



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:45 PM GMT

PDB ID : 2P6F
Title : Crystal structures of *Saccharomyces cerevisiae* N-myristoyltransferase with
bound myristoyl-CoA and inhibitors
Authors : Wu, J.; Ding, J.
Deposited on : 2007-03-18
Resolution : 3.10 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>

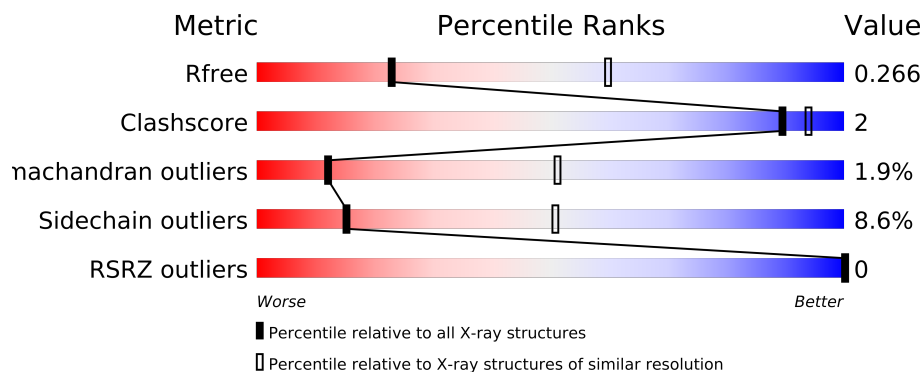
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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	455	
1	B	455	
1	C	455	
1	D	455	
1	E	455	
1	F	455	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	GN8	A	701	-	X
3	GN8	B	702	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
3	GN8	C	703	-	X
3	GN8	D	704	-	X
3	GN8	E	705	-	X
3	GN8	F	706	-	X

2 Entry composition i

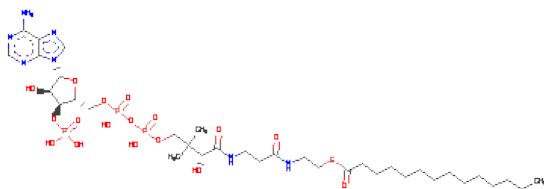
There are 3 unique types of molecules in this entry. The entry contains 21988 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glycylpeptide N-tetradecanoyltransferase.

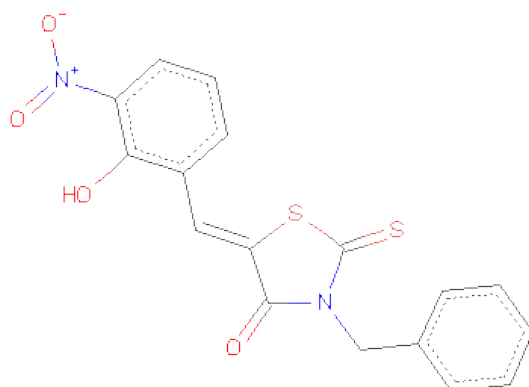
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	B	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	C	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	D	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	E	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	F	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			

- 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		
2	C	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- Molecule 3 is (Z)-3-BENZYL-5-(2-HYDROXY-3-NITROBENZYLIDENE)-2-THIOXOTHIAZOLIDIN-4-ONE (three-letter code: GN8) (formula: C₁₇H₁₂N₂O₄S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			25	17	2	4	2		
3	B	1	Total	C	N	O	S	0	0
			25	17	2	4	2		
3	C	1	Total	C	N	O	S	0	0
			25	17	2	4	2		
3	D	1	Total	C	N	O	S	0	0
			25	17	2	4	2		
3	E	1	Total	C	N	O	S	0	0
			25	17	2	4	2		

Continued on next page...

Continued from previous page...

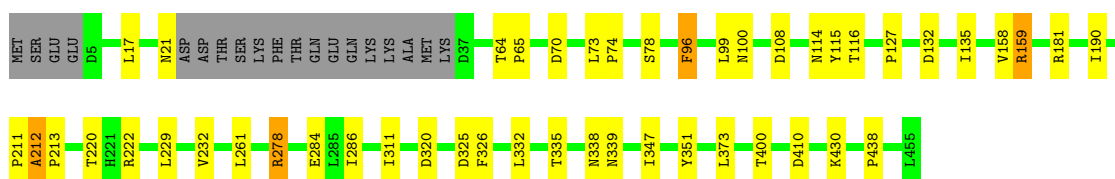
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	S	0	0
			25	17	2	4	2		

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.

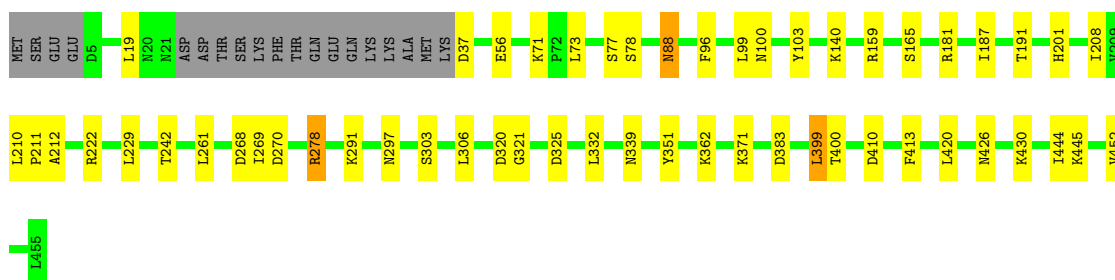
- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain A:



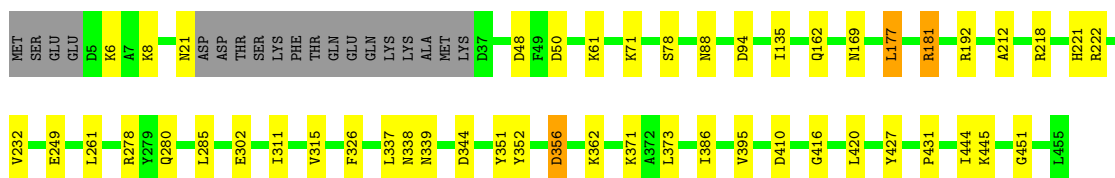
- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain B:



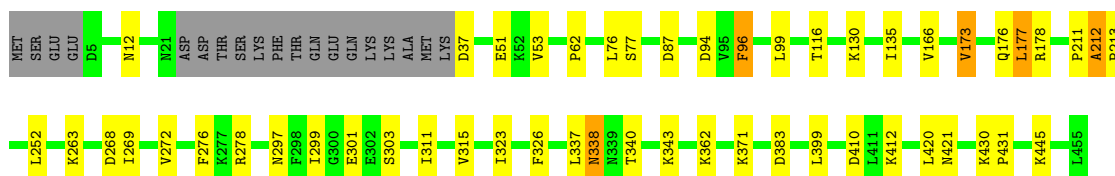
- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain C:



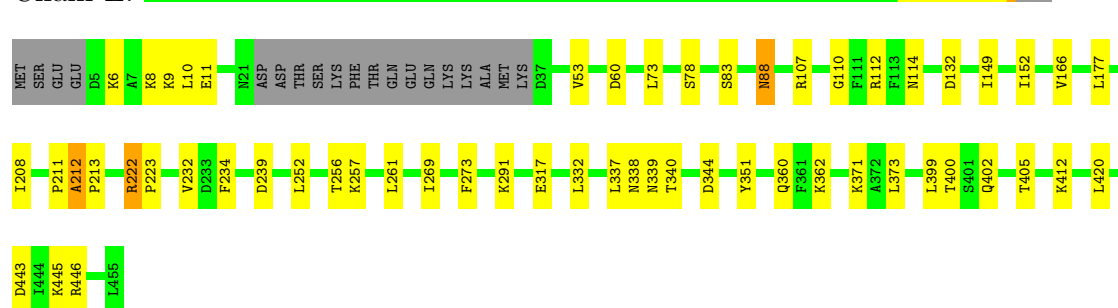
- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain D:



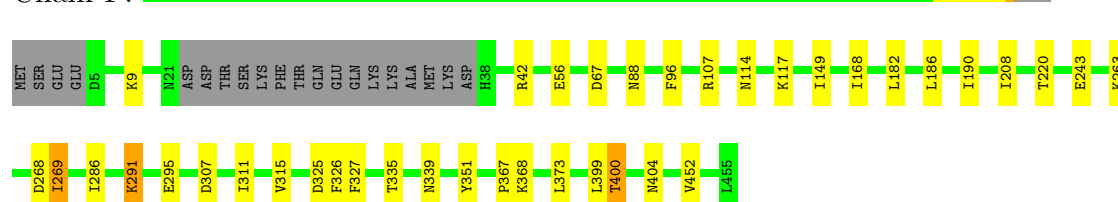
- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain E:



- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.76Å 151.49Å 133.94Å 90.00° 107.46° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 14.98 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-3.10) 97.4 (14.98-2.89)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.270 , 0.332 0.270 , 0.266	Depositor DCC
R_{free} test set	3185 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	7 of 77399 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	21988	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 44.18 % 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 1.5840e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MYA, GN8

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	0.38	0/3666	0.51	0/4957
1	B	0.38	0/3666	0.51	0/4957
1	C	0.39	0/3666	0.53	1/4957 (0.0%)
1	D	0.38	0/3666	0.53	1/4957 (0.0%)
1	E	0.38	0/3666	0.52	0/4957
1	F	0.38	0/3658	0.52	0/4946
All	All	0.38	0/21988	0.52	2/29731 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	177	LEU	CA-CB-CG	5.51	127.98	115.30
1	C	177	LEU	CA-CB-CG	5.09	127.00	115.30

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	3578	0	0	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3578	0	0	7	0
1	C	3578	0	0	7	0
1	D	3578	0	0	5	0
1	E	3578	0	0	13	0
1	F	3570	0	0	1	0
2	A	63	0	0	0	0
2	B	63	0	0	0	0
2	C	63	0	0	0	0
2	D	63	0	0	0	0
2	E	63	0	0	0	0
2	F	63	0	0	0	0
3	A	25	0	0	2	0
3	B	25	0	0	1	0
3	C	25	0	0	1	0
3	D	25	0	0	1	0
3	E	25	0	0	1	0
3	F	25	0	0	1	0
All	All	21988	0	0	48	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 2.

All (48) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:703:GN8:CAK	3:C:703:GN8:SAP	2.76	0.72
1:E:211:PRO:O	1:E:212:ALA:CB	2.50	0.59
3:B:702:GN8:SAP	3:B:702:GN8:CAK	2.90	0.59
3:F:706:GN8:CAK	3:F:706:GN8:SAP	2.91	0.58
1:D:211:PRO:O	1:D:212:ALA:CB	2.53	0.56
3:A:701:GN8:CAK	3:A:701:GN8:SAP	2.93	0.55
1:E:83:SER:OG	1:E:132:ASP:OD2	2.26	0.54
1:B:278:ARG:NH1	1:B:278:ARG:CG	2.71	0.54
3:D:704:GN8:SAP	3:D:704:GN8:CAK	2.96	0.54
1:C:337:LEU:O	1:C:339:ASN:N	2.41	0.53
1:E:212:ALA:N	1:E:213:PRO:CD	2.72	0.52
1:A:278:ARG:CG	1:A:278:ARG:NH1	2.72	0.52
1:E:443:ASP:OD2	1:E:446:ARG:NH2	2.43	0.52
1:A:159:ARG:N	1:A:284:GLU:O	2.44	0.51
1:A:212:ALA:N	1:A:213:PRO:CD	2.73	0.51
1:A:211:PRO:O	1:A:212:ALA:CB	2.61	0.49
1:E:399:LEU:O	1:E:400:THR:OG1	2.31	0.48
1:E:8:LYS:O	1:E:11:GLU:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:8:LYS:O	1:E:10:LEU:N	2.47	0.47
1:F:399:LEU:O	1:F:400:THR:OG1	2.32	0.47
1:E:107:ARG:O	1:E:112:ARG:NH2	2.47	0.47
1:D:96:PHE:CD1	1:D:96:PHE:C	2.88	0.47
1:C:181:ARG:NH1	1:C:181:ARG:CG	2.78	0.47
1:D:173:VAL:O	1:D:178:ARG:NH2	2.48	0.47
1:C:232:VAL:O	1:C:232:VAL:CG1	2.63	0.47
1:E:222:ARG:NH1	1:E:223:PRO:O	2.47	0.46
1:E:232:VAL:CG1	1:E:232:VAL:O	2.63	0.46
1:B:399:LEU:O	1:B:400:THR:OG1	2.34	0.46
1:C:192:ARG:NH1	1:C:192:ARG:CG	2.79	0.46
1:A:159:ARG:NH2	1:A:430:LYS:O	2.49	0.45
1:E:110:GLY:O	1:E:337:LEU:N	2.51	0.44
1:B:201:HIS:ND1	1:B:426:ASN:O	2.50	0.44
1:A:232:VAL:O	1:A:232:VAL:CG1	2.65	0.43
1:A:100:ASN:OD1	1:A:115:TYR:N	2.52	0.43
1:D:212:ALA:N	1:D:213:PRO:CD	2.81	0.43
3:A:701:GN8:CAS	3:A:701:GN8:SAE	3.07	0.42
1:B:187:ILE:O	1:B:191:THR:OG1	2.38	0.42
1:B:159:ARG:NH2	1:B:430:LYS:O	2.53	0.42
1:C:352:TYR:CE1	1:C:451:GLY:O	2.73	0.42
3:E:705:GN8:CAK	3:E:705:GN8:SAP	3.08	0.42
1:E:269:ILE:O	1:E:273:PHE:N	2.53	0.42
1:D:272:VAL:O	1:D:276:PHE:N	2.53	0.41
1:A:96:PHE:CD1	1:A:96:PHE:C	2.94	0.41
1:C:218:ARG:NE	1:C:416:GLY:O	2.54	0.41
1:C:356:ASP:C	1:C:356:ASP:OD1	2.58	0.41
1:E:88:ASN:C	1:E:88:ASN:ND2	2.75	0.40
1:B:56:GLU:OE2	1:B:159:ARG:NH2	2.55	0.40
1:B:96:PHE:O	1:B:100:ASN:N	2.54	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	432/455 (95%)	391 (90%)	33 (8%)	8 (2%)	12	51
1	B	432/455 (95%)	382 (88%)	38 (9%)	12 (3%)	8	39
1	C	432/455 (95%)	376 (87%)	50 (12%)	6 (1%)	16	58
1	D	432/455 (95%)	376 (87%)	44 (10%)	12 (3%)	8	39
1	E	432/455 (95%)	391 (90%)	35 (8%)	6 (1%)	16	58
1	F	431/455 (95%)	373 (86%)	52 (12%)	6 (1%)	16	58
All	All	2591/2730 (95%)	2289 (88%)	252 (10%)	50 (2%)	12	51

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ALA
1	B	78	SER
1	C	302	GLU
1	D	135	ILE
1	D	212	ALA
1	D	301	GLU
1	E	9	LYS
1	E	212	ALA
1	B	77	SER
1	B	413	PHE
1	C	78	SER
1	D	51	GLU
1	D	77	SER
1	B	88	ASN
1	B	140	LYS
1	B	303	SER
1	C	338	ASN
1	C	427	TYR
1	D	76	LEU
1	D	337	LEU
1	E	78	SER
1	E	338	ASN
1	F	56	GLU
1	A	158	VAL
1	B	306	LEU
1	B	321	GLY
1	D	303	SER
1	D	338	ASN
1	D	412	LYS
1	F	42	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	269	ILE
1	F	291	LYS
1	A	65	PRO
1	A	78	SER
1	A	159	ARG
1	B	269	ILE
1	B	291	LYS
1	C	212	ALA
1	C	431	PRO
1	E	402	GLN
1	E	412	LYS
1	F	400	THR
1	A	400	THR
1	D	62	PRO
1	A	74	PRO
1	B	211	PRO
1	D	431	PRO
1	B	212	ALA
1	F	367	PRO
1	A	127	PRO

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	394/413 (95%)	361 (92%)	33 (8%)	16	52
1	B	394/413 (95%)	361 (92%)	33 (8%)	16	52
1	C	394/413 (95%)	358 (91%)	36 (9%)	14	45
1	D	394/413 (95%)	358 (91%)	36 (9%)	14	45
1	E	394/413 (95%)	362 (92%)	32 (8%)	17	53
1	F	393/413 (95%)	359 (91%)	34 (9%)	15	49
All	All	2363/2478 (95%)	2159 (91%)	204 (9%)	15	51

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	21	ASN
1	A	64	THR
1	A	70	ASP
1	A	73	LEU
1	A	96	PHE
1	A	99	LEU
1	A	108	ASP
1	A	114	ASN
1	A	116	THR
1	A	132	ASP
1	A	135	ILE
1	A	181	ARG
1	A	190	ILE
1	A	220	THR
1	A	222	ARG
1	A	229	LEU
1	A	261	LEU
1	A	278	ARG
1	A	286	ILE
1	A	311	ILE
1	A	320	ASP
1	A	325	ASP
1	A	326	PHE
1	A	332	LEU
1	A	335	THR
1	A	338	ASN
1	A	339	ASN
1	A	347	ILE
1	A	351	TYR
1	A	373	LEU
1	A	410	ASP
1	A	438	PRO
1	B	19	LEU
1	B	37	ASP
1	B	71	LYS
1	B	73	LEU
1	B	88	ASN
1	B	99	LEU
1	B	103	TYR
1	B	165	SER
1	B	181	ARG
1	B	208	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	210	LEU
1	B	222	ARG
1	B	229	LEU
1	B	242	THR
1	B	261	LEU
1	B	268	ASP
1	B	270	ASP
1	B	278	ARG
1	B	297	ASN
1	B	320	ASP
1	B	325	ASP
1	B	332	LEU
1	B	339	ASN
1	B	351	TYR
1	B	362	LYS
1	B	371	LYS
1	B	383	ASP
1	B	399	LEU
1	B	410	ASP
1	B	420	LEU
1	B	444	ILE
1	B	445	LYS
1	B	452	VAL
1	C	6	LYS
1	C	8	LYS
1	C	21	ASN
1	C	48	ASP
1	C	50	ASP
1	C	61	LYS
1	C	71	LYS
1	C	88	ASN
1	C	94	ASP
1	C	135	ILE
1	C	162	GLN
1	C	169	ASN
1	C	177	LEU
1	C	181	ARG
1	C	221	HIS
1	C	222	ARG
1	C	249	GLU
1	C	261	LEU
1	C	278	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	280	GLN
1	C	285	LEU
1	C	311	ILE
1	C	315	VAL
1	C	326	PHE
1	C	344	ASP
1	C	351	TYR
1	C	356	ASP
1	C	362	LYS
1	C	371	LYS
1	C	373	LEU
1	C	386	ILE
1	C	395	VAL
1	C	410	ASP
1	C	420	LEU
1	C	444	ILE
1	C	445	LYS
1	D	12	ASN
1	D	37	ASP
1	D	53	VAL
1	D	87	ASP
1	D	94	ASP
1	D	96	PHE
1	D	99	LEU
1	D	116	THR
1	D	130	LYS
1	D	166	VAL
1	D	173	VAL
1	D	176	GLN
1	D	177	LEU
1	D	252	LEU
1	D	263	LYS
1	D	268	ASP
1	D	269	ILE
1	D	278	ARG
1	D	297	ASN
1	D	299	ILE
1	D	311	ILE
1	D	315	VAL
1	D	323	ILE
1	D	326	PHE
1	D	338	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	340	THR
1	D	343	LYS
1	D	362	LYS
1	D	371	LYS
1	D	383	ASP
1	D	399	LEU
1	D	410	ASP
1	D	420	LEU
1	D	421	ASN
1	D	430	LYS
1	D	445	LYS
1	E	6	LYS
1	E	53	VAL
1	E	60	ASP
1	E	73	LEU
1	E	88	ASN
1	E	114	ASN
1	E	149	ILE
1	E	152	ILE
1	E	166	VAL
1	E	177	LEU
1	E	208	ILE
1	E	222	ARG
1	E	234	PHE
1	E	239	ASP
1	E	252	LEU
1	E	256	THR
1	E	257	LYS
1	E	261	LEU
1	E	291	LYS
1	E	317	GLU
1	E	332	LEU
1	E	339	ASN
1	E	340	THR
1	E	344	ASP
1	E	351	TYR
1	E	360	GLN
1	E	362	LYS
1	E	371	LYS
1	E	373	LEU
1	E	405	THR
1	E	420	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	445	LYS
1	F	9	LYS
1	F	67	ASP
1	F	88	ASN
1	F	96	PHE
1	F	107	ARG
1	F	114	ASN
1	F	117	LYS
1	F	149	ILE
1	F	168	ILE
1	F	182	LEU
1	F	186	LEU
1	F	190	ILE
1	F	208	ILE
1	F	220	THR
1	F	243	GLU
1	F	263	LYS
1	F	268	ASP
1	F	269	ILE
1	F	286	ILE
1	F	291	LYS
1	F	295	GLU
1	F	307	ASP
1	F	311	ILE
1	F	315	VAL
1	F	325	ASP
1	F	326	PHE
1	F	327	PHE
1	F	335	THR
1	F	339	ASN
1	F	351	TYR
1	F	368	LYS
1	F	373	LEU
1	F	404	ASN
1	F	452	VAL

Some 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 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 ⓘ

12 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	601	-	64,65,65	0.68	1 (1%)	87,91,91	1.59	13 (14%)
3	GN8	A	701	-	27,27,27	4.00	7 (25%)	38,38,38	3.19	13 (34%)
2	MYA	B	602	-	64,65,65	0.67	1 (1%)	87,91,91	1.66	12 (13%)
3	GN8	B	702	-	27,27,27	3.96	7 (25%)	38,38,38	3.20	13 (34%)
2	MYA	C	603	-	64,65,65	0.67	1 (1%)	87,91,91	1.58	12 (13%)
3	GN8	C	703	-	27,27,27	3.96	7 (25%)	38,38,38	3.24	12 (31%)
2	MYA	D	604	-	64,65,65	0.71	1 (1%)	87,91,91	1.53	11 (12%)
3	GN8	D	704	-	27,27,27	3.97	7 (25%)	38,38,38	3.24	13 (34%)
2	MYA	E	605	-	64,65,65	0.66	1 (1%)	87,91,91	1.60	13 (14%)
3	GN8	E	705	-	27,27,27	4.12	12 (44%)	38,38,38	3.18	13 (34%)
2	MYA	F	606	-	64,65,65	0.70	1 (1%)	87,91,91	1.57	12 (13%)
3	GN8	F	706	-	27,27,27	3.98	8 (29%)	38,38,38	3.14	13 (34%)

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	601	-	1/1/12/14	0/63/80/80	0/1/3/3
3	GN8	A	701	-	-	0/10/28/28	0/3/3/3
2	MYA	B	602	-	1/1/12/14	0/63/80/80	0/1/3/3
3	GN8	B	702	-	-	0/10/28/28	0/3/3/3
2	MYA	C	603	-	1/1/12/14	0/63/80/80	0/1/3/3
3	GN8	C	703	-	-	0/10/28/28	0/3/3/3
2	MYA	D	604	-	1/1/12/14	0/63/80/80	0/1/3/3
3	GN8	D	704	-	-	0/10/28/28	0/3/3/3
2	MYA	E	605	-	1/1/12/14	0/63/80/80	0/1/3/3
3	GN8	E	705	-	-	0/10/28/28	0/3/3/3
2	MYA	F	606	-	1/1/12/14	0/63/80/80	0/1/3/3
3	GN8	F	706	-	-	0/10/28/28	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	705	GN8	CAF-CAW	13.05	1.50	1.34
3	A	701	GN8	CAF-CAW	12.90	1.49	1.34
3	D	704	GN8	CAF-CAW	12.86	1.49	1.34
3	F	706	GN8	CAF-CAW	12.82	1.49	1.34
3	B	702	GN8	CAF-CAW	12.73	1.49	1.34
3	C	703	GN8	CAF-CAW	12.62	1.49	1.34
3	C	703	GN8	OAD-NAY	10.31	1.40	1.23
3	D	704	GN8	OAD-NAY	10.23	1.40	1.23
3	A	701	GN8	OAD-NAY	10.18	1.39	1.23
3	F	706	GN8	OAD-NAY	10.17	1.39	1.23
3	E	705	GN8	OAD-NAY	10.16	1.39	1.23
3	B	702	GN8	OAD-NAY	10.14	1.39	1.23
3	C	703	GN8	OAB-NAY	7.81	1.40	1.25
3	A	701	GN8	OAB-NAY	7.71	1.40	1.25
3	B	702	GN8	OAB-NAY	7.66	1.40	1.25
3	D	704	GN8	OAB-NAY	7.64	1.40	1.25
3	E	705	GN8	OAB-NAY	7.64	1.40	1.25
3	F	706	GN8	OAB-NAY	7.57	1.39	1.25
3	A	701	GN8	CAT-NAY	-6.25	1.36	1.46
3	F	706	GN8	CAT-NAY	-6.21	1.36	1.46
3	B	702	GN8	CAT-NAY	-6.12	1.37	1.46
3	E	705	GN8	CAT-NAY	-5.98	1.37	1.46
3	C	703	GN8	CAT-NAY	-5.97	1.37	1.46
3	D	704	GN8	CAT-NAY	-5.91	1.37	1.46
3	E	705	GN8	CAU-CAW	-4.75	1.39	1.48
3	A	701	GN8	CAU-CAW	-4.67	1.39	1.48
3	C	703	GN8	CAV-SAE	4.63	1.78	1.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	706	GN8	CAU-CAW	-4.63	1.39	1.48
3	F	706	GN8	CAV-SAE	4.62	1.78	1.66
3	E	705	GN8	CAV-SAE	4.62	1.78	1.66
3	B	702	GN8	CAV-SAE	4.60	1.77	1.66
3	A	701	GN8	CAV-SAE	4.59	1.77	1.66
3	B	702	GN8	CAU-CAW	-4.58	1.39	1.48
3	D	704	GN8	CAV-SAE	4.57	1.77	1.66
3	C	703	GN8	CAU-CAW	-4.57	1.39	1.48
3	D	704	GN8	CAU-CAW	-4.54	1.39	1.48
3	E	705	GN8	CAM-CAS	3.21	1.46	1.38
3	D	704	GN8	OAA-CAU	2.87	1.29	1.23
3	C	703	GN8	OAA-CAU	2.82	1.29	1.23
3	E	705	GN8	CAH-CAG	2.81	1.46	1.37
3	B	702	GN8	OAA-CAU	2.78	1.29	1.23
3	F	706	GN8	OAA-CAU	2.77	1.29	1.23
3	E	705	GN8	OAA-CAU	2.67	1.29	1.23
3	A	701	GN8	OAA-CAU	2.67	1.29	1.23
2	D	604	MYA	C4A-N9A	-2.58	1.34	1.37
2	A	601	MYA	C4A-N9A	-2.50	1.34	1.37
2	E	605	MYA	C4A-N9A	-2.46	1.34	1.37
3	E	705	GN8	CAL-CAS	2.38	1.44	1.38
2	F	606	MYA	C4A-N9A	-2.32	1.34	1.37
2	B	602	MYA	C4A-N9A	-2.30	1.34	1.37
3	E	705	GN8	CAG-CAI	2.22	1.44	1.37
2	C	603	MYA	C4A-N9A	-2.17	1.34	1.37
3	E	705	GN8	CAU-NAX	-2.08	1.35	1.39
3	F	706	GN8	CAU-NAX	-2.05	1.35	1.39

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	MYA	N3A-C2A-N1A	-9.52	120.75	128.71
2	C	603	MYA	N3A-C2A-N1A	-9.16	121.05	128.71
2	D	604	MYA	N3A-C2A-N1A	-9.09	121.11	128.71
2	F	606	MYA	N3A-C2A-N1A	-8.99	121.20	128.71
2	A	601	MYA	N3A-C2A-N1A	-8.90	121.26	128.71
2	E	605	MYA	N3A-C2A-N1A	-8.90	121.27	128.71
3	C	703	GN8	CAF-CAW-CAU	8.53	129.11	120.44
3	B	702	GN8	SAP-CAV-NAX	8.40	118.67	110.00
3	D	704	GN8	SAP-CAV-NAX	8.34	118.60	110.00
3	A	701	GN8	SAP-CAV-NAX	8.34	118.60	110.00
3	C	703	GN8	SAP-CAV-NAX	8.23	118.49	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	706	GN8	SAP-CAV-NAX	8.18	118.44	110.00
3	E	705	GN8	SAP-CAV-NAX	8.16	118.42	110.00
3	C	703	GN8	CAF-CAW-SAP	-7.79	119.87	129.26
3	A	701	GN8	CAF-CAW-CAU	7.40	127.96	120.44
3	F	706	GN8	CAF-CAW-CAU	7.37	127.92	120.44
3	B	702	GN8	CAF-CAW-CAU	7.34	127.89	120.44
3	D	704	GN8	CAF-CAW-CAU	7.13	127.68	120.44
3	B	702	GN8	CAV-SAP-CAW	-6.82	86.33	92.89
3	D	704	GN8	CAV-SAP-CAW	-6.76	86.39	92.89
3	A	701	GN8	CAV-SAP-CAW	-6.73	86.41	92.89
3	F	706	GN8	CAV-SAP-CAW	-6.72	86.43	92.89
3	C	703	GN8	CAV-SAP-CAW	-6.69	86.45	92.89
3	B	702	GN8	CAF-CAW-SAP	-6.65	121.25	129.26
3	E	705	GN8	CAV-SAP-CAW	-6.63	86.51	92.89
3	F	706	GN8	CAF-CAW-SAP	-6.61	121.29	129.26
3	A	701	GN8	CAF-CAW-SAP	-6.58	121.33	129.26
3	D	704	GN8	CAF-CAW-SAP	-6.42	121.53	129.26
3	E	705	GN8	CAF-CAW-CAU	5.88	126.42	120.44
3	E	705	GN8	CAO-NAX-CAV	5.78	132.01	122.48
3	E	705	GN8	OAA-CAU-CAW	-5.54	119.73	126.44
3	E	705	GN8	CAW-CAU-NAX	5.46	118.89	110.11
3	D	704	GN8	CAN-CAT-CAQ	-5.42	119.11	121.78
3	D	704	GN8	CAO-NAX-CAV	5.35	131.30	122.48
3	A	701	GN8	CAO-NAX-CAV	5.34	131.29	122.48
3	A	701	GN8	CAW-CAU-NAX	5.18	118.44	110.11
3	E	705	GN8	CAN-CAT-CAQ	-5.17	119.23	121.78
3	B	702	GN8	CAO-NAX-CAV	5.14	130.95	122.48
3	A	701	GN8	OAA-CAU-CAW	-5.14	120.22	126.44
3	D	704	GN8	OAA-CAU-CAW	-5.08	120.28	126.44
3	E	705	GN8	CAF-CAW-SAP	-5.05	123.18	129.26
3	D	704	GN8	CAW-CAU-NAX	5.03	118.20	110.11
3	B	702	GN8	CAW-CAU-NAX	4.99	118.13	110.11
3	C	703	GN8	OAA-CAU-CAW	-4.92	120.48	126.44
3	E	705	GN8	CAV-NAX-CAU	-4.92	105.77	116.72
3	F	706	GN8	CAW-CAU-NAX	4.91	118.01	110.11
3	F	706	GN8	OAA-CAU-CAW	-4.90	120.51	126.44
3	B	702	GN8	OAA-CAU-CAW	-4.89	120.52	126.44
3	A	701	GN8	CAV-NAX-CAU	-4.89	105.84	116.72
3	F	706	GN8	CAO-NAX-CAV	4.84	130.46	122.48
3	D	704	GN8	CAV-NAX-CAU	-4.81	106.01	116.72
3	B	702	GN8	CAV-NAX-CAU	-4.81	106.01	116.72
3	F	706	GN8	CAV-NAX-CAU	-4.66	106.33	116.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	703	GN8	CAW-CAU-NAX	4.63	117.56	110.11
3	F	706	GN8	CAN-CAT-CAQ	-4.60	119.52	121.78
3	C	703	GN8	CAV-NAX-CAU	-4.60	106.48	116.72
3	B	702	GN8	CAN-CAT-CAQ	-4.38	119.62	121.78
3	E	705	GN8	CAS-CAO-NAX	4.36	119.35	113.01
3	C	703	GN8	CAN-CAT-CAQ	-4.32	119.66	121.78
2	F	606	MYA	N3A-C4A-N9A	4.29	133.18	125.43
2	C	603	MYA	N3A-C4A-N9A	4.23	133.07	125.43
2	B	602	MYA	N3A-C4A-N9A	4.23	133.06	125.43
3	D	704	GN8	CAS-CAO-NAX	4.19	119.11	113.01
3	C	703	GN8	CAR-CAF-CAW	-4.17	123.46	130.48
2	A	601	MYA	N3A-C4A-N9A	4.16	132.94	125.43
2	D	604	MYA	N3A-C4A-N9A	4.14	132.90	125.43
3	A	701	GN8	CAN-CAT-CAQ	-4.03	119.80	121.78
2	E	605	MYA	N3A-C4A-N9A	3.96	132.59	125.43
3	C	703	GN8	CAO-NAX-CAV	3.80	128.75	122.48
3	B	702	GN8	CAS-CAO-NAX	3.63	118.29	113.01
2	E	605	MYA	C2-C3-N4	-3.62	104.32	112.50
2	B	602	MYA	C7-N8-C9	3.59	129.94	122.57
3	A	701	GN8	SAP-CAV-SAE	-3.54	116.26	123.36
3	D	704	GN8	SAP-CAV-SAE	-3.50	116.34	123.36
3	C	703	GN8	SAP-CAV-SAE	-3.46	116.42	123.36
3	F	706	GN8	SAP-CAV-SAE	-3.45	116.44	123.36
3	B	702	GN8	SAP-CAV-SAE	-3.36	116.63	123.36
2	B	602	MYA	C6-C7-N8	-3.33	104.69	111.87
2	A	601	MYA	P2A-O3A-P1A	-3.32	121.95	131.68
3	E	705	GN8	SAP-CAV-SAE	-3.31	116.73	123.36
3	A	701	GN8	CAS-CAO-NAX	3.28	117.79	113.01
2	C	603	MYA	C2-C3-N4	-3.19	105.28	112.50
2	B	602	MYA	C2-C3-N4	-3.18	105.30	112.50
2	B	602	MYA	P2A-O3A-P1A	-3.14	122.47	131.68
2	A	601	MYA	C4M-C3M-C2M	-3.08	108.42	114.64
2	E	605	MYA	C6-C7-N8	-3.07	105.25	111.87
2	E	605	MYA	P2A-O3A-P1A	-3.04	122.77	131.68
2	F	606	MYA	C4M-C3M-C2M	-3.03	108.53	114.64
2	F	606	MYA	C2-C3-N4	-3.01	105.70	112.50
2	E	605	MYA	C11-C10-C9	3.00	115.64	112.73
2	A	601	MYA	C2-C3-N4	-2.96	105.81	112.50
2	B	602	MYA	C14-C11-C10	2.92	113.89	108.82
2	C	603	MYA	C5A-C4A-N3A	-2.92	119.35	125.70
2	F	606	MYA	C5A-C4A-N3A	-2.90	119.38	125.70
2	B	602	MYA	C5A-C4A-N3A	-2.85	119.49	125.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	605	MYA	C5A-C4A-N3A	-2.84	119.51	125.70
3	B	702	GN8	CAR-CAF-CAW	-2.84	125.70	130.48
2	D	604	MYA	P2A-O3A-P1A	-2.80	123.47	131.68
2	D	604	MYA	C5A-C4A-N3A	-2.78	119.66	125.70
2	A	601	MYA	C5A-C4A-N3A	-2.76	119.68	125.70
2	D	604	MYA	C7-N8-C9	2.76	128.25	122.57
3	F	706	GN8	CAR-CAF-CAW	-2.76	125.83	130.48
3	E	705	GN8	CAR-CAQ-CAT	2.74	120.79	117.35
2	A	601	MYA	C14-C11-C10	2.71	113.51	108.82
3	D	704	GN8	CAR-CAQ-CAT	2.64	120.66	117.35
2	D	604	MYA	C14-C11-C10	2.62	113.37	108.82
3	A	701	GN8	CAR-CAF-CAW	-2.58	126.14	130.48
2	F	606	MYA	C7-N8-C9	2.58	127.86	122.57
3	F	706	GN8	CAS-CAO-NAX	2.57	116.75	113.01
2	F	606	MYA	P2A-O3A-P1A	-2.56	124.17	131.68
3	A	701	GN8	CAR-CAQ-CAT	2.54	120.54	117.35
2	C	603	MYA	P2A-O3A-P1A	-2.54	124.24	131.68
3	F	706	GN8	CAR-CAQ-CAT	2.51	120.50	117.35
2	C	603	MYA	O4X-C1X-N9A	2.46	110.73	108.44
2	C	603	MYA	C4A-C5A-N7A	-2.44	107.43	109.52
2	F	606	MYA	C6-C7-N8	-2.44	106.60	111.87
2	E	605	MYA	C7-N8-C9	2.44	127.59	122.57
3	C	703	GN8	CAR-CAQ-CAT	2.43	120.40	117.35
2	C	603	MYA	C7-N8-C9	2.43	127.56	122.57
2	B	602	MYA	C4A-C5A-N7A	-2.42	107.45	109.52
3	B	702	GN8	CAR-CAQ-CAT	2.41	120.38	117.35
2	D	604	MYA	C6-C7-N8	-2.40	106.69	111.87
2	A	601	MYA	C7-N8-C9	2.39	127.48	122.57
2	A	601	MYA	O4X-C1X-N9A	2.39	110.66	108.44
2	D	604	MYA	C2-C3-N4	-2.38	107.13	112.50
2	C	603	MYA	C6-C7-N8	-2.35	106.80	111.87
2	E	605	MYA	C3-N4-C5	2.33	127.57	122.84
2	E	605	MYA	C4A-C5A-N7A	-2.32	107.53	109.52
3	E	705	GN8	CAL-CAS-CAM	2.32	122.07	118.16
3	D	704	GN8	CAR-CAF-CAW	-2.29	126.63	130.48
2	B	602	MYA	C2A-N3A-C4A	2.29	120.53	114.01
2	C	603	MYA	C2A-N3A-C4A	2.29	120.52	114.01
2	E	605	MYA	O4X-C1X-N9A	2.28	110.56	108.44
2	F	606	MYA	C2A-N3A-C4A	2.27	120.47	114.01
2	C	603	MYA	C3-N4-C5	2.26	127.44	122.84
2	F	606	MYA	C4A-C5A-N7A	-2.25	107.59	109.52
2	E	605	MYA	C14-C11-C10	2.22	112.66	108.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	MYA	C4A-C5A-N7A	-2.21	107.62	109.52
2	A	601	MYA	C3-N4-C5	2.21	127.34	122.84
2	E	605	MYA	C2A-N3A-C4A	2.21	120.30	114.01
2	D	604	MYA	C4A-C5A-N7A	-2.20	107.64	109.52
2	C	603	MYA	C4M-C3M-C2M	-2.20	110.21	114.64
2	D	604	MYA	C2A-N3A-C4A	2.19	120.25	114.01
2	B	602	MYA	C3-N4-C5	2.17	127.25	122.84
2	A	601	MYA	C2A-N3A-C4A	2.16	120.15	114.01
2	F	606	MYA	C14-C11-C10	2.13	112.51	108.82
2	D	604	MYA	C4M-C3M-C2M	-2.12	110.36	114.64
2	B	602	MYA	C8A-N9A-C4A	2.05	108.46	106.90
2	F	606	MYA	C3-N4-C5	2.03	126.96	122.84
2	A	601	MYA	C8A-N9A-C4A	2.02	108.44	106.90

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	603	MYA	C10
2	D	604	MYA	C10
2	E	605	MYA	C10
2	A	601	MYA	C10
2	F	606	MYA	C10
2	B	602	MYA	C10

There are no torsion outliers.

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	436/455 (95%)	-0.37	0 100 100	16, 31, 54, 69	0
1	B	436/455 (95%)	-0.39	0 100 100	15, 29, 56, 66	0
1	C	436/455 (95%)	-0.27	0 100 100	15, 42, 65, 104	0
1	D	436/455 (95%)	-0.36	0 100 100	17, 34, 54, 69	0
1	E	436/455 (95%)	-0.41	0 100 100	15, 26, 48, 65	0
1	F	435/455 (95%)	-0.23	0 100 100	17, 47, 66, 106	0
All	All	2615/2730 (95%)	-0.34	0 100 100	15, 34, 61, 106	0

There are no RSRZ outliers to report.

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(\AA^2)	Q<0.9
3	GN8	D	704	25/25	0.40	9.84	59,68,77,78	0
3	GN8	F	706	25/25	0.37	4.96	65,72,76,78	0
3	GN8	C	703	25/25	0.36	4.50	60,66,73,74	0
3	GN8	B	702	25/25	0.39	4.50	67,72,78,78	0
3	GN8	E	705	25/25	0.41	4.12	62,67,73,74	0
3	GN8	A	701	25/25	0.35	3.70	50,62,72,73	0
2	MYA	C	603	63/63	0.22	0.12	47,50,55,55	0
2	MYA	F	606	63/63	0.21	-0.07	53,60,65,66	0
2	MYA	E	605	63/63	0.14	-0.62	13,25,30,32	0
2	MYA	D	604	63/63	0.16	-0.67	25,39,43,43	0
2	MYA	B	602	63/63	0.13	-0.71	16,26,29,31	0
2	MYA	A	601	63/63	0.13	-0.84	21,31,44,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.