Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2021 – 11:03 am BST

PDB ID	:	6TW8
Title	:	Leishmania major N-myristoyltransferase in complex with indazole inhibitor IMP-917
Authors	:	Brannigan, J.A.
Deposited on	:	2020-01-12
Resolution	:	1.79 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:

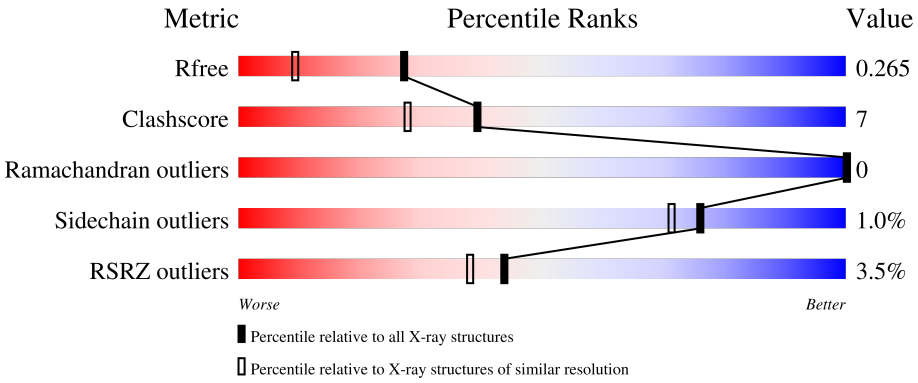
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

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 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	AAA	418	3% 88% 10%
1	CCC	418	4% 85% 13%

2 Entry composition

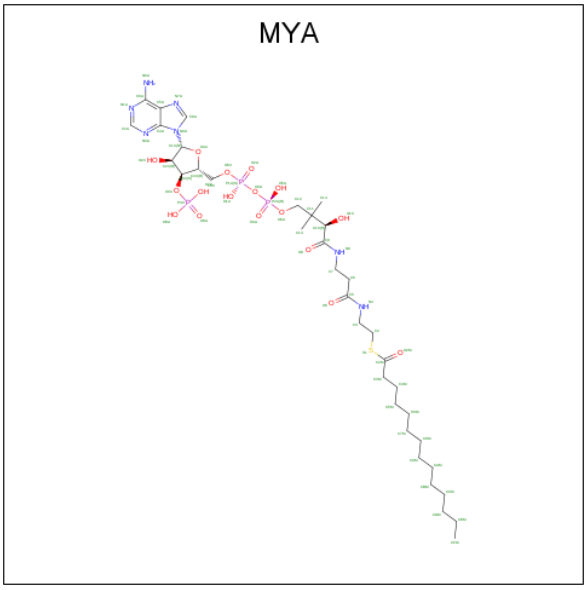
There are 5 unique types of molecules in this entry. The entry contains 7792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycylpeptide N-tetradecanoyltransferase.

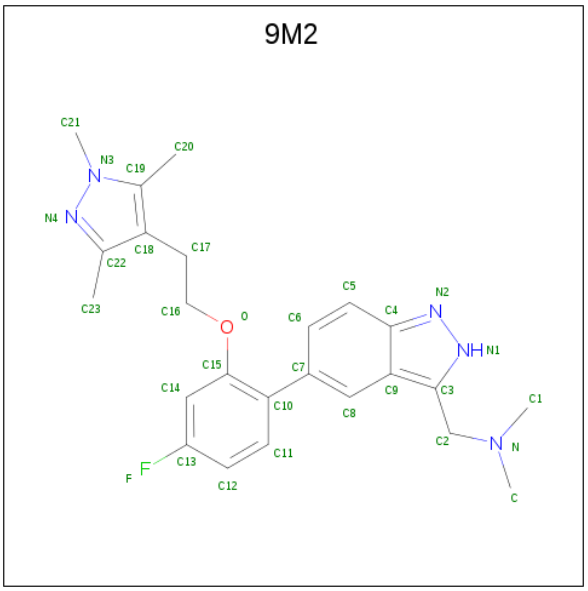
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	411	Total	C	N	O	S	0	22	0
			3472	2254	575	626	17			
1	CCC	411	Total	C	N	O	S	0	26	0
			3496	2281	573	625	17			

- Molecule 2 is TETRADECANOYL-COA (three-letter code: MYA) (formula: $C_{35}H_{62}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	CCC	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- Molecule 3 is 1-[5-[4-fluoranyl-2-[2-(1,3,5-trimethylpyrazol-4-yl)ethoxy]phenyl]-2 {H}-indazol-3-yl]- {N}, {N}-dimethyl-methanamine (three-letter code: 9M2) (formula: $C_{24}H_{28}FN_5O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C F N O 31 24 1 5 1	0	0
3	CCC	1	Total C F N O 31 24 1 5 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total Mg 1 1	0	0
4	CCC	1	Total Mg 1 1	0	0

- Molecule 5 is water.

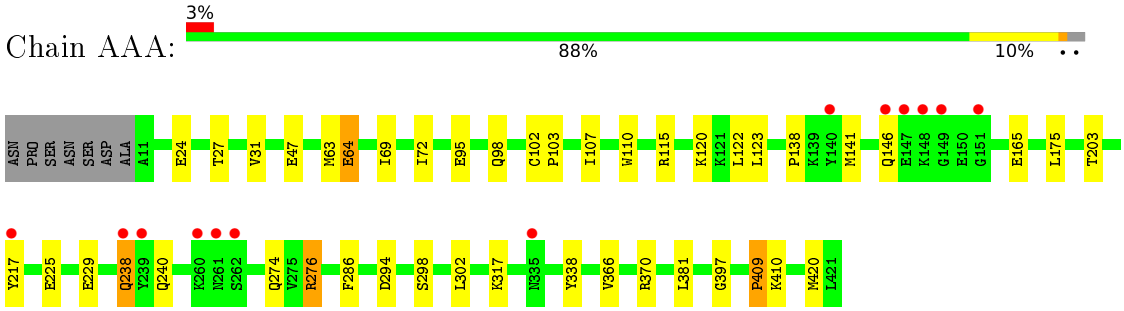
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	320	Total O 320 320	0	0
5	CCC	314	Total O 314 314	0	0

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.

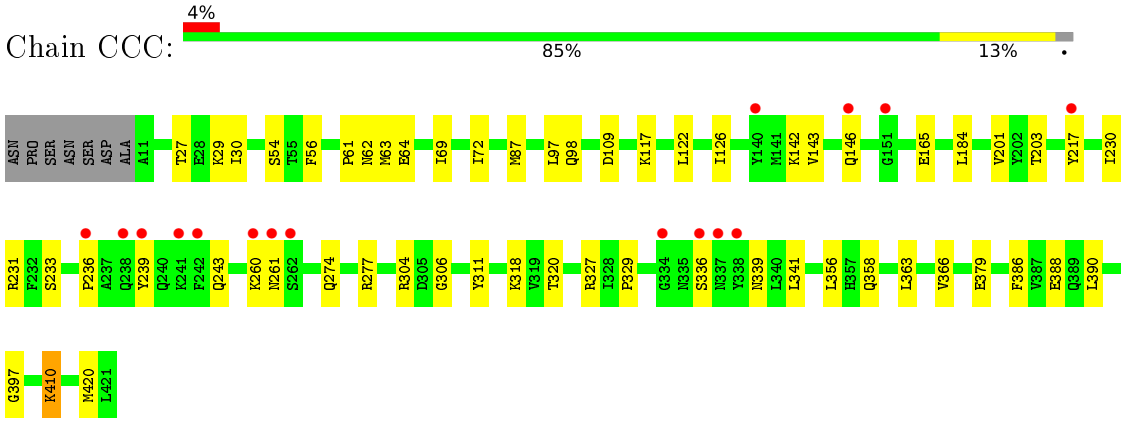
- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain AAA:



- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain CCC:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.02Å 89.82Å 97.18Å 90.00° 104.27° 90.00°	Depositor
Resolution (Å)	65.00 – 1.79 65.00 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.7 (65.00-1.79) 99.7 (65.00-1.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.218 , 0.265 0.218 , 0.265	Depositor DCC
R_{free} test set	4145 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7792	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0639e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 9M2, MYA, MG

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	AAA	0.47	2/3638 (0.1%)	0.82	4/4942 (0.1%)
1	CCC	0.49	2/3674 (0.1%)	0.81	1/4992 (0.0%)
All	All	0.48	4/7312 (0.1%)	0.81	5/9934 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	388	GLU	CD-OE1	7.67	1.34	1.25
1	CCC	379	GLU	CD-OE2	-6.13	1.19	1.25
1	AAA	64[A]	GLU	C-O	5.33	1.33	1.23
1	AAA	64[B]	GLU	C-O	5.33	1.33	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CCC	304	ARG	CG-CD-NE	-7.59	95.86	111.80
1	AAA	276	ARG	CG-CD-NE	-5.65	99.93	111.80
1	AAA	115	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	AAA	64[A]	GLU	CA-C-O	5.10	130.81	120.10
1	AAA	64[B]	GLU	CA-C-O	5.10	130.81	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3472	0	3465	50	0
1	CCC	3496	0	3521	58	0
2	AAA	63	0	58	0	0
2	CCC	63	0	58	0	0
3	AAA	31	0	0	0	0
3	CCC	31	0	0	0	0
4	AAA	1	0	0	0	0
4	CCC	1	0	0	0	0
5	AAA	320	0	0	6	0
5	CCC	314	0	0	5	0
All	All	7792	0	7102	105	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 7.

All (105) 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:CCC:69[A]:ILE:CD1	1:CCC:98[A]:GLN:NE2	1.69	1.49
1:CCC:69[A]:ILE:HD13	1:CCC:98[A]:GLN:NE2	1.13	1.42
1:AAA:69:ILE:HD13	1:AAA:98[A]:GLN:OE1	1.21	1.32
1:CCC:98[B]:GLN:HG2	5:CCC:1366:HOH:O	1.54	1.08
1:AAA:69:ILE:CD1	1:AAA:98[A]:GLN:OE1	2.02	1.06
1:AAA:141[B]:MET:HA	1:AAA:141[B]:MET:CE	1.88	1.03
1:CCC:69[A]:ILE:HD13	1:CCC:98[A]:GLN:CD	1.80	1.02
1:AAA:203:THR:HG23	1:AAA:420:MET:CE	1.92	0.98
1:CCC:69[A]:ILE:HD12	1:CCC:98[A]:GLN:NE2	1.81	0.91
1:AAA:203:THR:HG23	1:AAA:420:MET:HE3	1.52	0.91
1:AAA:141[B]:MET:HA	1:AAA:141[B]:MET:HE2	1.57	0.84
1:AAA:24:GLU:OE1	1:AAA:410[B]:LYS:HE2	1.82	0.80
1:AAA:141[A]:MET:HE3	5:AAA:1107:HOH:O	1.81	0.80
1:AAA:69:ILE:HD13	1:AAA:98[A]:GLN:CD	2.00	0.80
1:AAA:203:THR:HG23	1:AAA:420:MET:HE2	1.63	0.79
1:AAA:120[B]:LYS:NZ	1:AAA:120[B]:LYS:HB3	1.97	0.79
1:AAA:141[B]:MET:HA	1:AAA:141[B]:MET:HE3	1.65	0.78
1:AAA:120[B]:LYS:HB3	1:AAA:120[B]:LYS:HZ3	1.48	0.78
1:CCC:69[A]:ILE:HD13	1:CCC:98[A]:GLN:CG	2.16	0.74
1:AAA:410[B]:LYS:HE3	5:AAA:1342:HOH:O	1.88	0.74
1:CCC:69[A]:ILE:HD11	1:CCC:98[A]:GLN:NE2	2.01	0.72
1:CCC:63:MET:SD	1:CCC:72[B]:ILE:CD1	2.79	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:261:ASN:HD21	1:CCC:358:GLN:HE21	1.39	0.70
1:CCC:410[A]:LYS:NZ	1:CCC:410[A]:LYS:HB2	2.07	0.69
1:CCC:62:ASN:OD1	1:CCC:64[B]:GLU:HG3	1.91	0.68
1:AAA:47[B]:GLU:OE1	5:AAA:1101:HOH:O	2.11	0.68
1:AAA:63:MET:O	1:AAA:69:ILE:HD11	1.95	0.67
1:CCC:261:ASN:ND2	1:CCC:358:GLN:HE21	1.94	0.65
1:AAA:217[A]:TYR:HE2	1:AAA:397:GLY:HA3	1.62	0.64
1:AAA:274:GLN:HG3	5:AAA:1166:HOH:O	1.98	0.63
1:AAA:146:GLN:HA	1:AAA:146:GLN:OE1	1.98	0.61
1:CCC:217[A]:TYR:CZ	1:CCC:397:GLY:HA3	2.36	0.60
1:CCC:109:ASP:OD2	5:CCC:1102:HOH:O	2.17	0.60
1:AAA:217[A]:TYR:CE2	1:AAA:397:GLY:HA3	2.38	0.59
1:CCC:274:GLN:HG3	5:CCC:1126:HOH:O	2.02	0.59
1:CCC:63:MET:HE1	1:CCC:69[B]:ILE:HD12	1.85	0.57
1:CCC:143:VAL:O	1:CCC:146:GLN:HB2	2.04	0.57
1:CCC:63:MET:SD	1:CCC:72[B]:ILE:HD13	2.44	0.56
1:AAA:165[A]:GLU:OE2	5:AAA:1102:HOH:O	2.17	0.56
1:CCC:126:ILE:HG22	1:CCC:184[B]:LEU:HD12	1.88	0.55
1:CCC:261:ASN:OD1	1:CCC:358:GLN:NE2	2.39	0.55
1:AAA:317:LYS:HD2	1:AAA:317:LYS:N	2.22	0.55
1:CCC:201:VAL:HG22	1:CCC:420:MET:HE2	1.89	0.54
1:AAA:298[B]:SER:OG	1:AAA:302:LEU:HD12	2.07	0.54
1:CCC:217[A]:TYR:OH	1:CCC:397:GLY:HA3	2.08	0.53
1:CCC:142:LYS:O	1:CCC:146:GLN:HG2	2.09	0.52
1:CCC:236:PRO:HG2	1:CCC:239:TYR:CD2	2.45	0.52
1:CCC:277[B]:ARG:HG3	1:CCC:277[B]:ARG:NH1	2.25	0.51
1:AAA:217[A]:TYR:CE2	1:AAA:397:GLY:CA	2.94	0.51
1:AAA:217[A]:TYR:CE2	1:AAA:397:GLY:N	2.79	0.51
1:CCC:165[B]:GLU:OE2	5:CCC:1103:HOH:O	2.19	0.51
1:AAA:203:THR:CG2	1:AAA:420:MET:HE2	2.39	0.50
1:AAA:238:GLN:H	1:AAA:238:GLN:NE2	2.09	0.50
1:CCC:63:MET:CE	1:CCC:69[B]:ILE:HD12	2.41	0.50
1:CCC:277[B]:ARG:HG3	1:CCC:277[B]:ARG:HH11	1.76	0.50
1:CCC:201:VAL:HG22	1:CCC:420:MET:CE	2.42	0.49
1:AAA:141[B]:MET:HE2	1:AAA:141[B]:MET:CA	2.38	0.49
1:CCC:230:ILE:HD11	1:CCC:341:LEU:HD13	1.94	0.49
1:AAA:141[A]:MET:CE	5:AAA:1107:HOH:O	2.51	0.49
1:AAA:238:GLN:H	1:AAA:238:GLN:HE21	1.60	0.48
1:CCC:336:SER:O	1:CCC:339:ASN:HB3	2.13	0.48
1:CCC:363:LEU:HD23	1:CCC:363:LEU:C	2.34	0.48
1:CCC:203:THR:HG23	1:CCC:420:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:261:ASN:CG	1:CCC:358:GLN:HE21	2.17	0.48
1:AAA:27:THR:HG22	1:AAA:410[B]:LYS:HG2	1.96	0.47
1:AAA:47[B]:GLU:H	1:AAA:47[B]:GLU:HG3	1.49	0.47
1:AAA:123:LEU:HB3	1:AAA:175:LEU:HD13	1.97	0.47
1:AAA:366:VAL:O	1:AAA:370:ARG:HG2	2.14	0.47
1:AAA:123:LEU:HD22	1:AAA:175:LEU:HD11	1.96	0.46
1:CCC:318[A]:LYS:HD3	1:CCC:320:THR:CG2	2.46	0.46
1:AAA:217[A]:TYR:HE2	1:AAA:397:GLY:CA	2.28	0.46
1:CCC:87[B]:MET:HE1	1:CCC:231:ARG:HB2	1.98	0.46
1:CCC:236:PRO:O	1:CCC:239:TYR:N	2.45	0.46
1:CCC:29:LYS:HB2	1:CCC:29:LYS:HE2	1.77	0.45
1:AAA:95:GLU:HG3	1:CCC:336:SER:CB	2.47	0.45
1:CCC:386:PHE:O	1:CCC:390[B]:LEU:HB2	2.16	0.45
1:CCC:410[A]:LYS:HB2	1:CCC:410[A]:LYS:HZ1	1.81	0.45
1:CCC:261:ASN:HD21	1:CCC:358:GLN:HG2	1.82	0.45
1:CCC:311:TYR:CZ	1:CCC:366:VAL:HG11	2.52	0.45
1:AAA:276:ARG:HD2	1:AAA:294:ASP:OD1	2.17	0.45
1:CCC:56:PHE:O	1:CCC:117[A]:LYS:HE3	2.17	0.44
1:AAA:102:CYS:N	1:AAA:103:PRO:CD	2.80	0.44
1:CCC:63:MET:SD	1:CCC:72[B]:ILE:HD12	2.56	0.44
1:CCC:54:SER:O	1:CCC:117[A]:LYS:HD2	2.17	0.44
1:AAA:64[B]:GLU:HA	1:AAA:69:ILE:HD11	2.00	0.44
1:CCC:69[B]:ILE:HD11	1:CCC:97:LEU:HB2	2.01	0.43
1:AAA:338:TYR:OH	1:CCC:306:GLY:HA2	2.18	0.43
1:AAA:72:ILE:HD13	1:AAA:122:LEU:HD21	1.99	0.43
1:CCC:327:ARG:CZ	1:CCC:329:PRO:HG3	2.48	0.43
1:AAA:107:ILE:HD12	1:AAA:110:TRP:CZ2	2.53	0.42
1:CCC:72[A]:ILE:HD13	1:CCC:122:LEU:HD21	2.01	0.42
1:CCC:117[A]:LYS:HE2	5:CCC:1360:HOH:O	2.19	0.42
1:AAA:31:VAL:HA	1:AAA:141[A]:MET:HE2	2.03	0.41
1:AAA:138:PRO:HG2	1:AAA:409:PRO:HG2	2.03	0.41
1:AAA:141[B]:MET:CE	1:AAA:141[B]:MET:CA	2.77	0.41
1:AAA:95:GLU:HG3	1:CCC:336:SER:OG	2.21	0.41
1:AAA:120[B]:LYS:NZ	1:AAA:120[B]:LYS:CB	2.67	0.41
1:AAA:225:GLU:O	1:AAA:229[A]:GLU:HG2	2.20	0.41
1:CCC:69[A]:ILE:CD1	1:CCC:98[A]:GLN:CG	2.91	0.41
1:CCC:203:THR:HG23	1:CCC:420:MET:HE3	2.02	0.41
1:CCC:27:THR:HA	1:CCC:30:ILE:HD12	2.02	0.40
1:CCC:217[A]:TYR:CZ	1:CCC:397:GLY:CA	3.03	0.40
1:CCC:356[B]:LEU:HD23	1:CCC:356[B]:LEU:HA	1.78	0.40
1:CCC:61:PRO:HG2	1:CCC:72[B]:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:286:PHE:CE2	1:AAA:381:LEU:HA	2.57	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	AAA	431/418 (103%)	418 (97%)	13 (3%)	0	100	100
1	CCC	435/418 (104%)	423 (97%)	12 (3%)	0	100	100
All	All	866/836 (104%)	841 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	384/368 (104%)	381 (99%)	3 (1%)	81	78
1	CCC	388/368 (105%)	383 (99%)	5 (1%)	69	62
All	All	772/736 (105%)	764 (99%)	8 (1%)	76	71

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	238	GLN
1	AAA	240	GLN
1	AAA	409	PRO
1	CCC	233	SER
1	CCC	243	GLN
1	CCC	260	LYS
1	CCC	410[A]	LYS
1	CCC	410[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	MYA	CCC	1001	4	54,65,65	0.89	2 (3%)	67,91,91	1.43	5 (7%)
3	9M2	CCC	1002	-	31,34,34	2.47	9 (29%)	39,49,49	2.27	15 (38%)
3	9M2	AAA	1002	-	31,34,34	2.44	8 (25%)	39,49,49	1.73	10 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MYA	AAA	1001	4	54,65,65	0.93	4 (7%)	67,91,91	1.30	5 (7%)

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	MYA	CCC	1001	4	-	3/59/80/80	0/3/3/3
3	9M2	CCC	1002	-	-	0/13/14/14	0/4/4/4
3	9M2	AAA	1002	-	-	0/13/14/14	0/4/4/4
2	MYA	AAA	1001	4	-	5/59/80/80	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	1002	9M2	C2-C3	8.20	1.54	1.51
3	CCC	1002	9M2	C2-C3	7.94	1.54	1.51
3	CCC	1002	9M2	C18-C22	7.34	1.52	1.39
3	AAA	1002	9M2	C18-C22	6.26	1.50	1.39
3	AAA	1002	9M2	C19-N3	-4.86	1.30	1.37
3	AAA	1002	9M2	C19-C18	3.93	1.47	1.39
3	CCC	1002	9M2	C19-C18	3.72	1.46	1.39
3	CCC	1002	9M2	C19-N3	-3.40	1.32	1.37
3	AAA	1002	9M2	C10-C15	2.93	1.46	1.40
3	AAA	1002	9M2	O-C15	-2.80	1.32	1.37
3	CCC	1002	9M2	C10-C15	2.73	1.46	1.40
2	AAA	1001	MYA	O10-C10	2.71	1.47	1.42
3	AAA	1002	9M2	C8-C9	-2.53	1.37	1.42
3	CCC	1002	9M2	C9-C4	2.49	1.49	1.42
3	CCC	1002	9M2	C5-C6	2.35	1.41	1.36
3	CCC	1002	9M2	O-C15	-2.27	1.33	1.37
2	AAA	1001	MYA	O4X-C1X	2.20	1.44	1.41
2	AAA	1001	MYA	C2X-C1X	-2.17	1.50	1.53
3	AAA	1002	9M2	C5-C6	2.14	1.41	1.36
2	CCC	1001	MYA	C3-N4	2.12	1.51	1.46
2	CCC	1001	MYA	O10-C10	2.03	1.46	1.42
2	AAA	1001	MYA	C8A-N7A	2.02	1.38	1.34
3	CCC	1002	9M2	C8-C9	-2.01	1.38	1.42

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	CCC	1001	MYA	O2M-C2M-C3M	6.08	119.85	109.02
2	AAA	1001	MYA	O2M-C2M-C3M	5.78	119.31	109.02
3	CCC	1002	9M2	C17-C18-C19	-5.48	123.45	127.30
3	CCC	1002	9M2	C6-C5-C4	-4.56	115.10	120.84
2	CCC	1001	MYA	N3A-C2A-N1A	-4.32	121.92	128.68
3	CCC	1002	9M2	C17-C18-C22	4.22	130.26	127.30
2	AAA	1001	MYA	N3A-C2A-N1A	-4.22	122.08	128.68
3	AAA	1002	9M2	C3-C2-N	4.08	119.29	113.48
3	CCC	1002	9M2	C3-N1-N2	3.95	114.62	106.98
3	AAA	1002	9M2	C22-N4-N3	3.87	107.68	104.35
3	CCC	1002	9M2	C22-N4-N3	3.80	107.62	104.35
3	CCC	1002	9M2	C8-C9-C4	3.56	123.12	118.26
3	AAA	1002	9M2	C6-C5-C4	-3.40	116.55	120.84
2	CCC	1001	MYA	O4X-C1X-C2X	-3.40	101.96	106.93
3	CCC	1002	9M2	C3-C2-N	3.12	117.93	113.48
3	AAA	1002	9M2	C8-C9-C4	3.05	122.43	118.26
3	CCC	1002	9M2	C7-C8-C9	-3.01	115.70	122.30
3	CCC	1002	9M2	C11-C12-C13	3.01	121.48	118.36
2	CCC	1001	MYA	C4M-C3M-C2M	-2.82	106.02	113.80
3	AAA	1002	9M2	C5-C4-N2	2.76	134.68	130.19
2	AAA	1001	MYA	C4M-C3M-C2M	-2.53	106.82	113.80
3	CCC	1002	9M2	F-C13-C14	2.48	121.80	118.25
3	AAA	1002	9M2	C7-C10-C15	2.45	127.77	122.33
3	CCC	1002	9M2	C21-N3-C19	-2.45	125.62	128.82
3	CCC	1002	9M2	C6-C7-C8	2.40	121.85	118.09
3	AAA	1002	9M2	C23-C22-N4	2.38	124.93	119.78
3	AAA	1002	9M2	C19-N3-N4	2.38	115.00	112.10
3	CCC	1002	9M2	C23-C22-N4	2.36	124.86	119.78
3	AAA	1002	9M2	C3-N1-N2	2.34	111.50	106.98
2	AAA	1001	MYA	O8A-P3X-O9A	2.25	119.51	110.68
3	AAA	1002	9M2	C18-C19-N3	-2.22	105.02	106.79
2	CCC	1001	MYA	C3-C2-S1	-2.21	105.33	114.36
3	CCC	1002	9M2	C5-C6-C7	2.18	124.53	121.00
3	CCC	1002	9M2	C5-C4-N2	2.17	133.72	130.19
2	AAA	1001	MYA	P2A-O3A-P1A	-2.11	125.60	132.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	1001	MYA	S1-C2M-C3M-C4M
2	CCC	1001	MYA	S1-C2M-C3M-C4M
2	AAA	1001	MYA	C5M-C6M-C7M-C8M

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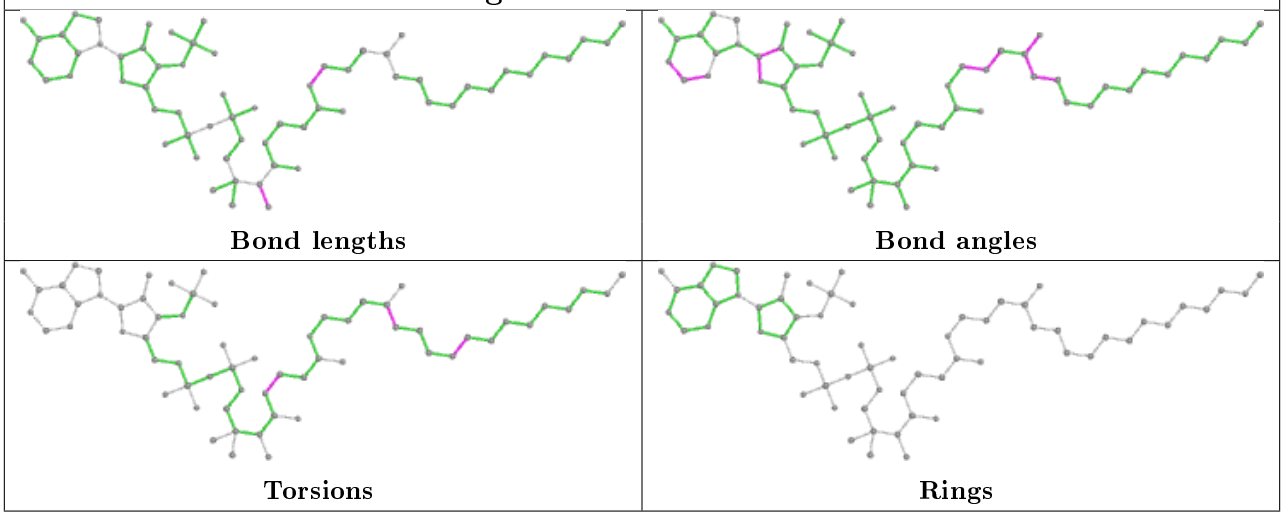
Mol	Chain	Res	Type	Atoms
2	CCC	1001	MYA	C6-C7-N8-C9
2	CCC	1001	MYA	C5M-C6M-C7M-C8M
2	AAA	1001	MYA	C8M-C9M-CAM-CBM
2	AAA	1001	MYA	P2A-O3A-P1A-O2A
2	AAA	1001	MYA	CAM-CBM-CCM-CDM

There are no ring outliers.

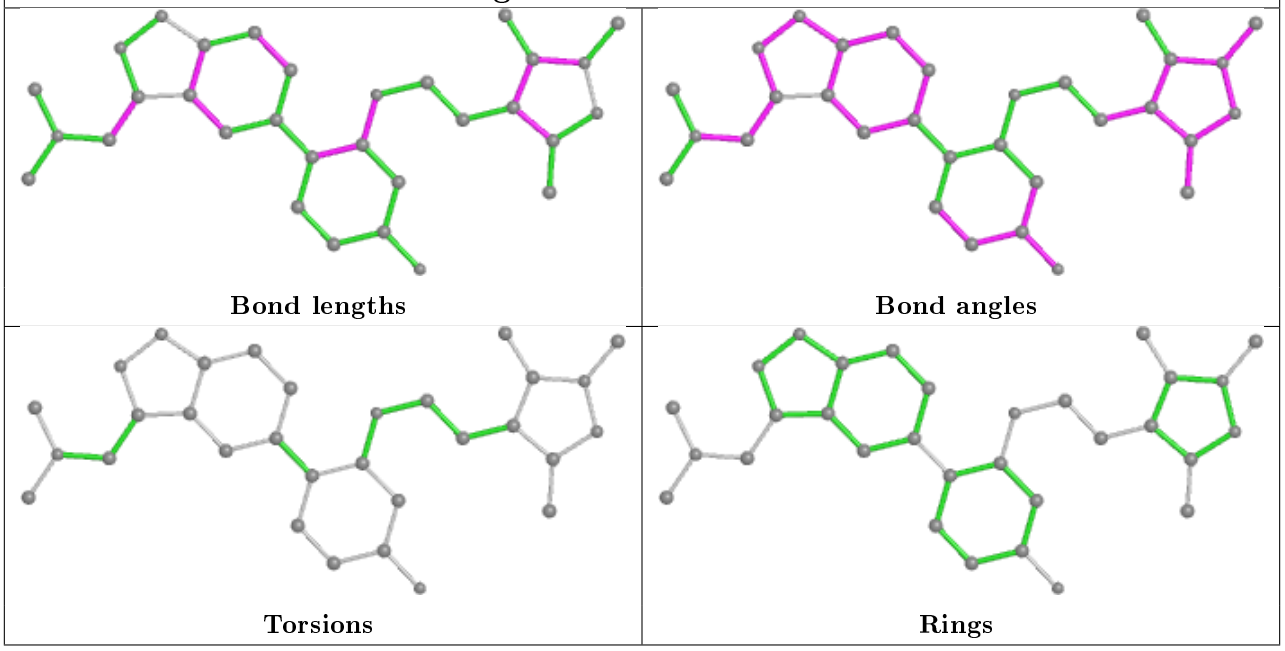
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

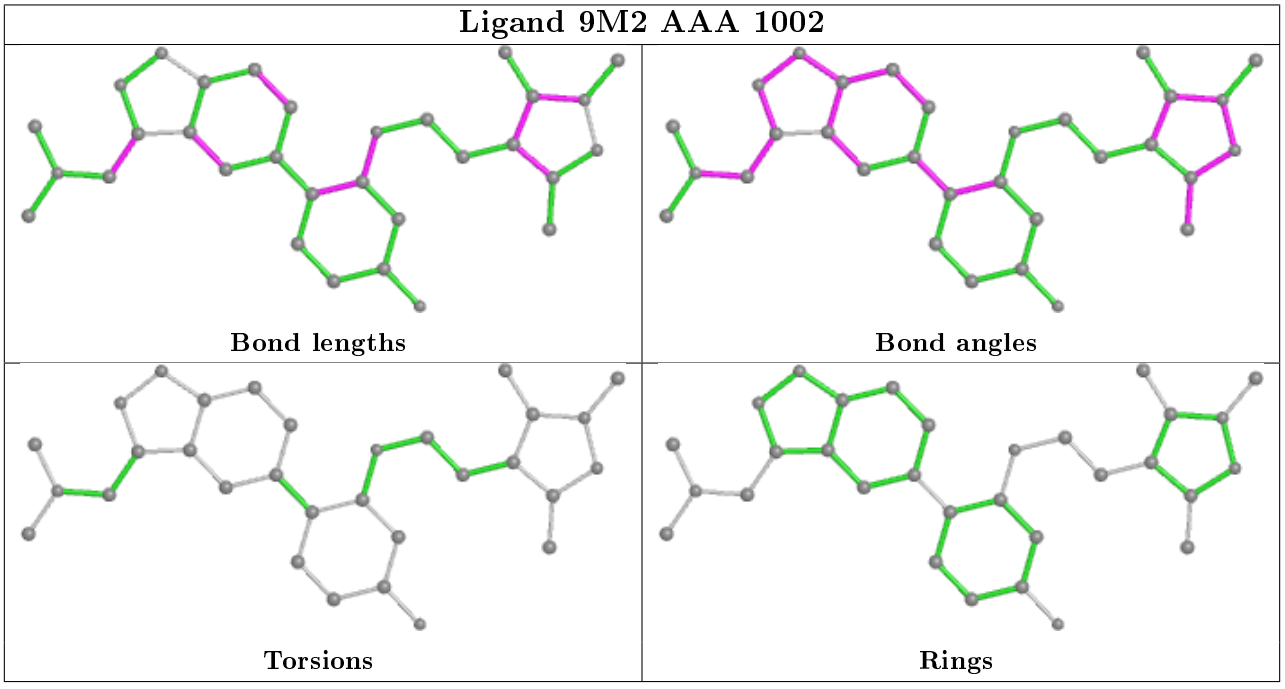
Ligand MYA CCC 1001



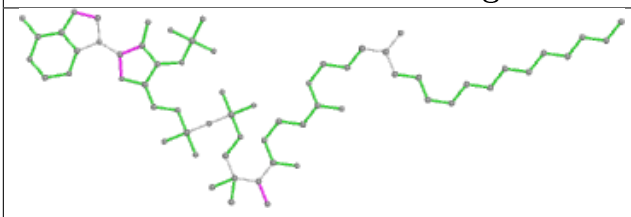
Ligand 9M2 CCC 1002



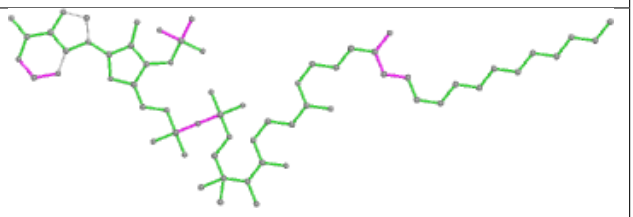
Ligand 9M2 AAA 1002



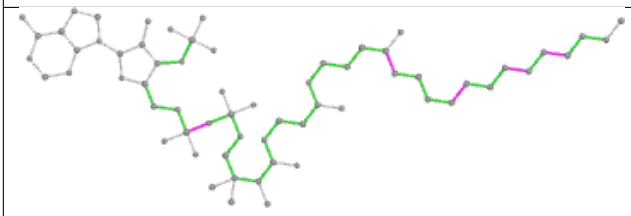
Ligand MYA AAA 1001



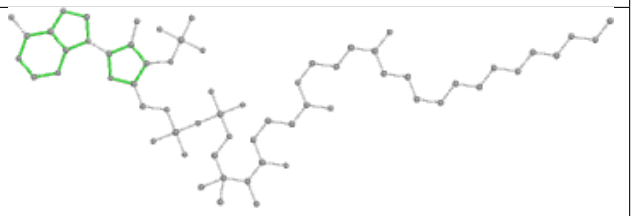
Bond lengths



Bond angles



Torsions



Rings

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, 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	AAA	411/418 (98%)	0.07	13 (3%) 47 41	9, 18, 41, 74	21 (5%)
1	CCC	411/418 (98%)	0.02	16 (3%) 39 33	9, 17, 39, 55	24 (5%)
All	All	822/836 (98%)	0.05	29 (3%) 44 38	9, 18, 40, 74	45 (5%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	146	GLN	5.4
1	AAA	262	SER	4.9
1	CCC	239	TYR	4.5
1	AAA	147	GLU	4.1
1	CCC	336	SER	4.1
1	AAA	149	GLY	3.8
1	AAA	261	ASN	3.8
1	AAA	140	TYR	3.6
1	CCC	140	TYR	3.6
1	CCC	334	GLY	3.5
1	CCC	338	TYR	3.4
1	AAA	148	LYS	3.4
1	CCC	236	PRO	3.4
1	CCC	242	PHE	3.3
1	CCC	262	SER	3.2
1	CCC	260	LYS	3.0
1	AAA	238	GLN	2.9
1	CCC	146	GLN	2.8
1	CCC	151	GLY	2.8
1	AAA	260	LYS	2.5
1	CCC	217[A]	TYR	2.4
1	AAA	335	ASN	2.3
1	AAA	217[A]	TYR	2.2
1	CCC	337	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	AAA	239	TYR	2.1
1	CCC	238	GLN	2.1
1	AAA	151	GLY	2.0
1	CCC	241	LYS	2.0
1	CCC	261	ASN	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 monosaccharides 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
3	9M2	CCC	1002	31/31	0.91	0.10	15,17,20,21	0
3	9M2	AAA	1002	31/31	0.95	0.09	13,15,21,22	0
2	MYA	AAA	1001	63/63	0.97	0.07	9,13,17,18	0
2	MYA	CCC	1001	63/63	0.97	0.07	10,13,17,17	0
4	MG	CCC	1003	1/1	0.98	0.07	27,27,27,27	0
4	MG	AAA	1003	1/1	0.99	0.06	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.