



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 08:56 PM EST

PDB ID : 3WBF
Title : Crystal Structure of meso-diaminopimelate dehydrogenase from *Symbiobacterium thermophilum* co-crystallized with NADP⁺ and DAP
Authors : Liu, W.D.; Li, Z.; Huang, C.H.; Guo, R.T.; Wu, Q.Q.; Zhu, D.M.
Deposited on : unknown
Resolution : 2.12 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

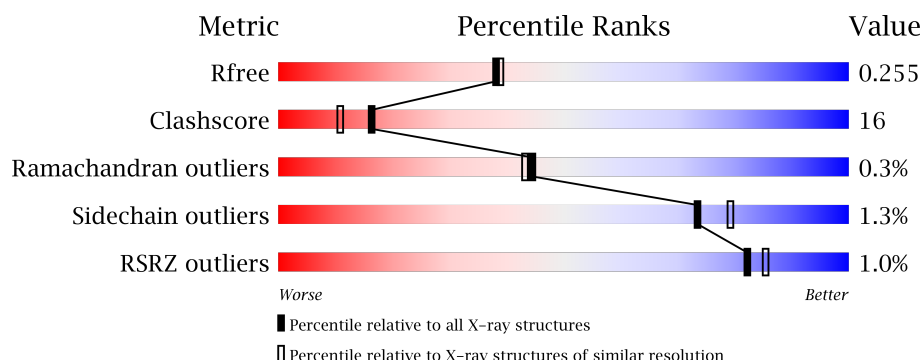
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 2.12 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}	100719	4988 (2.14-2.10)
Clashscore	112137	5557 (2.14-2.10)
Ramachandran outliers	110173	5504 (2.14-2.10)
Sidechain outliers	110143	5505 (2.14-2.10)
RSRZ outliers	101464	5021 (2.14-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	305	 77% 20% 2% 1%
1	B	305	 70% 26% 2% 1%
1	C	305	 71% 25% 2% 1%

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	API	A	301	-	-	-	X
2	API	B	301	-	-	-	X
2	API	C	301	-	-	-	X
3	GOL	A	303	-	-	-	X
3	GOL	A	305	-	-	-	X
3	GOL	B	302	-	-	-	X
3	GOL	B	303	-	-	X	X
3	GOL	B	304	-	-	-	X
3	GOL	B	305	-	-	X	-
3	GOL	C	303	-	-	-	X
3	GOL	C	304	-	-	-	X
3	GOL	C	306	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8462 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.

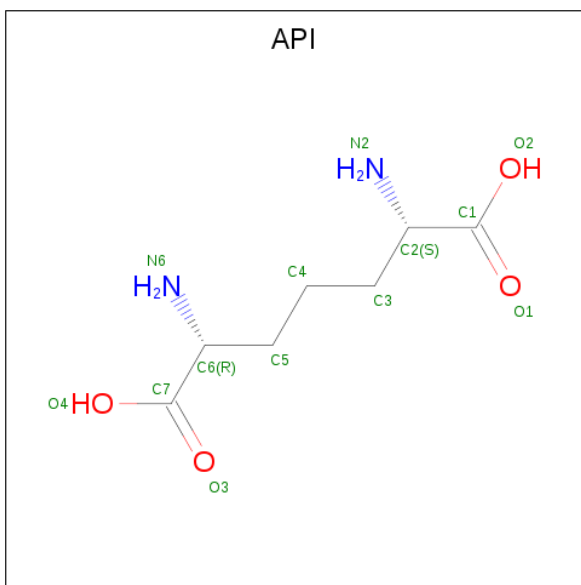
- Molecule 1 is a protein called Diaminopimelate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2259	1423	409	413	14			
1	B	297	Total	C	N	O	S	0	0	0
			2259	1423	409	413	14			
1	C	297	Total	C	N	O	S	0	0	0
			2259	1423	409	413	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q67PI3
A	-4	HIS	-	EXPRESSION TAG	UNP Q67PI3
A	-3	HIS	-	EXPRESSION TAG	UNP Q67PI3
A	-2	HIS	-	EXPRESSION TAG	UNP Q67PI3
A	-1	HIS	-	EXPRESSION TAG	UNP Q67PI3
A	0	HIS	-	EXPRESSION TAG	UNP Q67PI3
B	-5	HIS	-	EXPRESSION TAG	UNP Q67PI3
B	-4	HIS	-	EXPRESSION TAG	UNP Q67PI3
B	-3	HIS	-	EXPRESSION TAG	UNP Q67PI3
B	-2	HIS	-	EXPRESSION TAG	UNP Q67PI3
B	-1	HIS	-	EXPRESSION TAG	UNP Q67PI3
B	0	HIS	-	EXPRESSION TAG	UNP Q67PI3
C	-5	HIS	-	EXPRESSION TAG	UNP Q67PI3
C	-4	HIS	-	EXPRESSION TAG	UNP Q67PI3
C	-3	HIS	-	EXPRESSION TAG	UNP Q67PI3
C	-2	HIS	-	EXPRESSION TAG	UNP Q67PI3
C	-1	HIS	-	EXPRESSION TAG	UNP Q67PI3
C	0	HIS	-	EXPRESSION TAG	UNP Q67PI3

- Molecule 2 is 2,6-DIAMINOPIMELIC ACID (three-letter code: API) (formula: $C_7H_{14}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	7	2	4		
2	B	1	Total	C	N	O	0	0
			13	7	2	4		
2	C	1	Total	C	N	O	0	0
			13	7	2	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



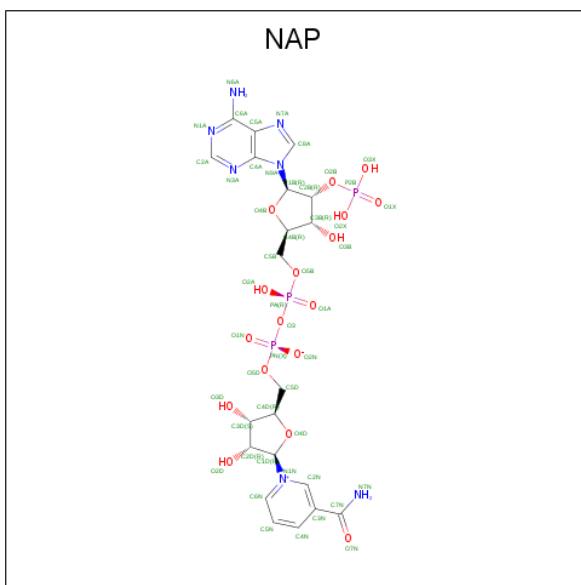
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	C	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	494	Total O 494 494	0	0
5	B	451	Total O 451 451	0	0
5	C	461	Total O 461 461	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	172.35Å 99.69Å 67.17Å 90.00° 108.52° 90.00°	Depositor
Resolution (Å)	30.00 – 2.12 25.09 – 2.11	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-2.12) 93.5 (25.09-2.11)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.49 (at 2.11Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.255 0.198 , 0.255	Depositor DCC
R_{free} test set	2910 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	1.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8462	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.51% 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, NAP, API

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	0.32	0/2301	0.64	0/3123
1	B	0.32	0/2301	0.65	0/3123
1	C	0.31	0/2301	0.65	1/3123 (0.0%)
All	All	0.32	0/6903	0.65	1/9369 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	250	ARG	N-CA-C	-5.06	97.33	111.00

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	2259	0	2298	58	0
1	B	2259	0	2298	97	0
1	C	2259	0	2298	82	0
2	A	13	0	12	2	0
2	B	13	0	12	2	0
2	C	13	0	12	2	0
3	A	36	0	48	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	32	19	0
3	C	36	0	48	8	0
4	A	48	0	25	3	0
4	B	48	0	25	4	0
4	C	48	0	25	3	0
5	A	494	0	0	15	0
5	B	451	0	0	12	0
5	C	461	0	0	12	0
All	All	8462	0	7133	227	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 16.

All (227) 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:259:GLN:HE22	3:B:303:GOL:H31	1.10	1.13
1:B:259:GLN:HE22	3:B:303:GOL:C3	1.67	1.06
1:B:299:VAL:HG21	1:C:97:LEU:HD11	1.37	1.04
1:A:172:ILE:HD12	1:B:176:MET:HE2	1.44	0.98
1:B:146:PHE:H	1:B:179:HIS:HE1	1.14	0.96
1:C:59:GLU:HG2	1:C:60:GLY:H	1.30	0.95
1:B:295:ILE:O	1:B:299:VAL:HG22	1.68	0.93
1:C:266:ARG:HG3	3:C:306:GOL:H31	1.49	0.92
1:B:238:GLY:H	1:C:259:GLN:HE21	1.17	0.92
1:B:146:PHE:H	1:B:179:HIS:CE1	1.88	0.89
1:B:259:GLN:NE2	3:B:303:GOL:H31	1.88	0.89
1:B:5:ARG:HD2	1:B:59:GLU:OE2	1.73	0.88
1:A:246:ARG:NH2	3:A:307:GOL:H12	1.92	0.84
1:B:299:VAL:CG2	1:C:97:LEU:HD11	2.08	0.82
1:B:122:ASP:H	4:B:306:NAP:H72N	1.26	0.81
1:B:259:GLN:HE21	1:C:238:GLY:H	1.27	0.81
1:C:5:ARG:HD3	1:C:59:GLU:OE2	1.80	0.81
1:B:102:ARG:HD3	5:B:542:HOH:O	1.82	0.80
1:B:270:ARG:HH21	3:B:305:GOL:H32	1.45	0.80
1:C:59:GLU:HG2	1:C:60:GLY:N	1.96	0.79
1:C:270:ARG:NH2	3:C:306:GOL:H12	2.01	0.76
1:B:259:GLN:NE2	1:C:238:GLY:H	1.83	0.75
1:C:56:SER:HB3	1:C:83:ARG:HH12	1.52	0.75
1:B:134:GLU:HG3	1:C:298:LEU:HD21	1.69	0.74
1:B:198:ARG:HD3	1:B:199:ALA:N	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HD3	3:A:302:GOL:O3	1.89	0.73
1:A:5:ARG:HG2	1:A:59:GLU:OE1	1.89	0.72
1:B:156:VAL:HA	1:B:159:LYS:HE3	1.71	0.72
1:B:31:VAL:HG11	1:B:59:GLU:HB2	1.70	0.72
1:C:122:ASP:H	4:C:308:NAP:H72N	1.38	0.72
1:A:122:ASP:H	4:A:308:NAP:H72N	1.38	0.71
1:C:106:PRO:O	1:C:110:GLU:HG3	1.90	0.71
1:B:3:LYS:HG3	5:B:646:HOH:O	1.91	0.71
1:C:59:GLU:CG	1:C:60:GLY:H	1.97	0.71
3:B:303:GOL:H12	1:C:138:PRO:HD2	1.72	0.70
1:C:56:SER:HB3	1:C:83:ARG:NH1	2.05	0.70
1:C:146:PHE:CD2	2:C:301:API:H2	2.26	0.70
2:A:301:API:H6	4:A:308:NAP:C4N	2.22	0.69
4:C:308:NAP:H3B	4:C:308:NAP:H8A	1.75	0.69
1:A:172:ILE:CD1	1:B:176:MET:HE2	2.22	0.68
1:C:130:ARG:HG3	1:C:231:MET:CE	2.24	0.68
1:B:238:GLY:N	1:C:259:GLN:HE21	1.91	0.67
1:B:145:ASN:ND2	1:B:177:GLY:H	1.94	0.66
1:B:259:GLN:NE2	3:B:303:GOL:C3	2.49	0.66
1:B:146:PHE:CD2	2:B:301:API:H2	2.32	0.65
1:B:270:ARG:NH2	3:B:305:GOL:H32	2.11	0.65
1:B:146:PHE:N	1:B:179:HIS:HE1	1.91	0.65
1:A:11:TYR:OH	1:A:45:GLU:HG3	1.97	0.65
1:C:266:ARG:CG	3:C:306:GOL:H31	2.26	0.64
1:C:130:ARG:HG3	1:C:231:MET:HE1	1.79	0.64
1:C:170:MET:HE1	5:C:427:HOH:O	1.97	0.64
1:A:120:GLY:O	1:A:124:GLY:HA3	1.98	0.63
1:C:75:GLU:HG2	5:C:822:HOH:O	1.99	0.63
1:B:186:GLU:HB2	1:B:219:VAL:HG23	1.79	0.63
4:B:306:NAP:H3B	4:B:306:NAP:H8A	1.80	0.62
3:B:303:GOL:H11	1:C:238:GLY:N	2.14	0.62
1:C:253:ASN:HB3	1:C:254:PRO:CD	2.29	0.62
2:B:301:API:H6	4:B:306:NAP:C4N	2.29	0.62
1:B:3:LYS:HD3	5:B:633:HOH:O	1.98	0.62
3:B:303:GOL:H11	1:C:238:GLY:H	1.63	0.62
1:B:270:ARG:HE	3:B:305:GOL:H32	1.65	0.62
1:B:145:ASN:HD21	1:B:177:GLY:H	1.48	0.62
1:A:101:ARG:HD3	5:A:789:HOH:O	2.01	0.61
3:B:303:GOL:H32	1:C:138:PRO:HG2	1.82	0.61
1:B:165:ARG:HH21	1:B:189:PRO:HD3	1.66	0.61
1:B:238:GLY:H	1:C:259:GLN:NE2	1.96	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:GLY:O	1:C:124:GLY:HA3	2.01	0.61
3:C:307:GOL:H12	5:C:529:HOH:O	2.00	0.61
1:C:37:LYS:HE3	5:C:787:HOH:O	2.01	0.60
1:B:198:ARG:C	1:B:198:ARG:HD3	2.21	0.60
1:A:18:ALA:HA	1:A:258:ALA:HB1	1.83	0.59
2:A:301:API:H6	4:A:308:NAP:C3N	2.33	0.58
1:B:203:ASP:O	1:B:207:VAL:HG13	2.03	0.58
1:A:59:GLU:CG	1:A:60:GLY:H	2.16	0.57
1:C:18:ALA:O	1:C:22:VAL:HG23	2.05	0.57
1:B:270:ARG:HE	3:B:305:GOL:C3	2.18	0.57
1:B:203:ASP:OD2	1:B:205:TYR:HB2	2.05	0.56
1:C:246:ARG:HD3	5:C:435:HOH:O	2.04	0.56
1:B:13:ASN:HD22	1:B:16:ARG:HH21	1.52	0.56
1:C:18:ALA:HA	1:C:258:ALA:HB1	1.88	0.56
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.71	0.56
1:A:253:ASN:HB3	1:A:254:PRO:CD	2.35	0.56
2:C:301:API:H6	4:C:308:NAP:C4N	2.35	0.56
1:A:106:PRO:O	1:A:110:GLU:HG3	2.06	0.56
1:B:253:ASN:HB3	1:B:254:PRO:CD	2.36	0.55
1:B:6:VAL:HG11	1:B:65:LEU:HD11	1.88	0.55
1:A:39:LEU:HD12	5:A:758:HOH:O	2.06	0.55
1:B:109:ARG:HD3	5:B:647:HOH:O	2.06	0.55
1:C:52:VAL:HB	5:C:463:HOH:O	2.06	0.55
1:A:37:LYS:HD3	5:A:660:HOH:O	2.07	0.55
1:B:299:VAL:HG23	1:B:299:VAL:OXT	2.06	0.55
1:B:24:ALA:HB3	3:B:303:GOL:H2	1.89	0.54
1:C:186:GLU:HB2	1:C:219:VAL:HG23	1.88	0.54
1:B:43:PRO:HB3	5:B:554:HOH:O	2.07	0.54
1:A:74:PRO:O	1:A:78:GLU:HG3	2.09	0.52
1:C:180:LYS:HE3	1:C:210:GLU:OE1	2.09	0.52
1:C:252:ASN:HB3	1:C:255:ALA:HB3	1.91	0.52
1:A:16:ARG:HG3	5:A:485:HOH:O	2.08	0.52
1:C:203:ASP:OD2	1:C:205:TYR:HB2	2.09	0.52
1:C:296:ARG:HD2	5:C:434:HOH:O	2.09	0.52
1:B:279:ILE:HD11	1:C:295:ILE:HD13	1.91	0.52
1:A:26:PRO:HA	5:A:803:HOH:O	2.09	0.52
1:C:74:PRO:HG2	5:C:841:HOH:O	2.10	0.52
1:B:292:GLU:CD	1:C:102:ARG:HH21	2.13	0.52
1:B:120:GLY:O	1:B:124:GLY:HA3	2.10	0.51
1:A:70:THR:HG23	1:A:91:TYR:CD1	2.45	0.51
1:A:176:MET:HG2	5:A:846:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:HG2	1:A:60:GLY:N	2.26	0.51
1:B:24:ALA:CB	3:B:303:GOL:H2	2.41	0.51
1:A:16:ARG:NH1	1:A:16:ARG:HG2	2.27	0.50
1:C:31:VAL:HG11	1:C:59:GLU:HB3	1.93	0.50
1:C:130:ARG:HH11	1:C:231:MET:HE3	1.77	0.49
1:A:59:GLU:CG	1:A:60:GLY:N	2.75	0.49
1:A:80:MET:HB2	1:A:87:THR:HG21	1.94	0.49
1:B:65:LEU:HD12	1:B:65:LEU:N	2.27	0.49
1:C:248:GLU:CD	3:C:303:GOL:H11	2.32	0.49
1:B:150:MET:HG2	1:B:152:MET:HE2	1.93	0.49
1:A:88:VAL:HG21	1:A:265:LEU:CA	2.43	0.49
1:B:88:VAL:HG21	1:B:265:LEU:CA	2.42	0.49
1:C:231:MET:SD	5:C:632:HOH:O	2.60	0.49
1:C:229:VAL:O	1:C:248:GLU:HA	2.13	0.49
1:A:52:VAL:HB	5:A:505:HOH:O	2.13	0.48
1:C:250:ARG:NH2	3:C:304:GOL:H31	2.27	0.48
1:C:130:ARG:NH1	1:C:231:MET:HE3	2.29	0.48
1:C:248:GLU:OE1	3:C:303:GOL:H11	2.14	0.48
1:A:212:ARG:HD3	5:A:695:HOH:O	2.14	0.48
1:A:41:ALA:N	5:A:755:HOH:O	2.45	0.48
1:B:3:LYS:N	5:B:641:HOH:O	2.46	0.48
1:B:80:MET:HB2	1:B:87:THR:HG21	1.96	0.48
1:C:253:ASN:HB3	1:C:254:PRO:HD3	1.95	0.48
1:B:270:ARG:NE	3:B:305:GOL:H32	2.27	0.48
1:C:55:ILE:HD11	1:C:61:VAL:HG11	1.96	0.48
1:B:18:ALA:HA	1:B:258:ALA:HB1	1.95	0.48
1:B:283:VAL:HG21	1:C:132:LEU:HD12	1.95	0.47
1:B:287:LEU:HD23	5:B:628:HOH:O	2.14	0.47
1:C:130:ARG:HG3	1:C:231:MET:HE2	1.96	0.47
1:C:168:LEU:HD21	1:C:170:MET:CE	2.45	0.47
1:B:292:GLU:HB3	5:B:843:HOH:O	2.14	0.47
1:A:19:LEU:HD23	1:A:19:LEU:C	2.34	0.47
1:B:134:GLU:HG2	5:B:437:HOH:O	2.13	0.47
1:A:3:LYS:N	5:A:553:HOH:O	2.48	0.47
1:B:88:VAL:HG21	1:B:265:LEU:N	2.29	0.47
1:A:101:ARG:HB2	1:A:117:ILE:HD11	1.96	0.47
1:B:259:GLN:HE21	1:C:238:GLY:N	2.05	0.47
1:B:259:GLN:HE22	3:B:303:GOL:H32	1.72	0.47
1:C:156:VAL:HA	1:C:159:LYS:HE3	1.95	0.47
1:A:65:LEU:HD12	1:A:65:LEU:N	2.30	0.47
1:C:97:LEU:HD12	1:C:97:LEU:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:OG1	1:A:233:ARG:NH1	2.48	0.47
1:C:168:LEU:HD13	1:C:223:MET:HG3	1.97	0.46
1:A:165:ARG:HD3	1:A:188:GLU:OE1	2.15	0.46
1:B:3:LYS:NZ	1:B:3:LYS:HB2	2.30	0.46
1:B:128:ILE:O	1:B:132:LEU:HD13	2.15	0.46
1:B:83:ARG:NH1	3:B:302:GOL:O1	2.47	0.46
1:B:35:ARG:O	1:B:53:THR:HA	2.16	0.46
1:C:6:VAL:HG12	1:C:7:ALA:N	2.31	0.46
1:B:39:LEU:HD12	5:B:687:HOH:O	2.16	0.46
1:B:6:VAL:CG1	1:B:7:ALA:N	2.80	0.45
1:C:198:ARG:HD2	5:C:667:HOH:O	2.14	0.45
1:C:152:MET:O	1:C:156:VAL:HG23	2.16	0.45
1:A:19:LEU:O	1:A:23:GLN:HG3	2.16	0.45
1:C:270:ARG:NE	3:C:306:GOL:H32	2.32	0.45
1:A:88:VAL:HG23	1:A:265:LEU:HD13	1.99	0.44
1:B:299:VAL:HG23	1:C:97:LEU:HD21	1.98	0.44
1:A:253:ASN:HB3	1:A:254:PRO:HD3	1.98	0.44
1:A:97:LEU:HD12	1:A:98:ALA:N	2.33	0.44
1:B:118:SER:HB3	1:B:123:PRO:CG	2.48	0.44
1:B:6:VAL:HG12	1:B:7:ALA:N	2.33	0.44
1:B:59:GLU:HB3	1:B:60:GLY:H	1.16	0.44
1:C:99:ASP:HA	1:C:102:ARG:NH1	2.32	0.44
1:B:276:TYR:CD1	1:B:276:TYR:N	2.86	0.44
1:B:54:ASP:OD2	1:B:56:SER:HB2	2.18	0.44
1:C:283:VAL:HA	1:C:286:TYR:CD2	2.53	0.44
1:A:238:GLY:HA3	5:A:596:HOH:O	2.17	0.43
1:B:152:MET:O	1:B:156:VAL:HG23	2.17	0.43
1:B:16:ARG:NE	5:B:555:HOH:O	2.51	0.43
1:A:16:ARG:HD2	5:A:651:HOH:O	2.17	0.43
1:A:168:LEU:HD13	1:A:223:MET:HG3	1.99	0.43
1:B:6:VAL:CG1	1:B:65:LEU:HD11	2.48	0.43
1:C:56:SER:OG	1:C:57:GLN:NE2	2.51	0.43
1:B:78:GLU:O	1:B:82:ARG:HG3	2.17	0.43
1:A:6:VAL:HG11	1:A:65:LEU:HD11	2.01	0.43
1:C:118:SER:HB3	1:C:123:PRO:CG	2.48	0.43
1:C:16:ARG:NH2	5:C:761:HOH:O	2.51	0.43
1:C:137:ALA:HA	1:C:236:VAL:O	2.19	0.43
1:B:168:LEU:HD13	1:B:223:MET:HG3	2.00	0.42
1:A:75:GLU:HG2	5:A:446:HOH:O	2.18	0.42
1:A:74:PRO:HG2	5:A:559:HOH:O	2.19	0.42
1:C:82:ARG:HA	1:C:111:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLY:O	1:B:16:ARG:HG3	2.19	0.42
1:C:16:ARG:HG3	1:C:17:TYR:N	2.34	0.42
1:B:6:VAL:CG1	1:B:65:LEU:CD1	2.98	0.42
1:A:31:VAL:HG11	1:A:59:GLU:HB3	2.00	0.42
1:B:31:VAL:CG1	1:B:59:GLU:HB2	2.45	0.42
1:A:132:LEU:O	1:A:136:MET:HG3	2.19	0.42
1:C:19:LEU:HD23	1:C:19:LEU:C	2.40	0.42
1:B:19:LEU:HD23	1:B:19:LEU:C	2.39	0.42
1:B:229:VAL:O	1:B:248:GLU:HA	2.19	0.42
1:A:31:VAL:CG1	1:A:59:GLU:HB3	2.50	0.42
1:B:132:LEU:O	1:B:136:MET:HG3	2.20	0.41
1:B:18:ALA:O	1:B:22:VAL:HG23	2.19	0.41
1:B:283:VAL:HG12	5:C:449:HOH:O	2.20	0.41
1:C:143:TYR:O	1:C:231:MET:HA	2.20	0.41
1:C:38:VAL:HG22	1:C:51:VAL:HG12	2.03	0.41
1:A:97:LEU:HD12	1:A:97:LEU:C	2.40	0.41
1:A:129:ILE:HG22	1:A:231:MET:SD	2.59	0.41
1:A:41:ALA:HA	5:A:748:HOH:O	2.20	0.41
1:A:90:SER:O	1:A:91:TYR:C	2.59	0.41
1:A:234:LYS:HG3	1:A:244:LEU:CD2	2.51	0.41
1:C:6:VAL:CG1	1:C:7:ALA:N	2.83	0.41
1:B:259:GLN:NE2	1:C:238:GLY:N	2.60	0.41
1:A:58:LEU:O	1:A:59:GLU:O	2.39	0.41
1:A:83:ARG:HD3	3:A:302:GOL:C3	2.51	0.41
1:B:128:ILE:HG23	1:C:283:VAL:HG11	2.03	0.41
1:B:159:LYS:HB3	5:B:443:HOH:O	2.21	0.41
1:C:45:GLU:OE1	1:C:45:GLU:N	2.33	0.41
1:B:68:VAL:HB	1:B:69:PRO:CD	2.51	0.41
1:A:88:VAL:HG21	1:A:265:LEU:HB2	2.03	0.41
1:B:165:ARG:HD2	1:B:186:GLU:OE2	2.20	0.41
1:B:36:ARG:NH2	4:B:306:NAP:H2B	2.35	0.41
1:C:105:ASP:HB3	1:C:106:PRO:CD	2.51	0.41
1:A:118:SER:HB3	1:A:123:PRO:CG	2.50	0.41
1:B:91:TYR:CE1	1:B:93:ILE:HB	2.56	0.41
1:A:6:VAL:CG1	1:A:65:LEU:CD1	2.99	0.40
1:B:270:ARG:CZ	3:B:305:GOL:H32	2.51	0.40
1:B:85:ILE:HD11	3:B:302:GOL:H31	2.04	0.40
1:C:80:MET:HB2	1:C:87:THR:HG21	2.03	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	295/305 (97%)	282 (96%)	12 (4%)	1 (0%)	44	43
1	B	295/305 (97%)	284 (96%)	10 (3%)	1 (0%)	44	43
1	C	295/305 (97%)	283 (96%)	11 (4%)	1 (0%)	44	43
All	All	885/915 (97%)	849 (96%)	33 (4%)	3 (0%)	44	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	B	59	GLU
1	C	59	GLU

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	235/243 (97%)	233 (99%)	2 (1%)	82	86
1	B	235/243 (97%)	231 (98%)	4 (2%)	66	71
1	C	235/243 (97%)	232 (99%)	3 (1%)	73	79
All	All	705/729 (97%)	696 (99%)	9 (1%)	73	79

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

Mol	Chain	Res	Type
1	A	37	LYS
1	A	227	HIS
1	B	96	ASP
1	B	159	LYS
1	B	198	ARG
1	B	290	ASP
1	C	16	ARG
1	C	227	HIS
1	C	290	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	241	HIS
1	B	13	ASN
1	B	145	ASN
1	B	179	HIS
1	B	259	GLN
1	C	259	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

22 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
2	API	A	301	-	2,12,12	0.29	0	1,15,15	0.44	0
3	GOL	A	302	-	5,5,5	0.25	0	5,5,5	0.24	0
3	GOL	A	303	-	5,5,5	0.25	0	5,5,5	0.27	0
3	GOL	A	304	-	5,5,5	0.26	0	5,5,5	0.24	0
3	GOL	A	305	-	5,5,5	0.26	0	5,5,5	0.14	0
3	GOL	A	306	-	5,5,5	0.26	0	5,5,5	0.24	0
3	GOL	A	307	-	5,5,5	0.26	0	5,5,5	0.25	0
4	NAP	A	308	-	44,52,52	1.71	5 (11%)	51,80,80	2.20	4 (7%)
2	API	B	301	-	2,12,12	0.26	0	1,15,15	0.76	0
3	GOL	B	302	-	5,5,5	0.26	0	5,5,5	0.24	0
3	GOL	B	303	-	5,5,5	0.27	0	5,5,5	0.27	0
3	GOL	B	304	-	5,5,5	0.25	0	5,5,5	0.27	0
3	GOL	B	305	-	5,5,5	0.26	0	5,5,5	0.23	0
4	NAP	B	306	-	44,52,52	1.72	5 (11%)	51,80,80	2.20	3 (5%)
2	API	C	301	-	2,12,12	0.26	0	1,15,15	0.63	0
3	GOL	C	302	-	5,5,5	0.27	0	5,5,5	0.21	0
3	GOL	C	303	-	5,5,5	0.26	0	5,5,5	0.26	0
3	GOL	C	304	-	5,5,5	0.26	0	5,5,5	0.24	0
3	GOL	C	305	-	5,5,5	0.25	0	5,5,5	0.23	0
3	GOL	C	306	-	5,5,5	0.26	0	5,5,5	0.24	0
3	GOL	C	307	-	5,5,5	0.26	0	5,5,5	0.25	0
4	NAP	C	308	-	44,52,52	1.73	5 (11%)	51,80,80	2.18	3 (5%)

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
2	API	A	301	-	-	0/6/14/14	0/0/0/0
3	GOL	A	302	-	-	0/4/4/4	0/0/0/0
3	GOL	A	303	-	-	0/4/4/4	0/0/0/0
3	GOL	A	304	-	-	0/4/4/4	0/0/0/0
3	GOL	A	305	-	-	0/4/4/4	0/0/0/0
3	GOL	A	306	-	-	0/4/4/4	0/0/0/0
3	GOL	A	307	-	-	0/4/4/4	0/0/0/0
4	NAP	A	308	-	-	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	API	B	301	-	-	0/6/14/14	0/0/0/0
3	GOL	B	302	-	-	0/4/4/4	0/0/0/0
3	GOL	B	303	-	-	0/4/4/4	0/0/0/0
3	GOL	B	304	-	-	0/4/4/4	0/0/0/0
3	GOL	B	305	-	-	0/4/4/4	0/0/0/0
4	NAP	B	306	-	-	0/27/67/67	0/5/5/5
2	API	C	301	-	-	0/6/14/14	0/0/0/0
3	GOL	C	302	-	-	0/4/4/4	0/0/0/0
3	GOL	C	303	-	-	0/4/4/4	0/0/0/0
3	GOL	C	304	-	-	0/4/4/4	0/0/0/0
3	GOL	C	305	-	-	0/4/4/4	0/0/0/0
3	GOL	C	306	-	-	0/4/4/4	0/0/0/0
3	GOL	C	307	-	-	0/4/4/4	0/0/0/0
4	NAP	C	308	-	-	0/27/67/67	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	308	NAP	C3N-C7N	-7.05	1.39	1.50
4	B	306	NAP	C3N-C7N	-7.04	1.39	1.50
4	A	308	NAP	C3N-C7N	-6.99	1.39	1.50
4	B	306	NAP	C5A-C4A	-3.10	1.33	1.40
4	A	308	NAP	C5A-C4A	-3.09	1.33	1.40
4	C	308	NAP	C5A-C4A	-3.06	1.33	1.40
4	A	308	NAP	O4B-C1B	2.14	1.44	1.41
4	C	308	NAP	O4B-C1B	2.26	1.44	1.41
4	B	306	NAP	O4B-C1B	2.33	1.44	1.41
4	A	308	NAP	C2A-N1A	3.43	1.40	1.33
4	C	308	NAP	C2A-N1A	3.46	1.40	1.33
4	B	306	NAP	C2A-N1A	3.49	1.40	1.33
4	A	308	NAP	C2A-N3A	4.94	1.40	1.32
4	B	306	NAP	C2A-N3A	4.96	1.40	1.32
4	C	308	NAP	C2A-N3A	5.01	1.40	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	308	NAP	N3A-C2A-N1A	-12.69	117.81	128.86
4	B	306	NAP	N3A-C2A-N1A	-12.66	117.83	128.86
4	A	308	NAP	N3A-C2A-N1A	-12.62	117.86	128.86
4	B	306	NAP	C4D-O4D-C1D	-6.59	102.75	109.77
4	A	308	NAP	C4D-O4D-C1D	-6.15	103.22	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	308	NAP	C4D-O4D-C1D	-6.09	103.28	109.77
4	A	308	NAP	C4B-O4B-C1B	-2.68	106.92	109.77
4	A	308	NAP	C3N-C7N-N7N	-2.38	115.06	117.77
4	C	308	NAP	C3N-C7N-N7N	-2.23	115.22	117.77
4	B	306	NAP	C3N-C7N-N7N	-2.22	115.24	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	API	2	0
3	A	302	GOL	2	0
3	A	307	GOL	1	0
4	A	308	NAP	3	0
2	B	301	API	2	0
3	B	302	GOL	2	0
3	B	303	GOL	11	0
3	B	305	GOL	6	0
4	B	306	NAP	4	0
2	C	301	API	2	0
3	C	303	GOL	2	0
3	C	304	GOL	1	0
3	C	306	GOL	4	0
3	C	307	GOL	1	0
4	C	308	NAP	3	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	297/305 (97%)	-0.14	1 (0%) 93 94	13, 23, 43, 54	1 (0%)
1	B	297/305 (97%)	-0.08	5 (1%) 70 75	15, 24, 45, 56	1 (0%)
1	C	297/305 (97%)	-0.08	3 (1%) 82 85	12, 23, 38, 47	2 (0%)
All	All	891/915 (97%)	-0.10	9 (1%) 82 85	12, 23, 43, 56	4 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	PRO	4.1
1	C	208	ARG	3.4
1	B	59	GLU	2.7
1	B	162	PRO	2.5
1	C	59	GLU	2.4
1	B	195	GLU	2.3
1	B	165	ARG	2.3
1	C	191	ALA	2.2
1	A	119	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	A	305	6/6	0.66	0.23	8.82	41,43,44,45	0
3	GOL	C	306	6/6	0.65	0.29	8.82	32,34,37,37	0
3	GOL	B	303	6/6	0.84	0.22	7.05	24,29,30,31	0
3	GOL	B	302	6/6	0.68	0.25	6.37	53,56,57,59	0
3	GOL	C	303	6/6	0.80	0.19	5.76	43,43,44,44	0
3	GOL	C	304	6/6	0.85	0.22	5.64	51,53,54,54	0
2	API	C	301	13/13	0.87	0.19	4.10	24,28,31,32	0
3	GOL	B	304	6/6	0.82	0.22	3.51	65,65,66,67	0
2	API	B	301	13/13	0.88	0.19	3.47	28,32,33,33	0
2	API	A	301	13/13	0.93	0.16	2.90	29,31,34,34	0
3	GOL	A	303	6/6	0.70	0.20	2.83	53,55,55,57	0
3	GOL	A	304	6/6	0.81	0.20	1.85	56,56,57,57	0
3	GOL	C	305	6/6	0.86	0.14	0.53	36,40,41,41	0
3	GOL	A	302	6/6	0.86	0.16	0.33	55,55,56,58	0
4	NAP	C	308	48/48	0.94	0.12	-0.19	15,21,32,34	0
4	NAP	B	306	48/48	0.95	0.10	-0.71	15,21,33,36	0
4	NAP	A	308	48/48	0.96	0.09	-0.83	15,22,24,25	0
3	GOL	C	302	6/6	0.70	0.25	-	52,53,54,54	0
3	GOL	B	305	6/6	0.72	0.25	-	72,73,74,74	0
3	GOL	A	307	6/6	0.68	0.23	-	59,59,61,62	0
3	GOL	C	307	6/6	0.64	0.25	-	39,46,47,49	0
3	GOL	A	306	6/6	0.84	0.18	-	53,53,54,54	0

6.5 Other polymers

There are no such residues in this entry.