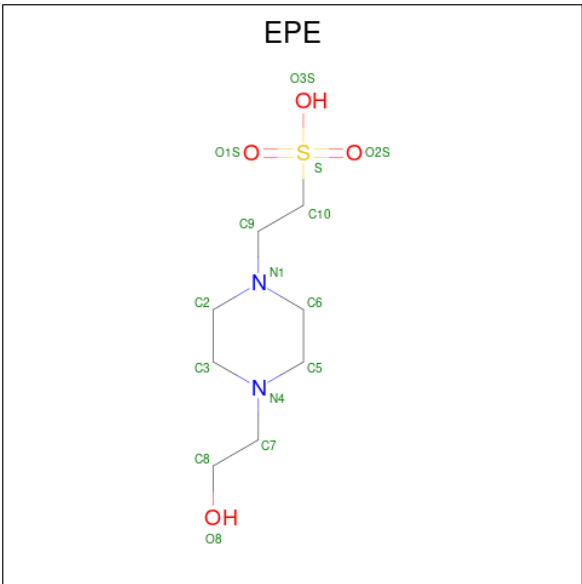
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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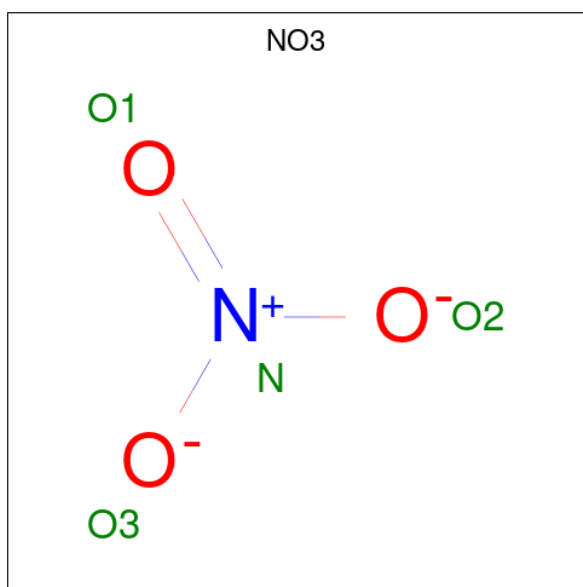
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

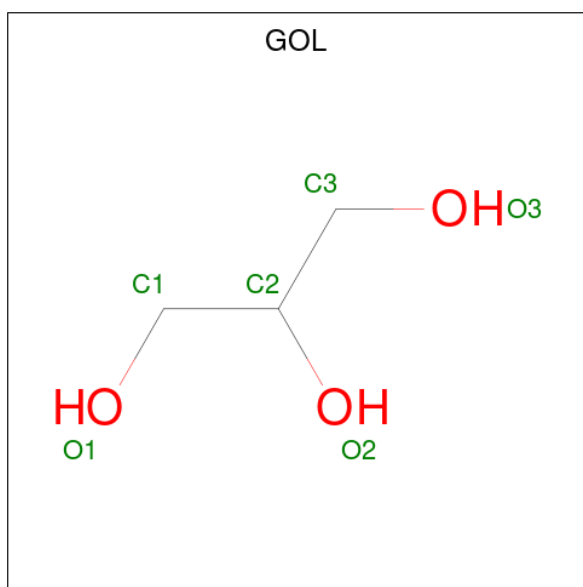
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		

- Molecule 7 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

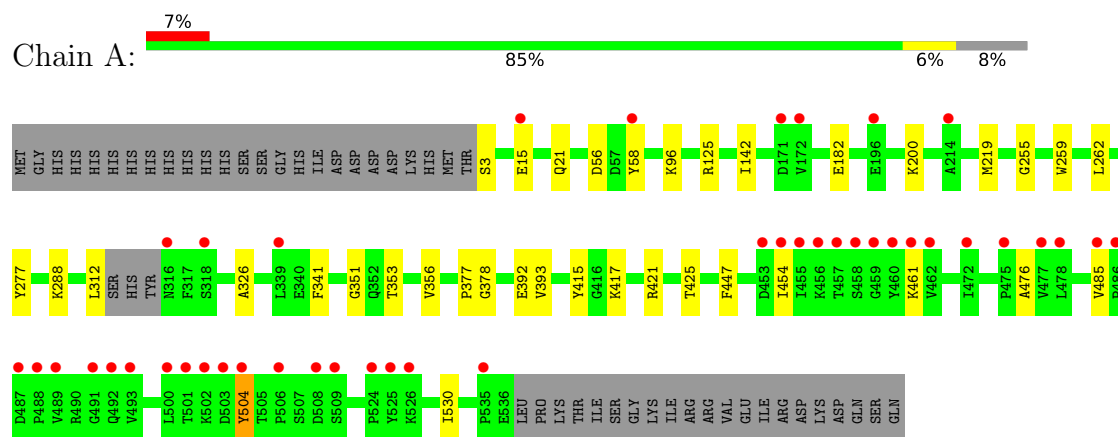
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	204	Total	O	0	0
			204	204		
9	B	225	Total	O	0	0
			225	225		

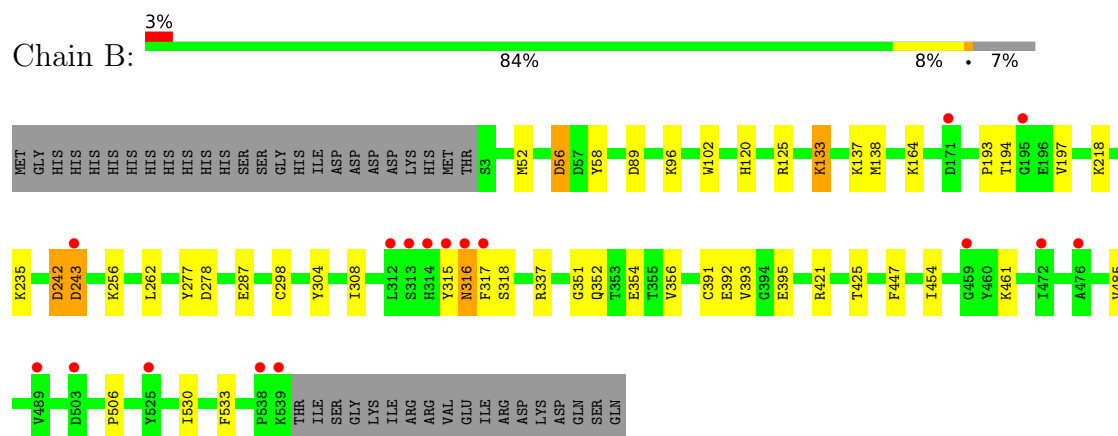
3 Residue-property plots [i](#)

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: AMP-binding protein



- Molecule 1: AMP-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.70Å 96.37Å 141.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.10 29.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.88-2.10) 99.9 (29.88-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.175 , 0.207 (Not available) , 0.203	Depositor DCC
R_{free} test set	4326 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9016	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, PGE, FOR, EPE, 1PE, NO3

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	0.58	1/4317 (0.0%)	0.78	0/5869
1	B	0.59	0/4360	0.81	1/5933 (0.0%)
All	All	0.59	1/8677 (0.0%)	0.80	1/11802 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	504	TYR	C-O	7.24	1.32	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	ASP	N-CA-C	-6.59	100.53	110.28

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	A	4191	0	3993	32	0
1	B	4233	0	4033	41	0
2	A	2	0	0	0	0
2	B	2	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	14	5	0
3	B	20	0	28	2	0
4	A	32	0	44	2	0
5	A	30	0	34	2	0
5	B	15	0	17	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
8	A	24	0	32	9	0
8	B	18	0	24	1	0
9	A	204	0	0	4	0
9	B	225	0	0	3	0
All	All	9016	0	8219	74	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 4.

All (74) 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:256:LYS:NZ	2:B:999:FOR:C	1.76	1.44
1:B:256:LYS:HZ3	2:B:999:FOR:C	1.32	1.28
1:B:242:ASP:O	1:B:243:ASP:CB	1.91	1.14
1:B:242:ASP:O	1:B:243:ASP:HB2	1.23	1.00
1:B:256:LYS:HZ1	2:B:999:FOR:C	1.59	0.93
1:B:315:TYR:O	1:B:317:PHE:N	2.18	0.76
1:B:56:ASP:HB3	1:B:58:TYR:H	1.50	0.74
9:A:1093:HOH:O	1:B:218:LYS:HE3	1.89	0.73
1:A:454:ILE:HD13	1:A:461:LYS:HE2	1.72	0.71
1:A:56:ASP:HB3	1:A:58:TYR:H	1.53	0.70
8:A:1005:GOL:H31	9:A:1169:HOH:O	1.94	0.67
1:B:391:CYS:HB3	1:B:395:GLU:HG3	1.77	0.66
1:B:485:VAL:HG21	1:B:530:ILE:HD12	1.77	0.66
1:A:485:VAL:HG21	1:A:530:ILE:HD12	1.79	0.64
1:A:353:THR:HG23	8:A:1005:GOL:H12	1.80	0.64
1:B:277:TYR:CZ	5:B:998:EPE:H61	2.34	0.62
8:A:1005:GOL:C3	9:A:1169:HOH:O	2.47	0.62
1:B:447:PHE:CD2	8:B:1003:GOL:H12	2.36	0.61
1:A:415:TYR:CE1	8:A:1004:GOL:H31	2.36	0.61
1:B:352:GLN:HG2	1:B:354:GLU:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:MET:HE1	1:B:102:TRP:CD1	2.38	0.59
1:B:256:LYS:CE	2:B:999:FOR:C	2.73	0.57
1:B:256:LYS:NZ	1:B:298:CYS:SG	2.77	0.57
1:A:277:TYR:CZ	5:A:996:EPE:H61	2.40	0.57
1:A:417:LYS:O	1:B:133:LYS:HE3	2.05	0.56
1:B:392:GLU:O	1:B:395:GLU:HG2	2.04	0.56
1:B:421:ARG:O	1:B:425:THR:HG23	2.06	0.55
1:B:304:TYR:O	1:B:308:ILE:HG12	2.08	0.54
1:A:353:THR:CG2	8:A:1005:GOL:H12	2.38	0.54
1:A:421:ARG:O	1:A:425:THR:HG23	2.10	0.52
1:A:312:LEU:HD12	1:A:341:PHE:HB3	1.92	0.51
1:B:351:GLY:H	3:B:993:PGE:H52	1.75	0.51
1:B:278:ASP:OD2	9:B:1270:HOH:O	2.19	0.51
1:A:378:GLY:HA3	8:A:1002:GOL:H2	1.93	0.51
1:A:392:GLU:HG3	1:A:393:VAL:N	2.26	0.51
1:A:461:LYS:H	4:A:994:1PE:H261	1.77	0.50
1:B:52:MET:HE1	1:B:102:TRP:CG	2.46	0.50
1:A:326:ALA:HB1	4:A:994:1PE:H221	1.93	0.49
1:B:454:ILE:HD13	1:B:461:LYS:HE3	1.94	0.49
1:B:287:GLU:HG3	1:B:315:TYR:CE1	2.47	0.49
1:A:96:LYS:HG3	1:A:142:ILE:HD13	1.93	0.48
1:A:447:PHE:CD2	8:A:1003:GOL:H31	2.49	0.48
1:B:242:ASP:O	1:B:243:ASP:HB3	2.03	0.48
1:B:506:PRO:HB3	1:B:533:PHE:CD2	2.48	0.48
1:B:315:TYR:O	1:B:316:ASN:C	2.56	0.48
1:B:287:GLU:HG3	1:B:315:TYR:CD1	2.50	0.47
1:B:392:GLU:HG3	1:B:393:VAL:N	2.30	0.47
1:B:235:LYS:HE2	9:B:1115:HOH:O	2.14	0.46
1:B:96:LYS:HD3	1:B:120:HIS:CG	2.50	0.46
1:A:288:LYS:HE2	3:A:991:PGE:H32	1.98	0.46
1:B:193:PRO:HB3	1:B:197:VAL:HG13	1.96	0.46
1:B:425:THR:HG21	9:B:1320:HOH:O	2.16	0.46
1:A:288:LYS:HZ3	3:A:991:PGE:H62	1.81	0.45
1:A:425:THR:HG21	9:A:1189:HOH:O	2.15	0.45
1:A:255:GLY:H	8:A:1005:GOL:H11	1.80	0.45
1:A:277:TYR:CE2	5:A:996:EPE:H61	2.52	0.44
1:B:194:THR:O	1:B:197:VAL:HG12	2.18	0.44
1:B:242:ASP:O	1:B:242:ASP:OD2	2.36	0.43
1:A:288:LYS:NZ	3:A:991:PGE:H62	2.33	0.43
1:A:392:GLU:CG	1:A:393:VAL:N	2.82	0.43
1:A:288:LYS:NZ	3:A:991:PGE:H22	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLN:HA	1:A:377:PRO:HG3	2.01	0.42
1:A:259:TRP:HH2	1:A:351:GLY:HA3	1.84	0.42
1:A:288:LYS:HZ3	3:A:991:PGE:H22	1.84	0.42
1:B:242:ASP:OD2	1:B:242:ASP:C	2.63	0.42
1:A:312:LEU:HD12	1:A:341:PHE:CB	2.50	0.42
1:A:353:THR:HG23	8:A:1005:GOL:C1	2.48	0.42
1:B:308:ILE:HD12	1:B:337:ARG:HD3	2.02	0.41
1:A:476:ALA:HA	1:A:504:TYR:CD2	2.56	0.41
1:A:219:MET:O	1:A:415:TYR:HA	2.21	0.40
1:B:89:ASP:CG	1:B:137:LYS:HD3	2.46	0.40
1:B:138:MET:HE2	1:B:164:LYS:HB3	2.04	0.40
1:B:287:GLU:HB3	3:B:992:PGE:H2	2.03	0.40
1:A:392:GLU:CG	1:A:393:VAL:H	2.34	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	530/580 (91%)	522 (98%)	6 (1%)	2 (0%)	30	28
1	B	537/580 (93%)	524 (98%)	9 (2%)	4 (1%)	18	15
All	All	1067/1160 (92%)	1046 (98%)	15 (1%)	6 (1%)	21	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	ASP
1	B	316	ASN
1	A	262	LEU
1	B	262	LEU
1	A	356	VAL

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Mol	Chain	Res	Type
1	B	356	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/503 (87%)	433 (99%)	5 (1%)	65	74
1	B	444/503 (88%)	440 (99%)	4 (1%)	70	78
All	All	882/1006 (88%)	873 (99%)	9 (1%)	68	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	15	GLU
1	A	125	ARG
1	A	182	GLU
1	A	200	LYS
1	B	56	ASP
1	B	125	ARG
1	B	133	LYS
1	B	318	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	ASN
1	B	336	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	1PE	A	995	-	15,15,15	0.53	0	14,14,14	0.20	0
8	GOL	B	1004	-	5,5,5	0.44	0	5,5,5	0.39	0
8	GOL	B	1002	-	5,5,5	0.33	0	5,5,5	0.42	0
3	PGE	A	991	-	9,9,9	0.56	0	8,8,8	0.24	0
7	NO3	A	1001	-	1,3,3	3.10	1 (100%)	0,3,3	-	-
8	GOL	A	1003	-	5,5,5	0.36	0	5,5,5	0.29	0
8	GOL	A	1002	-	5,5,5	0.40	0	5,5,5	0.70	0
4	1PE	A	994	-	15,15,15	0.51	0	14,14,14	0.37	0
8	GOL	B	1003	-	5,5,5	0.33	0	5,5,5	0.48	0
7	NO3	B	1001	-	1,3,3	3.17	1 (100%)	0,3,3	-	-
5	EPE	B	998	-	15,15,15	0.92	1 (6%)	19,20,20	1.82	5 (26%)
2	FOR	B	999	-	0,1,1	-	-	-	-	-
5	EPE	A	996	-	15,15,15	1.06	1 (6%)	19,20,20	1.78	4 (21%)
8	GOL	A	1004	-	5,5,5	0.28	0	5,5,5	0.74	0
3	PGE	B	992	-	9,9,9	0.46	0	8,8,8	0.19	0
2	FOR	A	999	-	0,1,1	-	-	-	-	-
3	PGE	B	993	-	9,9,9	0.58	0	8,8,8	0.36	0
8	GOL	A	1005	-	5,5,5	0.53	0	5,5,5	0.66	0
5	EPE	A	997	-	15,15,15	0.87	1 (6%)	19,20,20	1.71	3 (15%)

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	1PE	A	995	-	-	10/13/13/13	-
5	EPE	B	998	-	-	1/9/19/19	0/1/1/1
8	GOL	A	1003	-	-	0/4/4/4	-
3	PGE	B	992	-	-	2/7/7/7	-
8	GOL	B	1004	-	-	2/4/4/4	-
8	GOL	B	1002	-	-	0/4/4/4	-
8	GOL	A	1002	-	-	2/4/4/4	-
3	PGE	A	991	-	-	6/7/7/7	-
4	1PE	A	994	-	-	10/13/13/13	-
5	EPE	A	996	-	-	1/9/19/19	0/1/1/1
8	GOL	B	1003	-	-	2/4/4/4	-
3	PGE	B	993	-	-	4/7/7/7	-
8	GOL	A	1005	-	-	2/4/4/4	-
8	GOL	A	1004	-	-	3/4/4/4	-
5	EPE	A	997	-	-	6/9/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	996	EPE	C10-S	3.64	1.82	1.77
7	B	1001	NO3	O1-N	3.17	1.39	1.24
5	B	998	EPE	C10-S	3.13	1.82	1.77
7	A	1001	NO3	O1-N	3.10	1.39	1.24
5	A	997	EPE	C10-S	2.97	1.81	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	998	EPE	C5-N4-C3	5.08	119.78	108.84
5	A	996	EPE	C5-N4-C3	4.63	118.82	108.84
5	A	997	EPE	C5-N4-C3	4.13	117.75	108.84
5	A	996	EPE	O1S-S-C10	3.75	112.40	106.73
5	A	997	EPE	O3S-S-C10	3.50	112.85	106.00
5	A	997	EPE	C7-N4-C5	3.06	119.40	111.24
5	B	998	EPE	O1S-S-C10	2.82	110.99	106.73
5	A	996	EPE	C7-N4-C5	2.58	118.11	111.24
5	A	996	EPE	C7-N4-C3	2.39	117.62	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	998	EPE	C7-N4-C3	2.24	117.21	111.24
5	B	998	EPE	C7-N4-C5	2.14	116.95	111.24
5	B	998	EPE	C2-C3-N4	2.03	114.74	110.65

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	997	EPE	C9-C10-S-O1S
5	A	997	EPE	C9-C10-S-O3S
8	A	1002	GOL	O1-C1-C2-C3
8	A	1004	GOL	O1-C1-C2-C3
8	A	1005	GOL	C1-C2-C3-O3
8	A	1005	GOL	O2-C2-C3-O3
8	B	1004	GOL	C1-C2-C3-O3
8	B	1004	GOL	O2-C2-C3-O3
3	A	991	PGE	O2-C3-C4-O3
4	A	994	1PE	OH4-C13-C23-OH3
4	A	995	1PE	OH4-C13-C23-OH3
3	B	993	PGE	O2-C3-C4-O3
4	A	995	1PE	OH6-C15-C25-OH5
3	A	991	PGE	O3-C5-C6-O4
3	B	993	PGE	O1-C1-C2-O2
3	A	991	PGE	O1-C1-C2-O2
4	A	995	1PE	OH2-C12-C22-OH3
8	A	1002	GOL	O1-C1-C2-O2
8	A	1004	GOL	O1-C1-C2-O2
4	A	995	1PE	OH5-C14-C24-OH4
4	A	994	1PE	OH7-C16-C26-OH6
5	A	997	EPE	C10-C9-N1-C2
5	A	997	EPE	C10-C9-N1-C6
4	A	994	1PE	OH2-C12-C22-OH3
8	A	1004	GOL	O2-C2-C3-O3
5	B	998	EPE	C8-C7-N4-C3
4	A	994	1PE	C24-C14-OH5-C25
8	B	1003	GOL	O1-C1-C2-O2
5	A	997	EPE	C9-C10-S-O2S
8	B	1003	GOL	O1-C1-C2-C3
4	A	994	1PE	C12-C22-OH3-C23
3	A	991	PGE	C4-C3-O2-C2
4	A	994	1PE	C25-C15-OH6-C26
3	B	993	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	A	995	1PE	C13-C23-OH3-C22
4	A	995	1PE	C24-C14-OH5-C25
4	A	995	1PE	C12-C22-OH3-C23
5	A	996	EPE	C8-C7-N4-C3
4	A	995	1PE	OH7-C16-C26-OH6
4	A	994	1PE	OH5-C14-C24-OH4
4	A	995	1PE	C15-C25-OH5-C14
4	A	994	1PE	C23-C13-OH4-C24
3	B	992	PGE	O3-C5-C6-O4
3	B	992	PGE	C3-C4-O3-C5
3	B	993	PGE	C3-C4-O3-C5
3	A	991	PGE	C1-C2-O2-C3
3	A	991	PGE	C3-C4-O3-C5
4	A	995	1PE	C25-C15-OH6-C26
4	A	994	1PE	C16-C26-OH6-C15
5	A	997	EPE	N4-C7-C8-O8
4	A	994	1PE	OH6-C15-C25-OH5

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	991	PGE	5	0
8	A	1003	GOL	1	0
8	A	1002	GOL	1	0
4	A	994	1PE	2	0
8	B	1003	GOL	1	0
5	B	998	EPE	1	0
2	B	999	FOR	4	0
5	A	996	EPE	2	0
8	A	1004	GOL	1	0
3	B	992	PGE	1	0
3	B	993	PGE	1	0
8	A	1005	GOL	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	531/580 (91%)	0.22	43 (8%)	18 19	15, 27, 38, 44	3 (0%)
1	B	537/580 (92%)	-0.03	17 (3%)	50 53	13, 25, 38, 49	2 (0%)
All	All	1068/1160 (92%)	0.09	60 (5%)	30 32	13, 26, 38, 49	5 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	316	ASN	4.9
1	B	315	TYR	4.6
1	A	318	SER	4.3
1	B	314	HIS	3.9
1	A	459	GLY	3.6
1	A	504	TYR	3.5
1	B	312	LEU	3.5
1	A	503	ASP	3.5
1	A	196	GLU	3.5
1	A	501	THR	3.3
1	B	313	SER	3.3
1	A	486	PRO	3.3
1	A	460	TYR	3.3
1	A	454	ILE	3.2
1	A	456	LYS	3.1
1	A	491	GLY	3.1
1	A	485	VAL	3.1
1	A	461	LYS	3.1
1	A	455	ILE	3.0
1	A	493	VAL	3.0
1	A	462	VAL	2.9
1	B	243	ASP	2.9
1	A	488	PRO	2.9
1	A	525	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	172	VAL	2.9
1	A	457	THR	2.9
1	B	489	VAL	2.8
1	A	489	VAL	2.8
1	B	503	ASP	2.8
1	A	500	LEU	2.7
1	A	458	SER	2.6
1	B	459	GLY	2.6
1	A	58	TYR	2.6
1	A	524	PRO	2.6
1	B	317	PHE	2.5
1	B	472	ILE	2.5
1	A	492	GLN	2.5
1	A	478	LEU	2.5
1	A	15	GLU	2.4
1	A	171	ASP	2.4
1	A	506	PRO	2.4
1	A	477	VAL	2.3
1	A	453	ASP	2.3
1	A	502	LYS	2.3
1	B	476	ALA	2.3
1	A	535	PRO	2.2
1	B	195	GLY	2.2
1	A	316	ASN	2.2
1	A	508	ASP	2.2
1	A	487	ASP	2.2
1	A	339	LEU	2.2
1	A	526	LYS	2.2
1	B	539	LYS	2.2
1	B	538	PRO	2.1
1	A	472	ILE	2.1
1	B	171	ASP	2.1
1	B	525	TYR	2.1
1	A	509	SER	2.1
1	A	475	PRO	2.0
1	A	214	ALA	2.0

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

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

6.3 Carbohydrates [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
6	MG	B	1000	1/1	0.72	0.12	58,58,58,58	0
3	PGE	A	991	10/10	0.76	0.19	51,55,58,58	0
4	1PE	A	995	16/16	0.80	0.17	56,57,59,59	0
3	PGE	B	993	10/10	0.80	0.17	40,43,45,46	0
8	GOL	A	1005	6/6	0.82	0.24	42,44,46,46	0
8	GOL	A	1002	6/6	0.84	0.17	39,41,41,41	0
8	GOL	B	1004	6/6	0.84	0.17	41,43,44,45	0
4	1PE	A	994	16/16	0.85	0.15	45,48,55,55	0
8	GOL	A	1003	6/6	0.88	0.13	46,47,48,49	0
5	EPE	A	997	15/15	0.90	0.14	42,44,49,52	0
3	PGE	B	992	10/10	0.90	0.11	49,50,51,51	0
8	GOL	B	1003	6/6	0.90	0.14	33,37,38,40	0
5	EPE	A	996	15/15	0.90	0.15	31,40,44,44	0
8	GOL	A	1004	6/6	0.91	0.12	25,27,27,28	0
5	EPE	B	998	15/15	0.93	0.13	34,43,47,47	0
7	NO3	B	1001	4/4	0.93	0.16	37,37,37,38	0
7	NO3	A	1001	4/4	0.94	0.14	37,37,38,38	0
2	FOR	A	999	2/2	0.94	0.10	19,19,19,20	0
2	FOR	B	999	2/2	0.95	0.10	20,20,20,21	0
6	MG	A	1000	1/1	0.97	0.07	47,47,47,47	0
8	GOL	B	1002	6/6	0.97	0.11	24,26,27,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.