Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:02 PM GMT

PDB ID	:	1IIC
Title	:	Crystal Structure of Saccharomyces cerevisiae N-myristoyltransferase with Bound MyristoylCoA
Authors	:	Farazi, T.A.; Waksman, G.; Gordon, J.I.
Deposited on	:	2001-04-22
Resolution	:	2.20 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:

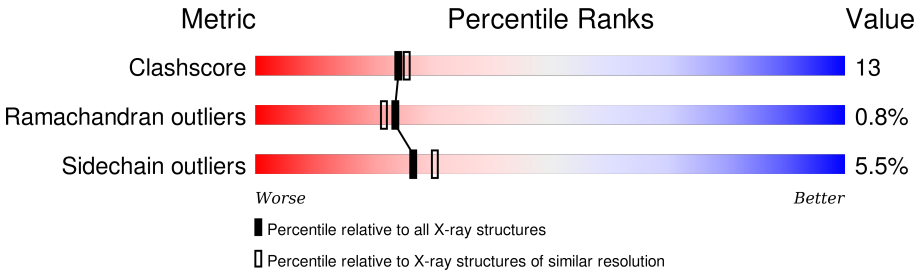
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	422	77% 21%
1	B	422	67% 30%

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	MYA	A	500	X	-	-	-
2	MYA	B	600	X	-	-	-

2 Entry composition

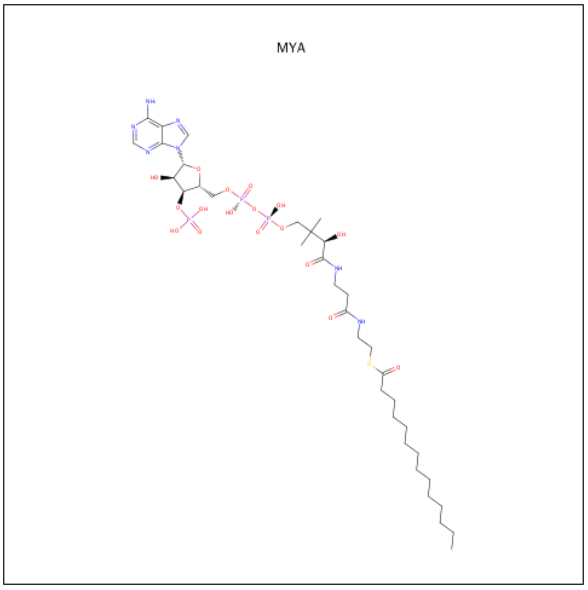
There are 3 unique types of molecules in this entry. The entry contains 7257 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PEPTIDE N-myristoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3440	2230	572	628	10			
1	B	422	Total	C	N	O	S	0	0	0
			3425	2219	570	626	10			

- 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	A	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	140	Total O 140 140	0	0
3	B	126	Total O 126 126	0	0

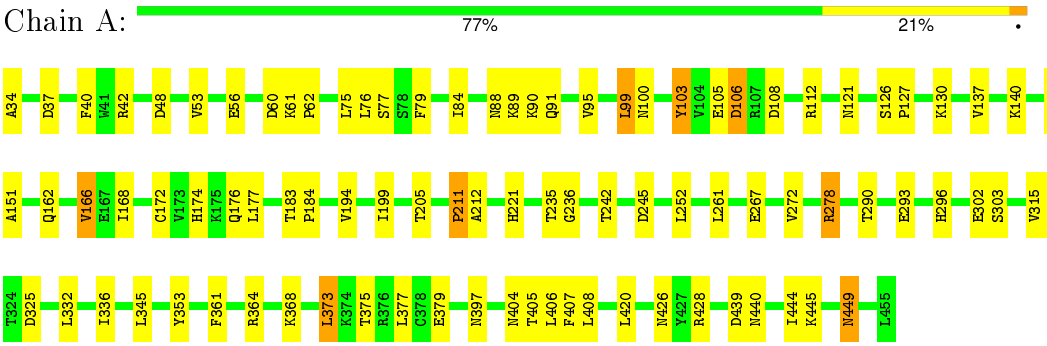
3 Residue-property plots (i)

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

Note EDS was not executed.

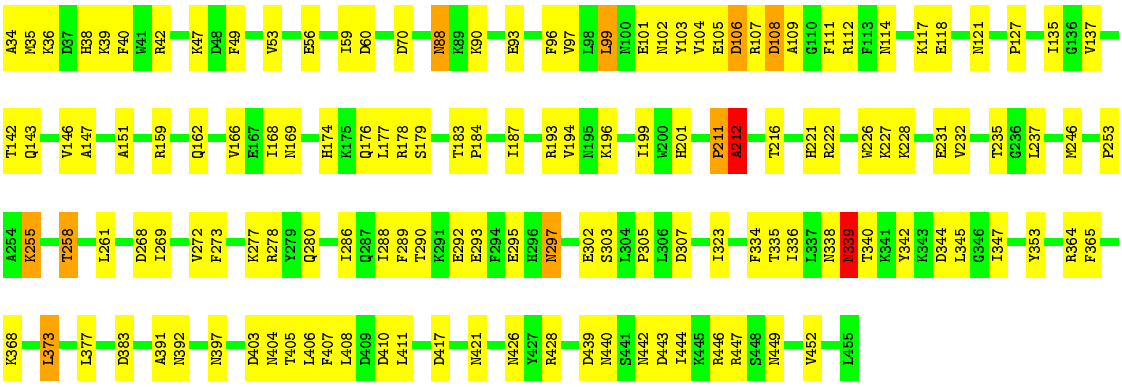
- Molecule 1: PEPTIDE N-myristoyltransferase

Chain A:



- Molecule 1: PEPTIDE N-myristoyltransferase

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	75.13Å 97.06Å 141.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.22 – 2.20	Depositor
% Data completeness (in resolution range)	91.7 (27.22-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	4.80	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.236 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7257	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.39	0/3529	0.64	1/4780 (0.0%)
1	B	0.38	0/3514	0.65	1/4763 (0.0%)
All	All	0.38	0/7043	0.64	2/9543 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	290	THR	N-CA-C	-5.32	96.63	111.00
1	B	212	ALA	N-CA-C	5.03	124.57	111.00

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	A	3440	0	3403	62	0
1	B	3425	0	3368	119	0
2	A	63	0	58	2	0
2	B	63	0	58	5	0
3	A	140	0	0	0	0
3	B	126	0	0	6	0
All	All	7257	0	6887	181	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 13.

All (181) 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:338:ASN:CG	1:B:339:ASN:H	1.64	0.98
1:B:336:ILE:HD11	1:B:345:LEU:HB2	1.49	0.95
1:B:60:ASP:H	1:B:426:ASN:HD21	1.13	0.94
1:B:151:ALA:HB1	1:B:166:VAL:HG11	1.49	0.94
1:A:88:ASN:HD22	1:A:91:GLN:H	1.14	0.90
1:B:174:HIS:HD2	1:B:176:GLN:H	1.20	0.90
1:A:322:LYS:HE3	1:A:322:LYS:HA	1.52	0.89
1:A:88:ASN:ND2	1:A:91:GLN:H	1.77	0.82
1:B:60:ASP:H	1:B:426:ASN:ND2	1.80	0.80
1:A:174:HIS:HD2	1:A:176:GLN:H	1.31	0.78
1:B:258:THR:HG23	1:B:383:ASP:OD1	1.86	0.76
1:B:338:ASN:CG	1:B:339:ASN:N	2.38	0.75
1:B:107:ARG:HH21	1:B:109:ALA:HB2	1.52	0.74
1:B:405:THR:HG22	1:B:447:ARG:HG2	1.70	0.74
1:A:373:LEU:HD22	1:A:377:LEU:HG	1.70	0.73
1:B:373:LEU:HD22	1:B:377:LEU:HG	1.71	0.73
1:B:273:PHE:CZ	1:B:277:LYS:HE3	2.24	0.72
1:B:273:PHE:CE2	1:B:277:LYS:HE3	2.24	0.72
1:A:322:LYS:HE3	1:A:322:LYS:CA	2.21	0.71
1:A:315:VAL:HG13	1:A:323:ILE:HG23	1.73	0.71
1:B:253:PRO:HB3	1:B:255:LYS:NZ	2.06	0.70
1:A:60:ASP:H	1:A:426:ASN:HD21	1.39	0.70
1:A:242:THR:HG23	1:A:245:ASP:H	1.57	0.69
1:B:99:LEU:O	1:B:103:TYR:HB2	1.93	0.68
1:B:34:ALA:HB1	1:B:38:HIS:NE2	2.08	0.68
1:B:406:LEU:HG	1:B:447:ARG:HD3	1.78	0.66
1:B:151:ALA:HB1	1:B:166:VAL:CG1	2.26	0.64
1:A:105:GLU:O	1:A:106:ASP:HB2	1.97	0.64
1:B:107:ARG:HH21	1:B:109:ALA:CB	2.10	0.64
1:B:290:THR:OG1	1:B:293:GLU:HG2	1.98	0.64
1:B:174:HIS:CD2	1:B:176:GLN:H	2.09	0.64
1:B:255:LYS:H	1:B:255:LYS:HE3	1.64	0.63
1:B:176:GLN:O	1:B:177:LEU:HD12	1.99	0.62
1:B:338:ASN:ND2	1:B:339:ASN:H	1.99	0.61
1:B:93:GLU:HA	1:B:96:PHE:CE2	2.36	0.61
1:B:106:ASP:C	1:B:108:ASP:N	2.55	0.60
1:A:205:THR:HB	1:A:420:LEU:HD11	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:THR:HG22	1:A:245:ASP:CG	2.22	0.60
1:B:70:ASP:OD1	1:B:196:LYS:HE2	2.02	0.60
1:B:221:HIS:ND1	1:B:397:ASN:ND2	2.50	0.60
1:B:286:ILE:HA	1:B:452:VAL:HG13	1.84	0.60
1:A:444:ILE:HD12	1:A:445:LYS:N	2.18	0.59
1:B:35:MET:HG3	1:B:49:PHE:HD1	1.67	0.59
1:A:183:THR:HB	1:A:184:PRO:HD3	1.84	0.59
1:A:60:ASP:H	1:A:426:ASN:ND2	2.01	0.58
1:B:405:THR:OG1	1:B:442:ASN:HB3	2.03	0.58
1:B:35:MET:HG3	1:B:49:PHE:CD1	2.38	0.58
1:B:106:ASP:C	1:B:108:ASP:H	2.07	0.58
1:B:194:VAL:CG1	1:B:199:ILE:HB	2.34	0.57
1:B:405:THR:HG21	1:B:443:ASP:O	2.05	0.57
1:B:127:PRO:HB3	1:B:292:GLU:OE2	2.05	0.57
1:B:176:GLN:C	1:B:177:LEU:HD12	2.25	0.56
1:A:151:ALA:HB1	1:A:166:VAL:HG11	1.88	0.56
1:B:253:PRO:HB3	1:B:255:LYS:HZ1	1.70	0.56
1:A:105:GLU:OE1	1:A:105:GLU:N	2.39	0.56
1:A:146:VAL:CG2	1:A:177:LEU:HD22	2.37	0.55
1:B:178:ARG:O	1:B:179:SER:HB2	2.08	0.54
1:B:289:PHE:HE2	1:B:297:ASN:ND2	2.06	0.54
1:A:439:ASP:O	1:A:440:ASN:HB2	2.08	0.53
1:A:34:ALA:HB1	1:A:37:ASP:OD2	2.07	0.53
1:A:151:ALA:HB1	1:A:166:VAL:CG1	2.39	0.53
1:B:174:HIS:HD2	1:B:176:GLN:N	1.99	0.53
1:A:99:LEU:O	1:A:103:TYR:HB2	2.09	0.53
1:B:258:THR:CG2	1:B:383:ASP:OD1	2.57	0.53
1:A:146:VAL:HG22	1:A:177:LEU:HD22	1.91	0.53
1:B:339:ASN:OD1	1:B:342:TYR:HD1	1.92	0.52
1:B:336:ILE:N	1:B:336:ILE:HD12	2.24	0.52
1:B:280:GLN:NE2	3:B:608:HOH:O	2.42	0.52
1:B:268:ASP:O	1:B:272:VAL:HG12	2.09	0.52
1:B:104:VAL:O	1:B:106:ASP:N	2.37	0.52
1:B:93:GLU:O	1:B:97:VAL:HG23	2.09	0.52
1:B:56:GLU:OE1	1:B:159:ARG:HD2	2.10	0.52
1:A:364:ARG:HH12	1:A:449:ASN:ND2	2.08	0.52
1:A:221:HIS:ND1	1:A:397:ASN:ND2	2.58	0.51
1:B:59:ILE:H	1:B:426:ASN:ND2	2.08	0.51
1:B:183:THR:HB	1:B:184:PRO:HD3	1.91	0.51
1:B:405:THR:CG2	1:B:447:ARG:HG2	2.39	0.51
1:B:39:LYS:HA	1:B:42:ARG:HD2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:HIS:O	1:B:42:ARG:HD2	2.10	0.51
1:B:280:GLN:HG2	1:B:286:ILE:HG21	1.91	0.51
1:B:444:ILE:HD12	1:B:444:ILE:C	2.31	0.51
1:A:100:ASN:O	1:A:112:ARG:HD2	2.11	0.51
1:B:290:THR:H	1:B:293:GLU:CG	2.23	0.50
1:B:201:HIS:HE1	3:B:650:HOH:O	1.93	0.50
1:B:47:LYS:O	1:B:212:ALA:HB3	2.11	0.50
1:B:168:ILE:HG13	2:B:600:MYA:HAMA	1.93	0.50
1:B:117:LYS:HE3	1:B:118:GLU:OE2	2.11	0.50
1:A:404:ASN:HA	1:A:407:PHE:CE2	2.47	0.50
1:A:127:PRO:HG2	1:A:293:GLU:HG2	1.92	0.50
1:A:194:VAL:CG1	1:A:199:ILE:HB	2.42	0.49
1:B:253:PRO:HB3	1:B:255:LYS:HZ2	1.78	0.49
1:A:168:ILE:HG13	2:A:500:MYA:HAMA	1.93	0.49
1:A:194:VAL:HG12	1:A:199:ILE:HB	1.94	0.49
1:B:187:ILE:HG12	2:B:600:MYA:H7MA	1.94	0.49
1:B:159:ARG:NH1	3:B:671:HOH:O	2.44	0.48
1:B:135:ILE:HD11	1:B:193:ARG:HD2	1.95	0.48
1:A:40:PHE:CD1	1:A:184:PRO:HB3	2.49	0.48
1:B:405:THR:HG23	1:B:444:ILE:HA	1.96	0.48
1:B:59:ILE:HG23	1:B:428:ARG:NH2	2.28	0.48
1:B:106:ASP:O	1:B:108:ASP:N	2.46	0.48
1:B:137:VAL:HB	1:B:147:ALA:HB3	1.94	0.48
1:B:353:TYR:HE2	1:B:404:ASN:HD21	1.61	0.47
1:B:302:GLU:O	1:B:303:SER:HB2	2.13	0.47
1:B:40:PHE:CD1	1:B:184:PRO:HB3	2.50	0.47
1:B:194:VAL:HG12	1:B:199:ILE:HB	1.95	0.47
1:A:375:THR:O	1:A:379:GLU:HG3	2.15	0.47
1:A:267:GLU:H	1:A:267:GLU:CD	2.18	0.47
1:B:53:VAL:HG13	1:B:428:ARG:HG2	1.95	0.47
1:A:404:ASN:HD22	1:A:404:ASN:N	2.11	0.47
1:A:84:ILE:HG21	1:A:95:VAL:HG21	1.97	0.46
1:B:112:ARG:HG2	1:B:335:THR:HB	1.97	0.46
1:A:53:VAL:HG13	1:A:428:ARG:HG2	1.97	0.46
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.81	0.46
1:B:216:THR:OG1	1:B:421:ASN:ND2	2.49	0.46
1:A:235:THR:HG22	1:A:236:GLY:N	2.31	0.46
1:B:373:LEU:CD2	1:B:377:LEU:HG	2.43	0.46
1:A:361:PHE:CE2	1:A:368:LYS:HB3	2.51	0.46
1:B:407:PHE:HB2	1:B:411:LEU:HD22	1.97	0.46
1:B:403:ASP:OD2	1:B:447:ARG:HD2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:GLN:HG3	3:B:657:HOH:O	2.15	0.45
1:A:444:ILE:C	1:A:444:ILE:HD12	2.37	0.45
1:B:334:PHE:CD1	1:B:347:ILE:HD11	2.52	0.45
1:B:268:ASP:HB3	1:B:323:ILE:CD1	2.47	0.45
1:B:162:GLN:HG2	1:B:288:ILE:CD1	2.46	0.45
1:B:305:PRO:HB2	1:B:307:ASP:OD1	2.16	0.45
1:B:168:ILE:CG2	2:B:600:MYA:H5M	2.47	0.44
1:A:88:ASN:HD22	1:A:91:GLN:N	1.96	0.44
1:B:101:GLU:HG2	1:B:102:ASN:OD1	2.17	0.44
1:A:99:LEU:HD22	1:A:172:CYS:CB	2.47	0.44
1:A:61:LYS:CG	1:A:62:PRO:HD2	2.48	0.44
1:B:406:LEU:CG	1:B:447:ARG:HD3	2.44	0.44
1:B:255:LYS:O	1:B:255:LYS:HD2	2.18	0.44
1:B:293:GLU:O	1:B:297:ASN:HB2	2.17	0.44
1:A:126:SER:HA	1:A:296:HIS:CD2	2.52	0.44
1:B:338:ASN:O	1:B:339:ASN:O	2.35	0.43
1:A:315:VAL:CG1	1:A:316:VAL:N	2.80	0.43
1:A:353:TYR:OH	1:A:404:ASN:ND2	2.51	0.43
1:A:302:GLU:O	1:A:303:SER:HB2	2.17	0.43
1:B:336:ILE:HD13	1:B:344:ASP:C	2.38	0.43
1:B:88:ASN:HD21	1:B:90:LYS:HB3	1.83	0.43
1:B:142:THR:O	1:B:143:GLN:HB2	2.18	0.43
1:B:365:PHE:CG	1:B:446:ARG:NH2	2.86	0.43
1:A:137:VAL:HB	1:A:147:ALA:HB3	2.00	0.43
1:B:269:ILE:CD1	1:B:295:GLU:HG3	2.48	0.43
1:B:237:LEU:C	1:B:237:LEU:HD23	2.39	0.43
1:A:278:ARG:CG	1:A:278:ARG:HH11	2.32	0.43
1:A:316:VAL:HB	1:A:325:ASP:HB2	2.00	0.43
1:A:242:THR:HG22	1:A:245:ASP:OD2	2.19	0.43
1:A:105:GLU:O	1:A:106:ASP:CB	2.65	0.43
1:B:439:ASP:O	1:B:440:ASN:HB2	2.19	0.43
1:B:168:ILE:HG21	2:B:600:MYA:H7M	1.99	0.43
1:B:142:THR:HA	3:B:679:HOH:O	2.19	0.43
1:B:53:VAL:CG1	1:B:428:ARG:HG2	2.49	0.42
1:A:373:LEU:HD13	1:A:406:LEU:HD12	2.02	0.42
1:B:228:LYS:O	1:B:232:VAL:HG22	2.20	0.42
1:B:109:ALA:HB3	1:B:111:PHE:CE2	2.55	0.42
1:B:280:GLN:HG2	1:B:280:GLN:O	2.19	0.42
1:A:56:GLU:HA	1:A:428:ARG:O	2.19	0.42
1:B:47:LYS:HG2	1:B:212:ALA:CB	2.50	0.42
1:A:168:ILE:HG21	2:A:500:MYA:H7M	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ALA:O	1:B:392:ASN:HB2	2.20	0.42
1:B:36:LYS:C	1:B:38:HIS:H	2.23	0.42
1:B:373:LEU:HD22	1:B:377:LEU:CG	2.47	0.41
1:A:405:THR:O	1:A:444:ILE:HG22	2.20	0.41
1:B:88:ASN:ND2	1:B:90:LYS:HB3	2.35	0.41
1:A:79:PHE:O	1:A:140:LYS:NZ	2.51	0.41
1:B:168:ILE:HG21	2:B:600:MYA:H5M	2.01	0.41
1:B:107:ARG:NH2	1:B:111:PHE:HE2	2.19	0.41
1:B:226:TRP:CE2	1:B:246:MET:HB3	2.56	0.41
1:B:368:LYS:HD3	3:B:696:HOH:O	2.20	0.41
1:A:336:ILE:HD11	1:A:345:LEU:HB2	2.03	0.41
1:B:364:ARG:HH12	1:B:449:ASN:ND2	2.19	0.41
1:A:75:LEU:O	1:A:76:LEU:C	2.59	0.41
1:B:99:LEU:N	1:B:99:LEU:HD23	2.36	0.40
1:B:227:LYS:O	1:B:231:GLU:HG2	2.20	0.40
1:B:102:ASN:O	1:B:178:ARG:NH2	2.51	0.40
1:A:272:VAL:HG22	1:A:323:ILE:HG21	2.03	0.40
1:B:35:MET:HA	1:B:49:PHE:CE1	2.56	0.40
1:B:302:GLU:O	1:B:303:SER:CB	2.69	0.40
1:B:336:ILE:HD11	1:B:345:LEU:CB	2.34	0.40
1:A:48:ASP:C	1:A:212:ALA:HB2	2.42	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	420/422 (100%)	391 (93%)	27 (6%)	2 (0%)	34	35
1	B	420/422 (100%)	393 (94%)	22 (5%)	5 (1%)	16	12
All	All	840/844 (100%)	784 (93%)	49 (6%)	7 (1%)	24	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ASP
1	B	339	ASN
1	B	105	GLU
1	B	106	ASP
1	B	212	ALA
1	A	211	PRO
1	B	211	PRO

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	375/381 (98%)	355 (95%)	20 (5%)	28	32
1	B	371/381 (97%)	350 (94%)	21 (6%)	25	29
All	All	746/762 (98%)	705 (94%)	41 (6%)	27	30

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	A	89	LYS
1	A	90	LYS
1	A	99	LEU
1	A	103	TYR
1	A	108	ASP
1	A	121	ASN
1	A	130	LYS
1	A	145	LEU
1	A	162	GLN
1	A	166	VAL
1	A	211	PRO
1	A	252	LEU
1	A	261	LEU
1	A	278	ARG
1	A	322	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	332	LEU
1	A	373	LEU
1	A	408	LEU
1	A	449	ASN
1	B	88	ASN
1	B	99	LEU
1	B	108	ASP
1	B	114	ASN
1	B	121	ASN
1	B	146	VAL
1	B	169	ASN
1	B	211	PRO
1	B	222	ARG
1	B	235	THR
1	B	255	LYS
1	B	258	THR
1	B	261	LEU
1	B	278	ARG
1	B	297	ASN
1	B	339	ASN
1	B	340	THR
1	B	373	LEU
1	B	408	LEU
1	B	410	ASP
1	B	417	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	114	ASN
1	A	162	GLN
1	A	174	HIS
1	A	195	ASN
1	A	201	HIS
1	A	296	HIS
1	A	297	ASN
1	A	397	ASN
1	A	404	ASN
1	A	421	ASN
1	A	426	ASN
1	A	437	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	449	ASN
1	B	88	ASN
1	B	114	ASN
1	B	174	HIS
1	B	195	ASN
1	B	201	HIS
1	B	280	GLN
1	B	297	ASN
1	B	397	ASN
1	B	404	ASN
1	B	421	ASN
1	B	426	ASN
1	B	437	ASN
1	B	449	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

2 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	MYA	A	500	-	53,65,65	1.36	9 (16%)	65,91,91	1.75	10 (15%)
2	MYA	B	600	-	53,65,65	1.36	9 (16%)	65,91,91	1.79	11 (16%)

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	A	500	-	1/1/12/14	0/59/80/80	0/3/3/3
2	MYA	B	600	-	1/1/12/14	0/59/80/80	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	MYA	C4A-N3A	-2.30	1.32	1.35
2	A	500	MYA	C4A-N3A	-2.24	1.32	1.35
2	B	600	MYA	C9-N8	2.04	1.37	1.33
2	A	500	MYA	C6-C5	2.08	1.55	1.51
2	B	600	MYA	C5-N4	2.16	1.38	1.33
2	A	500	MYA	C5-N4	2.16	1.38	1.33
2	A	500	MYA	C2-S1	2.31	1.84	1.81
2	B	600	MYA	C2-S1	2.36	1.84	1.81
2	B	600	MYA	P2A-O4A	2.39	1.59	1.51
2	B	600	MYA	P1A-O2A	2.58	1.60	1.51
2	A	500	MYA	P2A-O4A	2.64	1.60	1.51
2	A	500	MYA	P1A-O2A	2.64	1.60	1.51
2	B	600	MYA	P3X-O9A	2.70	1.60	1.51
2	A	500	MYA	P3X-O9A	2.92	1.60	1.51
2	A	500	MYA	O4X-C1X	3.23	1.45	1.41
2	B	600	MYA	O4X-C1X	3.41	1.45	1.41
2	B	600	MYA	C2A-N3A	4.00	1.39	1.32
2	A	500	MYA	C2A-N3A	4.04	1.39	1.32

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	MYA	N3A-C2A-N1A	-6.05	124.26	128.89
2	A	500	MYA	N3A-C2A-N1A	-6.01	124.30	128.89
2	B	600	MYA	P2A-O3A-P1A	-5.85	116.30	132.73
2	A	500	MYA	P2A-O3A-P1A	-5.83	116.35	132.73
2	B	600	MYA	P3X-O3X-C3X	-2.43	115.74	121.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	MYA	C14-C11-C13	-2.12	105.03	109.28
2	A	500	MYA	O1A-P1A-O3A	2.03	114.31	105.09
2	A	500	MYA	O5A-P2A-O3A	2.09	114.59	105.09
2	B	600	MYA	O3A-P2A-O6A	2.18	108.73	102.94
2	B	600	MYA	O5A-P2A-O3A	2.30	115.55	105.09
2	B	600	MYA	O4X-C1X-N9A	2.43	113.18	108.10
2	A	500	MYA	C1X-N9A-C4A	2.44	130.62	126.94
2	A	500	MYA	O2X-C2X-C3X	2.45	118.23	111.16
2	A	500	MYA	O3A-P2A-O6A	2.45	109.43	102.94
2	B	600	MYA	C1X-N9A-C4A	2.52	130.74	126.94
2	B	600	MYA	O2X-C2X-C3X	2.53	118.47	111.16
2	A	500	MYA	O4X-C1X-N9A	2.70	113.75	108.10
2	A	500	MYA	C14-C11-C10	4.74	117.99	109.34
2	B	600	MYA	C14-C11-C10	5.19	118.81	109.34
2	A	500	MYA	O2M-C2M-C3M	5.61	119.31	109.05
2	B	600	MYA	O2M-C2M-C3M	6.03	120.09	109.05

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	600	MYA	C10
2	A	500	MYA	C10

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	MYA	2	0
2	B	600	MYA	5	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.