



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 08:32 PM GMT

PDB ID : 2F59
Title : Lumazine synthase RibH1 from Brucella abortus (Gene BruAb1_0785, Swiss-Prot entry Q57DY1) complexed with inhibitor 5-Nitro-6-(D-Ribitylamino)-2,4(1H,3H)Pyrimidinedione
Authors : Klinke, S.; Zylberman, V.; Bonomi, H.R.; Haase, I.; Guimaraes, B.G.; Braden, B.C.; Bacher, A.; Fischer, M.; Goldbaum, F.A.
Deposited on : 2005-11-25
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

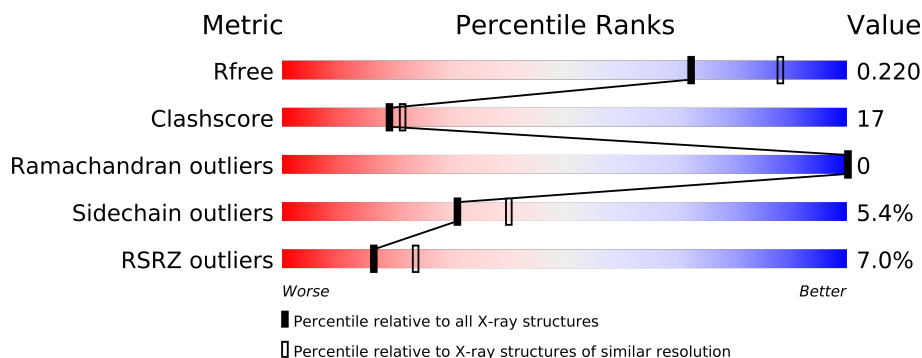
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	157	
1	B	157	
1	C	157	
1	D	157	
1	E	157	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	A	304	-	X
2	CA	C	305	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5793 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

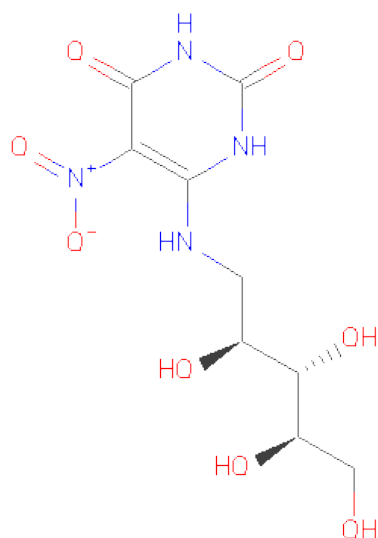
- Molecule 1 is a protein called 6,7-dimethyl-8-ribityllumazinesynthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1091	685	184	220	2			
1	B	146	Total	C	N	O	S	4	0	0
			1091	685	184	220	2			
1	C	146	Total	C	N	O	S	3	0	0
			1091	685	184	220	2			
1	D	147	Total	C	N	O	S	5	0	0
			1099	689	185	223	2			
1	E	146	Total	C	N	O	S	3	0	0
			1091	685	184	220	2			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	2	Total	Ca	0	0
			2	2		
2	D	1	Total	Ca	0	0
			1	1		
2	C	2	Total	Ca	0	0
			2	2		

- Molecule 3 is 5-NITRO-6-RIBITYL-AMINO-2,4(1H,3H)-PYRIMIDINEDIONE (three-letter code: INI) (formula: C₉H₁₄N₄O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	9	4	8		
3	B	1	Total	C	N	O	0	0
			21	9	4	8		
3	C	1	Total	C	N	O	0	0
			21	9	4	8		
3	D	1	Total	C	N	O	0	0
			21	9	4	8		
3	E	1	Total	C	N	O	0	0
			21	9	4	8		

- Molecule 4 is water.

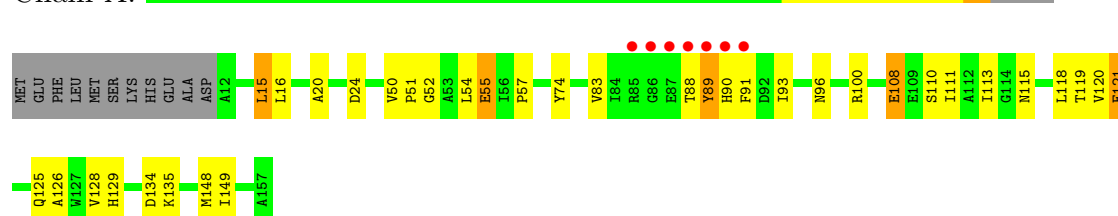
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	42	Total	O	0	0
			42	42		
4	C	43	Total	O	0	0
			43	43		
4	D	43	Total	O	0	0
			43	43		
4	E	38	Total	O	0	0
			38	38		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

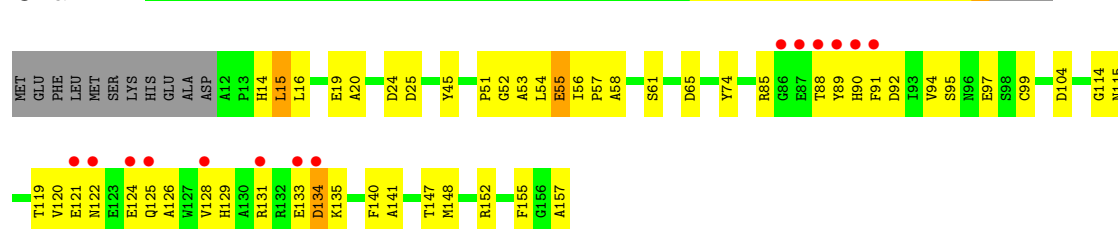
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase 1

Chain A:



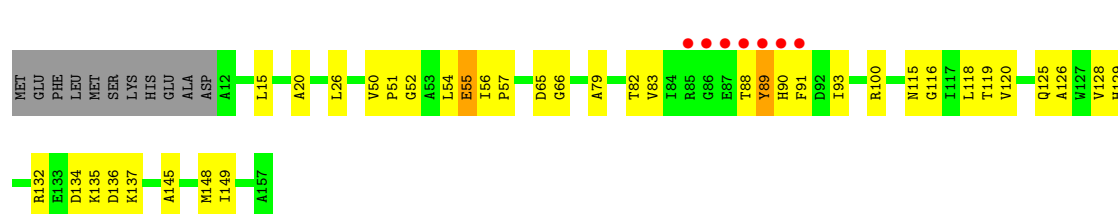
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase 1

Chain B:



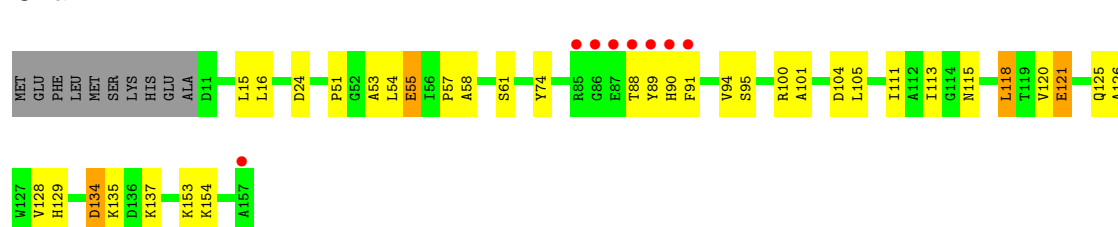
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase 1

Chain C:



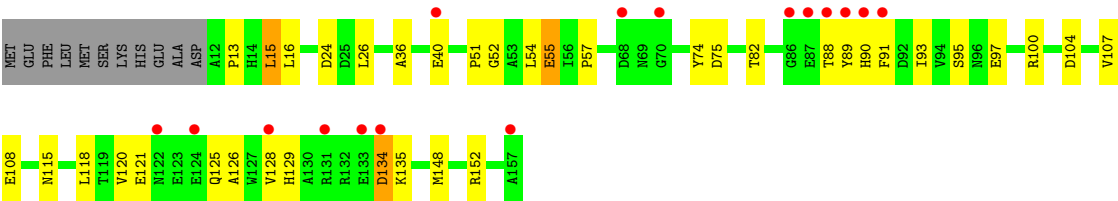
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase 1

Chain D:



● Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase 1

Chain E: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.32Å 95.32Å 171.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.50 – 2.30 33.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (33.50-2.30) 99.5 (33.48-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.241 0.220 , 0.220	Depositor DCC
R_{free} test set	2036 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 27.9	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 40644 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5793	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.35	0/1108	0.60	0/1502
1	B	0.35	0/1108	0.60	0/1502
1	C	0.36	0/1108	0.60	0/1502
1	D	0.35	0/1116	0.59	0/1513
1	E	0.35	0/1108	0.58	0/1502
All	All	0.35	0/5548	0.59	0/7521

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1091	0	1058	38	0
1	B	1091	0	1058	53	0
1	C	1091	0	1058	40	0
1	D	1099	0	1062	41	0
1	E	1091	0	1058	38	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	21	0	14	5	0
3	B	21	0	14	5	0
3	C	21	0	14	5	0
3	D	21	0	14	5	0
3	E	21	0	14	6	0
4	A	53	0	0	2	0
4	B	42	0	0	3	0
4	C	43	0	0	1	0
4	D	43	0	0	3	0
4	E	38	0	0	2	0
All	All	5793	0	5364	180	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (180) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:99:CYS:HB3	4:B:339:HOH:O	1.60	1.01
1:C:88:THR:HG22	1:C:90:HIS:H	1.27	0.99
1:A:120:VAL:HB	1:A:125:GLN:HG3	1.49	0.94
1:C:120:VAL:HB	1:C:125:GLN:HG3	1.47	0.93
1:A:129:HIS:HA	1:A:135:LYS:HB2	1.48	0.93
1:D:129:HIS:HA	1:D:135:LYS:HB2	1.52	0.92
1:D:88:THR:HG22	1:D:90:HIS:H	1.35	0.91
1:B:88:THR:HG22	1:B:90:HIS:H	1.38	0.89
1:D:120:VAL:HB	1:D:125:GLN:HG3	1.53	0.88
1:B:131:ARG:HH12	1:B:133:GLU:HB2	1.37	0.88
1:C:119:THR:O	1:D:88:THR:HG23	1.80	0.80
1:B:129:HIS:HA	1:B:135:LYS:HB2	1.65	0.79
1:D:88:THR:HB	1:D:91:PHE:CE1	2.19	0.78
1:A:88:THR:HG23	1:E:120:VAL:HA	1.67	0.77
1:B:88:THR:HB	1:B:91:PHE:CE1	2.22	0.74
1:D:128:VAL:O	1:D:134:ASP:HB3	1.89	0.72
1:C:118:LEU:HD11	1:C:129:HIS:HB3	1.73	0.70
1:B:128:VAL:O	1:B:134:ASP:HB3	1.90	0.70
1:B:131:ARG:NH1	1:B:133:GLU:HB2	2.06	0.70
1:E:118:LEU:HD21	1:E:129:HIS:HB2	1.73	0.70
1:D:51:PRO:HG2	1:D:55:GLU:OE2	1.92	0.70
1:D:100:ARG:HA	1:E:97:GLU:OE2	1.91	0.69
1:E:88:THR:HG22	1:E:90:HIS:H	1.58	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:100:ARG:HA	1:B:97:GLU:OE2	1.95	0.67
1:D:88:THR:HG22	1:D:90:HIS:N	2.10	0.66
1:D:118:LEU:HD13	1:D:137:LYS:HG2	1.79	0.65
1:E:128:VAL:O	1:E:134:ASP:HB3	1.96	0.65
1:A:51:PRO:HG2	1:A:55:GLU:OE2	1.95	0.64
1:C:57:PRO:HG2	4:C:311:HOH:O	1.98	0.64
1:D:137:LYS:HZ1	1:E:90:HIS:CE1	2.16	0.64
1:C:88:THR:HB	1:C:91:PHE:CE1	2.34	0.63
1:D:118:LEU:CD1	1:D:137:LYS:HG2	2.28	0.63
1:A:100:ARG:NH2	1:E:104:ASP:OD1	2.30	0.63
1:C:148:MET:HE2	1:D:55:GLU:HB2	1.81	0.63
1:B:119:THR:O	1:C:88:THR:HG23	1.98	0.63
1:A:88:THR:HB	1:A:91:PHE:CE1	2.34	0.62
1:A:118:LEU:HD21	1:A:129:HIS:HB2	1.80	0.62
1:E:57:PRO:HG2	4:E:217:HOH:O	2.00	0.62
1:D:121:GLU:HB2	1:D:125:GLN:NE2	2.16	0.61
1:D:88:THR:HB	1:D:91:PHE:HE1	1.64	0.61
1:B:120:VAL:HG21	1:B:126:ALA:HB2	1.81	0.61
1:E:120:VAL:HB	1:E:125:GLN:HG3	1.81	0.61
1:E:51:PRO:HG2	1:E:55:GLU:OE2	2.01	0.60
1:E:88:THR:O	1:E:91:PHE:HD1	1.85	0.60
1:D:88:THR:CG2	1:D:90:HIS:H	2.11	0.60
1:A:57:PRO:HG2	4:A:318:HOH:O	2.02	0.59
1:A:88:THR:HG22	1:A:90:HIS:H	1.67	0.59
1:A:88:THR:HB	1:A:91:PHE:HE1	1.68	0.59
1:E:120:VAL:HG21	1:E:126:ALA:HB2	1.87	0.57
1:E:129:HIS:HA	1:E:135:LYS:HB2	1.85	0.57
1:A:54:LEU:HD12	3:A:201:INI:H9	1.86	0.56
1:A:90:HIS:O	1:A:90:HIS:ND1	2.38	0.56
1:B:120:VAL:HB	1:B:125:GLN:HG3	1.88	0.56
1:B:121:GLU:HB3	1:B:125:GLN:NE2	2.21	0.56
1:B:15:LEU:HD23	1:B:15:LEU:N	2.21	0.55
1:C:118:LEU:HD11	1:C:129:HIS:CB	2.35	0.55
1:B:88:THR:HB	1:B:91:PHE:HE1	1.68	0.55
1:D:115:ASN:H	3:E:205:INI:C12	2.19	0.55
1:A:93:ILE:CD1	1:E:95:SER:HB3	2.37	0.54
1:C:120:VAL:HG21	1:C:126:ALA:HB2	1.89	0.54
1:C:129:HIS:HA	1:C:135:LYS:HB2	1.89	0.54
1:C:54:LEU:HD12	3:C:203:INI:H9	1.90	0.53
1:E:26:LEU:HD13	1:E:82:THR:HG21	1.91	0.53
1:C:118:LEU:HD13	1:C:137:LYS:HD2	1.91	0.53
1:D:54:LEU:HD12	3:D:204:INI:H9	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:19:GLU:O	1:B:19:GLU:HG3	2.08	0.52
1:C:128:VAL:O	1:C:134:ASP:HB3	2.10	0.52
1:C:118:LEU:CD1	1:C:137:LYS:HD2	2.39	0.52
1:D:118:LEU:HD21	1:D:129:HIS:HB2	1.91	0.52
1:D:90:HIS:O	1:D:94:VAL:HG23	2.09	0.52
1:D:88:THR:O	1:D:91:PHE:HD1	1.93	0.52
1:B:115:ASN:H	3:C:203:INI:C12	2.22	0.51
1:B:51:PRO:HG2	1:B:55:GLU:OE2	2.11	0.51
1:C:115:ASN:H	3:D:204:INI:C12	2.23	0.51
1:B:94:VAL:HG21	3:B:202:INI:H82	1.93	0.51
1:B:122:ASN:OD1	1:B:124:GLU:HB3	2.11	0.50
1:B:104:ASP:OD2	1:C:100:ARG:NH2	2.44	0.50
1:D:121:GLU:HB2	1:D:125:GLN:HE22	1.77	0.50
1:C:88:THR:HG22	1:C:90:HIS:N	2.11	0.49
1:E:88:THR:HB	1:E:91:PHE:CE1	2.47	0.49
1:A:115:ASN:H	3:B:202:INI:C12	2.26	0.49
1:A:148:MET:CE	1:B:55:GLU:HB2	2.43	0.49
1:E:36:ALA:O	1:E:40:GLU:HG3	2.13	0.49
1:C:79:ALA:O	1:C:116:GLY:N	2.44	0.49
1:A:55:GLU:HB2	1:E:148:MET:HE2	1.94	0.48
1:A:100:ARG:NH2	1:E:104:ASP:CG	2.67	0.48
1:C:20:ALA:HB2	1:C:56:ILE:HD11	1.94	0.48
1:B:134:ASP:HB3	1:B:135:LYS:H	1.45	0.48
1:A:88:THR:HG22	1:A:89:TYR:N	2.29	0.48
3:A:201:INI:H122	1:E:115:ASN:O	2.14	0.48
3:A:201:INI:C12	1:E:115:ASN:H	2.27	0.48
1:B:157:ALA:HB1	1:C:65:ASP:HB2	1.96	0.48
1:B:57:PRO:HG2	4:B:314:HOH:O	2.14	0.48
1:D:120:VAL:HG12	1:E:88:THR:HG23	1.95	0.47
1:A:119:THR:O	1:B:88:THR:HG23	2.14	0.47
1:C:52:GLY:HA3	3:C:203:INI:O10	2.14	0.47
1:E:54:LEU:HD12	3:E:205:INI:H9	1.95	0.47
1:B:53:ALA:HB3	1:B:94:VAL:CG1	2.45	0.47
1:B:52:GLY:HA3	3:B:202:INI:O10	2.14	0.47
1:C:125:GLN:HB3	4:D:325:HOH:O	2.15	0.47
1:B:122:ASN:OD1	1:B:125:GLN:HG2	2.15	0.47
1:A:57:PRO:HB2	1:E:107:VAL:CG2	2.44	0.47
1:B:15:LEU:O	1:B:45:TYR:HA	2.14	0.46
1:D:115:ASN:H	3:E:205:INI:H122	1.80	0.46
1:E:16:LEU:HB2	1:E:74:TYR:CD2	2.51	0.46
1:D:53:ALA:HB3	1:D:94:VAL:CG1	2.46	0.46
1:A:83:VAL:HG11	1:A:91:PHE:O	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:96:ASN:O	1:A:100:ARG:HB2	2.16	0.46
1:D:134:ASP:HB3	1:D:135:LYS:H	1.45	0.46
1:B:140:PHE:HE2	3:C:203:INI:H11	1.80	0.46
1:E:134:ASP:HB3	1:E:135:LYS:H	1.47	0.46
1:A:83:VAL:HA	3:A:201:INI:O4	2.16	0.46
1:B:95:SER:HB3	1:C:93:ILE:CD1	2.46	0.46
1:B:131:ARG:HH22	1:B:133:GLU:HG2	1.80	0.46
1:D:104:ASP:CG	1:E:100:ARG:HH22	2.19	0.46
1:A:108:GLU:HG3	4:A:339:HOH:O	2.16	0.45
1:C:83:VAL:HG11	1:C:91:PHE:O	2.17	0.45
1:B:119:THR:O	1:C:88:THR:CG2	2.65	0.45
1:B:131:ARG:NH1	1:B:131:ARG:HB3	2.31	0.45
1:A:20:ALA:HA	1:A:50:VAL:HG23	1.98	0.45
1:C:118:LEU:HD21	1:C:129:HIS:HB2	1.98	0.45
1:D:95:SER:HB3	1:E:93:ILE:HD11	1.97	0.45
1:B:54:LEU:HD12	3:B:202:INI:H9	1.98	0.45
1:A:110:SER:OG	1:B:65:ASP:OD2	2.30	0.45
1:D:16:LEU:HB2	1:D:74:TYR:CD2	2.52	0.45
1:B:94:VAL:CG2	3:B:202:INI:H82	2.47	0.44
1:B:58:ALA:O	1:B:61:SER:HB3	2.17	0.44
1:A:120:VAL:HG21	1:A:126:ALA:HB2	1.99	0.44
1:D:57:PRO:HG2	4:D:315:HOH:O	2.16	0.44
1:D:115:ASN:N	3:E:205:INI:H122	2.33	0.44
1:B:88:THR:HB	1:B:91:PHE:CD1	2.53	0.44
1:D:111:ILE:HD11	1:D:113:ILE:HD11	1.98	0.44
1:B:140:PHE:CE2	3:C:203:INI:H11	2.53	0.44
1:B:88:THR:O	1:B:91:PHE:HD1	2.01	0.44
1:D:120:VAL:HG21	1:D:126:ALA:HB2	2.00	0.44
1:E:121:GLU:HB3	1:E:125:GLN:NE2	2.33	0.43
1:D:115:ASN:O	3:E:205:INI:H122	2.17	0.43
1:C:20:ALA:HA	1:C:50:VAL:HG23	2.01	0.43
1:C:90:HIS:ND1	1:C:90:HIS:O	2.51	0.43
1:C:26:LEU:HD13	1:C:82:THR:HG21	2.00	0.43
1:A:20:ALA:HB1	1:A:52:GLY:C	2.39	0.43
1:A:57:PRO:HB2	1:E:107:VAL:HG21	2.00	0.43
1:B:155:PHE:O	1:C:66:GLY:HA3	2.19	0.43
1:E:152:ARG:NH1	4:E:243:HOH:O	2.52	0.43
1:E:15:LEU:CD2	1:E:15:LEU:N	2.82	0.43
1:E:52:GLY:HA3	3:E:205:INI:O10	2.18	0.43
1:B:20:ALA:HB2	1:B:56:ILE:HD11	2.00	0.42
1:C:115:ASN:H	3:D:204:INI:H122	1.85	0.42
1:A:16:LEU:HB2	1:A:74:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:114:GLY:HA3	1:B:141:ALA:O	2.19	0.42
1:A:128:VAL:O	1:A:134:ASP:HB3	2.20	0.42
1:E:13:PRO:HA	1:E:75:ASP:OD1	2.18	0.42
1:D:95:SER:HB3	1:E:93:ILE:CD1	2.50	0.42
1:C:145:ALA:O	1:C:149:ILE:HG13	2.20	0.42
1:D:153:LYS:HE3	1:D:153:LYS:HB2	1.88	0.42
1:A:125:GLN:O	1:A:129:HIS:HD2	2.02	0.41
1:A:52:GLY:HA3	3:A:201:INI:O10	2.20	0.41
1:A:121:GLU:HB3	1:A:125:GLN:NE2	2.34	0.41
1:C:132:ARG:HA	1:C:136:ASP:HB2	2.02	0.41
1:A:100:ARG:HA	1:B:97:GLU:CD	2.40	0.41
1:A:15:LEU:CD1	1:A:149:ILE:HD11	2.51	0.41
1:E:88:THR:HB	1:E:91:PHE:HE1	1.84	0.41
1:C:115:ASN:O	3:D:204:INI:H122	2.21	0.41
1:D:101:ALA:O	1:D:105:LEU:HB2	2.20	0.41
1:B:147:THR:HG21	1:C:51:PRO:HD3	2.03	0.41
1:B:25:ASP:HB2	4:B:311:HOH:O	2.19	0.41
1:D:154:LYS:NZ	4:D:347:HOH:O	2.54	0.41
1:C:115:ASN:N	3:D:204:INI:H122	2.36	0.41
1:B:95:SER:HB3	1:C:93:ILE:HD11	2.02	0.41
1:B:14:HIS:C	1:B:15:LEU:HD23	2.40	0.41
1:B:56:ILE:N	1:B:57:PRO:HD2	2.36	0.41
1:B:16:LEU:HB2	1:B:74:TYR:CD2	2.56	0.41
1:E:90:HIS:O	1:E:90:HIS:ND1	2.54	0.41
1:B:85:ARG:NH1	1:C:89:TYR:CE1	2.89	0.41
1:D:58:ALA:O	1:D:61:SER:HB3	2.21	0.41
1:E:88:THR:O	1:E:91:PHE:CD1	2.70	0.40
1:D:100:ARG:NH1	1:D:100:ARG:HG2	2.36	0.40
1:A:111:ILE:HD11	1:A:113:ILE:HD11	2.02	0.40
1:B:148:MET:CE	1:C:55:GLU:HB2	2.52	0.40
1:D:100:ARG:HH11	1:D:100:ARG:HG2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/157 (92%)	139 (96%)	5 (4%)	0	100	100
1	B	144/157 (92%)	142 (99%)	2 (1%)	0	100	100
1	C	144/157 (92%)	142 (99%)	2 (1%)	0	100	100
1	D	145/157 (92%)	142 (98%)	3 (2%)	0	100	100
1	E	144/157 (92%)	141 (98%)	3 (2%)	0	100	100
All	All	721/785 (92%)	706 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	108/118 (92%)	102 (94%)	6 (6%)	30	38
1	B	108/118 (92%)	101 (94%)	7 (6%)	24	30
1	C	108/118 (92%)	105 (97%)	3 (3%)	56	73
1	D	109/118 (92%)	102 (94%)	7 (6%)	25	31
1	E	108/118 (92%)	102 (94%)	6 (6%)	30	38
All	All	541/590 (92%)	512 (95%)	29 (5%)	31	40

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	24	ASP
1	A	55	GLU
1	A	89	TYR
1	A	108	GLU
1	A	121	GLU
1	B	15	LEU
1	B	24	ASP
1	B	55	GLU
1	B	89	TYR
1	B	92	ASP

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Mol	Chain	Res	Type
1	B	134	ASP
1	B	152	ARG
1	C	15	LEU
1	C	55	GLU
1	C	89	TYR
1	D	15	LEU
1	D	24	ASP
1	D	55	GLU
1	D	89	TYR
1	D	118	LEU
1	D	121	GLU
1	D	134	ASP
1	E	15	LEU
1	E	24	ASP
1	E	55	GLU
1	E	89	TYR
1	E	108	GLU
1	E	134	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	129	HIS
1	B	69	ASN
1	B	125	GLN
1	C	69	ASN
1	C	129	HIS
1	D	69	ASN
1	D	125	GLN
1	E	69	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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$
3	INI	A	201	-	21,21,21	3.50	9 (42%)	24,29,29	2.75	11 (45%)
3	INI	B	202	-	21,21,21	3.54	10 (47%)	24,29,29	2.84	10 (41%)
3	INI	C	203	-	21,21,21	3.55	9 (42%)	24,29,29	2.73	11 (45%)
3	INI	D	204	-	21,21,21	3.45	10 (47%)	24,29,29	2.77	11 (45%)
3	INI	E	205	-	21,21,21	3.50	10 (47%)	24,29,29	2.86	10 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	INI	A	201	-	-	1/17/19/19	0/1/1/1
3	INI	B	202	-	-	1/17/19/19	0/1/1/1
3	INI	C	203	-	-	1/17/19/19	0/1/1/1
3	INI	D	204	-	-	1/17/19/19	0/1/1/1
3	INI	E	205	-	-	1/17/19/19	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	205	INI	C11-C10	8.55	1.71	1.53
3	B	202	INI	C11-C10	8.43	1.71	1.53
3	C	203	INI	C11-C10	8.39	1.71	1.53
3	D	204	INI	C11-C10	8.33	1.70	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	INI	C11-C10	8.32	1.70	1.53
3	C	203	INI	C4-C5	8.01	1.57	1.42
3	A	201	INI	C4-C5	7.95	1.57	1.42
3	B	202	INI	C4-C5	7.68	1.57	1.42
3	D	204	INI	C4-C5	7.56	1.57	1.42
3	E	205	INI	C4-C5	7.39	1.56	1.42
3	B	202	INI	C6-N7	6.59	1.43	1.32
3	C	203	INI	C6-N7	6.56	1.43	1.32
3	E	205	INI	C6-N7	6.36	1.43	1.32
3	D	204	INI	C6-N7	6.27	1.43	1.32
3	A	201	INI	C6-N7	5.99	1.42	1.32
3	D	204	INI	C9-C10	4.60	1.63	1.53
3	A	201	INI	C9-C10	4.54	1.63	1.53
3	E	205	INI	C9-C10	4.38	1.62	1.53
3	B	202	INI	C9-C10	4.38	1.62	1.53
3	C	203	INI	C9-C10	4.33	1.62	1.53
3	D	204	INI	O51-N5	-4.23	1.17	1.25
3	B	202	INI	C8-C9	4.11	1.58	1.52
3	B	202	INI	O51-N5	-4.10	1.18	1.25
3	A	201	INI	C8-C9	4.09	1.58	1.52
3	C	203	INI	O51-N5	-4.05	1.18	1.25
3	A	201	INI	O51-N5	-4.03	1.18	1.25
3	E	205	INI	C8-C9	4.01	1.58	1.52
3	E	205	INI	O51-N5	-3.91	1.18	1.25
3	C	203	INI	C8-C9	3.71	1.58	1.52
3	D	204	INI	C8-C9	3.44	1.57	1.52
3	E	205	INI	C5-C6	3.01	1.48	1.41
3	A	201	INI	C5-C6	2.91	1.48	1.41
3	C	203	INI	C5-C6	2.90	1.48	1.41
3	B	202	INI	C12-C11	2.86	1.60	1.52
3	C	203	INI	C12-C11	2.78	1.60	1.52
3	D	204	INI	C5-C6	2.77	1.47	1.41
3	A	201	INI	C12-C11	2.66	1.60	1.52
3	B	202	INI	C5-C6	2.65	1.47	1.41
3	E	205	INI	C12-C11	2.56	1.59	1.52
3	D	204	INI	C12-C11	2.53	1.59	1.52
3	C	203	INI	C6-N1	2.34	1.41	1.35
3	E	205	INI	C6-N1	2.32	1.41	1.35
3	D	204	INI	C6-N1	2.21	1.40	1.35
3	A	201	INI	C6-N1	2.20	1.40	1.35
3	D	204	INI	O10-C10	-2.18	1.37	1.43
3	B	202	INI	C6-N1	2.17	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	INI	O10-C10	-2.17	1.37	1.43
3	E	205	INI	O10-C10	-2.08	1.37	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	INI	C12-C11-C10	7.58	129.57	112.38
3	E	205	INI	C12-C11-C10	7.34	129.02	112.38
3	D	204	INI	C12-C11-C10	7.13	128.56	112.38
3	A	201	INI	C12-C11-C10	7.04	128.35	112.38
3	C	203	INI	C12-C11-C10	6.96	128.16	112.38
3	E	205	INI	C4-C5-N5	-5.61	116.86	121.94
3	B	202	INI	C4-C5-N5	-5.18	117.25	121.94
3	C	203	INI	C4-C5-N5	-4.81	117.59	121.94
3	D	204	INI	O11-C11-C12	-4.57	98.54	109.20
3	E	205	INI	O11-C11-C12	-4.55	98.61	109.20
3	D	204	INI	C4-C5-N5	-4.53	117.84	121.94
3	A	201	INI	O11-C11-C12	-4.42	98.89	109.20
3	A	201	INI	C4-C5-N5	-4.42	117.94	121.94
3	B	202	INI	O11-C11-C12	-4.30	99.18	109.20
3	C	203	INI	O11-C11-C12	-4.07	99.71	109.20
3	A	201	INI	C8-N7-C6	-3.91	114.71	124.59
3	D	204	INI	C8-N7-C6	-3.65	115.38	124.59
3	B	202	INI	C8-N7-C6	-3.60	115.50	124.59
3	C	203	INI	C8-N7-C6	-3.60	115.50	124.59
3	A	201	INI	O11-C11-C10	-3.56	100.19	109.05
3	D	204	INI	O11-C11-C10	-3.53	100.25	109.05
3	E	205	INI	C8-N7-C6	-3.50	115.75	124.59
3	B	202	INI	O11-C11-C10	-3.47	100.41	109.05
3	D	204	INI	C8-C9-C10	3.42	122.53	110.94
3	C	203	INI	O11-C11-C10	-3.41	100.56	109.05
3	B	202	INI	O9-C9-C8	-3.41	102.25	109.72
3	E	205	INI	O11-C11-C10	-3.35	100.69	109.05
3	E	205	INI	C8-C9-C10	3.34	122.25	110.94
3	C	203	INI	O9-C9-C8	-3.28	102.52	109.72
3	A	201	INI	C8-C9-C10	3.27	122.01	110.94
3	C	203	INI	C8-C9-C10	3.24	121.92	110.94
3	B	202	INI	C4-C5-C6	3.22	116.76	114.55
3	B	202	INI	C8-C9-C10	3.18	121.72	110.94
3	E	205	INI	C11-C10-C9	3.08	120.21	113.25
3	E	205	INI	C4-C5-C6	3.07	116.65	114.55
3	C	203	INI	C11-C10-C9	3.04	120.12	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	INI	C11-C10-C9	3.02	120.08	113.25
3	A	201	INI	C11-C10-C9	2.98	119.98	113.25
3	A	201	INI	O9-C9-C8	-2.95	103.24	109.72
3	D	204	INI	C11-C10-C9	2.92	119.85	113.25
3	E	205	INI	O9-C9-C8	-2.92	103.31	109.72
3	A	201	INI	N7-C6-N1	-2.84	114.97	120.44
3	D	204	INI	O9-C9-C8	-2.79	103.60	109.72
3	C	203	INI	N7-C6-N1	-2.78	115.09	120.44
3	D	204	INI	N7-C6-N1	-2.76	115.14	120.44
3	E	205	INI	N7-C6-N1	-2.75	115.14	120.44
3	D	204	INI	C4-C5-C6	2.73	116.42	114.55
3	B	202	INI	N7-C6-N1	-2.58	115.48	120.44
3	C	203	INI	C4-C5-C6	2.58	116.31	114.55
3	A	201	INI	C4-C5-C6	2.55	116.29	114.55
3	D	204	INI	O12-C12-C11	-2.23	106.07	111.05
3	C	203	INI	O12-C12-C11	-2.02	106.52	111.05
3	A	201	INI	O12-C12-C11	-2.00	106.57	111.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	202	INI	N1-C6-N7-C8
3	D	204	INI	N1-C6-N7-C8
3	A	201	INI	N1-C6-N7-C8
3	C	203	INI	N1-C6-N7-C8
3	E	205	INI	N1-C6-N7-C8

There are no ring outliers.

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	146/157 (92%)	0.13	7 (4%)	29	39	18, 28, 47, 74	9 (6%)
1	B	146/157 (92%)	0.45	14 (9%)	8	14	19, 31, 56, 69	10 (6%)
1	C	146/157 (92%)	0.15	7 (4%)	29	39	19, 28, 46, 73	10 (6%)
1	D	147/157 (93%)	0.32	8 (5%)	25	34	19, 31, 53, 71	11 (7%)
1	E	146/157 (92%)	0.46	16 (10%)	6	10	20, 33, 58, 71	10 (6%)
All	All	731/785 (93%)	0.30	52 (7%)	16	23	18, 30, 56, 74	50 (6%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	86	GLY	13.5
1	D	89	TYR	13.0
1	D	90	HIS	10.7
1	A	90	HIS	9.7
1	B	90	HIS	8.6
1	A	89	TYR	8.3
1	C	87	GLU	7.9
1	A	91	PHE	7.4
1	B	86	GLY	7.3
1	C	89	TYR	7.3
1	C	88	THR	7.2
1	D	91	PHE	7.1
1	A	88	THR	7.0
1	C	91	PHE	7.0
1	A	86	GLY	6.6
1	C	90	HIS	6.6
1	B	89	TYR	6.2
1	C	86	GLY	6.0
1	E	88	THR	5.9
1	B	87	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
1	E	86	GLY	5.9
1	E	90	HIS	5.8
1	E	89	TYR	5.8
1	D	157	ALA	5.7
1	D	88	THR	5.4
1	B	91	PHE	5.1
1	A	87	GLU	4.9
1	B	88	THR	4.8
1	C	85	ARG	4.2
1	E	128	VAL	4.1
1	B	134	ASP	3.7
1	D	87	GLU	3.7
1	A	85	ARG	3.5
1	B	128	VAL	3.5
1	E	91	PHE	3.3
1	B	124	GLU	3.3
1	E	124	GLU	3.0
1	E	134	ASP	2.9
1	E	131	ARG	2.9
1	B	122	ASN	2.9
1	B	133	GLU	2.8
1	D	85	ARG	2.7
1	E	122	ASN	2.7
1	E	133	GLU	2.7
1	B	121	GLU	2.3
1	B	131	ARG	2.3
1	E	40	GLU	2.3
1	E	70	GLY	2.3
1	E	68	ASP	2.1
1	B	125	GLN	2.1
1	E	157	ALA	2.1
1	E	87	GLU	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CA	A	304	1/1	0.16	21.97	44,44,44,44	0
2	CA	C	305	1/1	0.14	5.29	44,44,44,44	0
3	INI	E	205	21/21	0.16	0.22	22,30,36,41	0
3	INI	B	202	21/21	0.17	0.12	21,28,36,40	0
3	INI	C	203	21/21	0.17	0.07	22,30,38,42	0
3	INI	D	204	21/21	0.17	-0.01	22,27,34,39	0
3	INI	A	201	21/21	0.16	-0.06	26,31,39,44	0
2	CA	D	306	1/1	0.10	-0.97	58,58,58,58	0
2	CA	A	301	1/1	0.15	-1.41	63,63,63,63	0
2	CA	B	302	1/1	0.10	-1.55	63,63,63,63	0
2	CA	C	303	1/1	0.06	-3.18	39,39,39,39	1

6.5 Other polymers ⓘ

There are no such residues in this entry.