Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 09:00 am BST

PDB ID	:	4C2Z
Title	:	Human N-myristoyltransferase (NMT1) with Myristoyl-CoA and inhibitor bound
Authors	:	Thinon, E.; Serwa, R.A.; Brannigan, J.A.; Brassat, U.; Wright, M.H.; Heal, W.P.; Wilkinson, A.J.; Mann, D.J.; Tate, E.W.
Deposited on	:	2013-08-20
Resolution	:	2.08 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

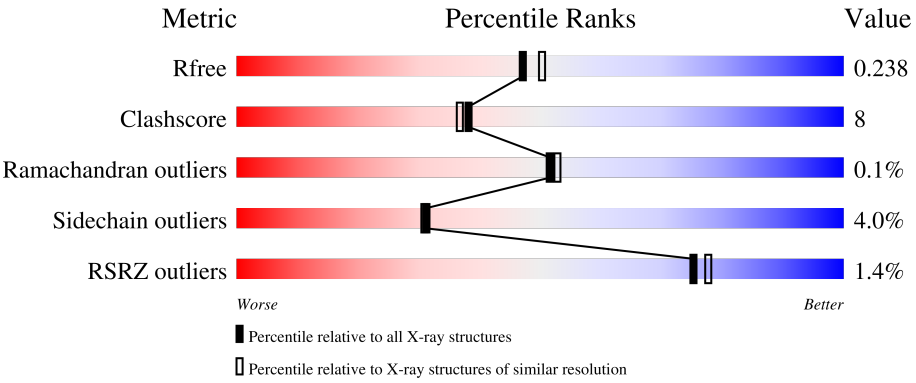
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

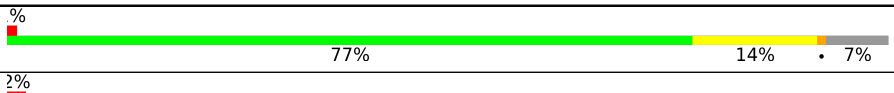
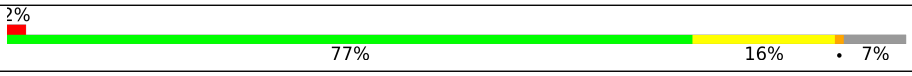
The reported resolution of this entry is 2.08 Å.

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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	A	410	
1	B	410	

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
3	646	B	1498	-	-	X	-
6	GOL	B	1502	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7221 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-TETRADECANOYLTRANSFERAS E 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	12	0
			3208	2084	544	564	16			
1	B	382	Total	C	N	O	S	0	15	0
			3226	2095	545	569	17			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	MET	-	expression tag	UNP P30419
A	88	GLY	-	expression tag	UNP P30419
A	89	SER	-	expression tag	UNP P30419
A	90	SER	-	expression tag	UNP P30419
A	91	HIS	-	expression tag	UNP P30419
A	92	HIS	-	expression tag	UNP P30419
A	93	HIS	-	expression tag	UNP P30419
A	94	HIS	-	expression tag	UNP P30419
A	95	HIS	-	expression tag	UNP P30419
A	96	HIS	-	expression tag	UNP P30419
A	97	SER	-	expression tag	UNP P30419
A	98	SER	-	expression tag	UNP P30419
A	99	GLY	-	expression tag	UNP P30419
A	100	LEU	-	expression tag	UNP P30419
A	101	GLU	-	expression tag	UNP P30419
A	102	VAL	-	expression tag	UNP P30419
A	103	LEU	-	expression tag	UNP P30419
A	104	PHE	-	expression tag	UNP P30419
A	105	GLN	-	expression tag	UNP P30419
A	106	GLY	-	expression tag	UNP P30419
A	107	PRO	-	expression tag	UNP P30419
A	108	HIS	-	expression tag	UNP P30419
B	87	MET	-	expression tag	UNP P30419
B	88	GLY	-	expression tag	UNP P30419

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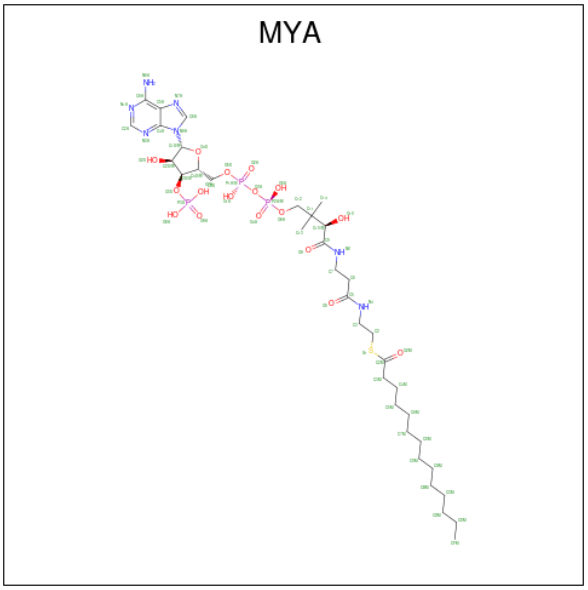
Chain	Residue	Modelled	Actual	Comment	Reference
B	89	SER	-	expression tag	UNP P30419
B	90	SER	-	expression tag	UNP P30419
B	91	HIS	-	expression tag	UNP P30419
B	92	HIS	-	expression tag	UNP P30419
B	93	HIS	-	expression tag	UNP P30419
B	94	HIS	-	expression tag	UNP P30419
B	95	HIS	-	expression tag	UNP P30419
B	96	HIS	-	expression tag	UNP P30419
B	97	SER	-	expression tag	UNP P30419
B	98	SER	-	expression tag	UNP P30419
B	99	GLY	-	expression tag	UNP P30419
B	100	LEU	-	expression tag	UNP P30419
B	101	GLU	-	expression tag	UNP P30419
B	102	VAL	-	expression tag	UNP P30419
B	103	LEU	-	expression tag	UNP P30419
B	104	PHE	-	expression tag	UNP P30419
B	105	GLN	-	expression tag	UNP P30419
B	106	GLY	-	expression tag	UNP P30419
B	107	PRO	-	expression tag	UNP P30419
B	108	HIS	-	expression tag	UNP P30419

- 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		

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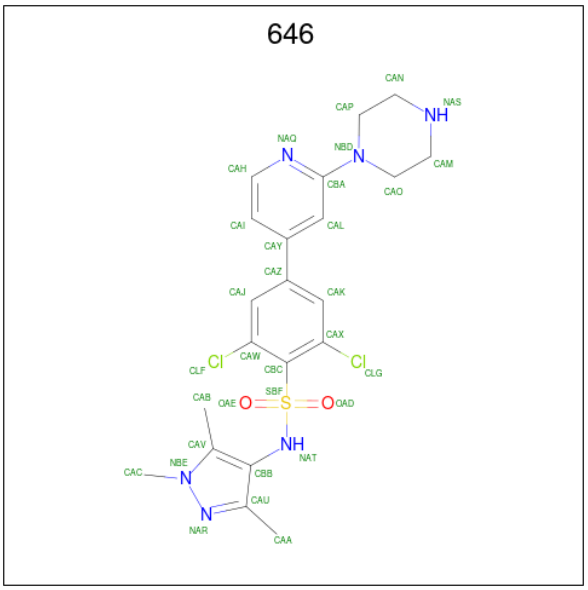
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- Molecule 3 is 2,6-dichloro-4-(2-piperazin-1-ylpyridin-4-yl)-N-(1,3,5-trimethyl-1H-pyrazol-4-yl)benzenesulfonamide (three-letter code: 646) (formula: $C_{21}H_{24}Cl_2N_6O_2S$).

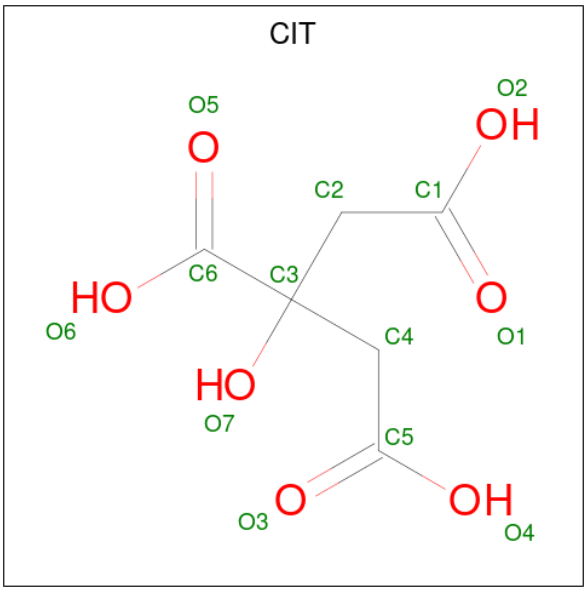


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			32	21	2	6	2	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			32	21	2	6	2	1		

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

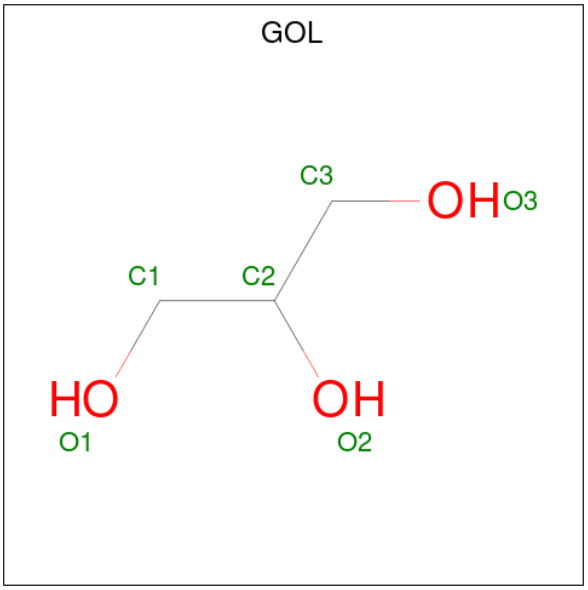
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 6 7	0	0
5	B	1	Total C O 13 6 7	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total Cl 3 3	0	0
7	B	5	Total Cl 5 5	0	0

- Molecule 8 is water.

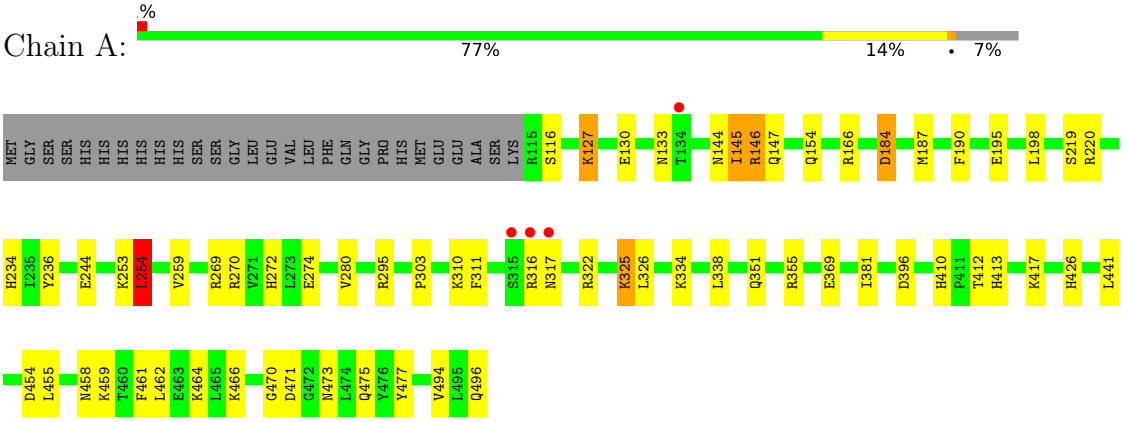
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	283	Total O 283 283	0	0
8	B	254	Total O 254 254	0	0

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.

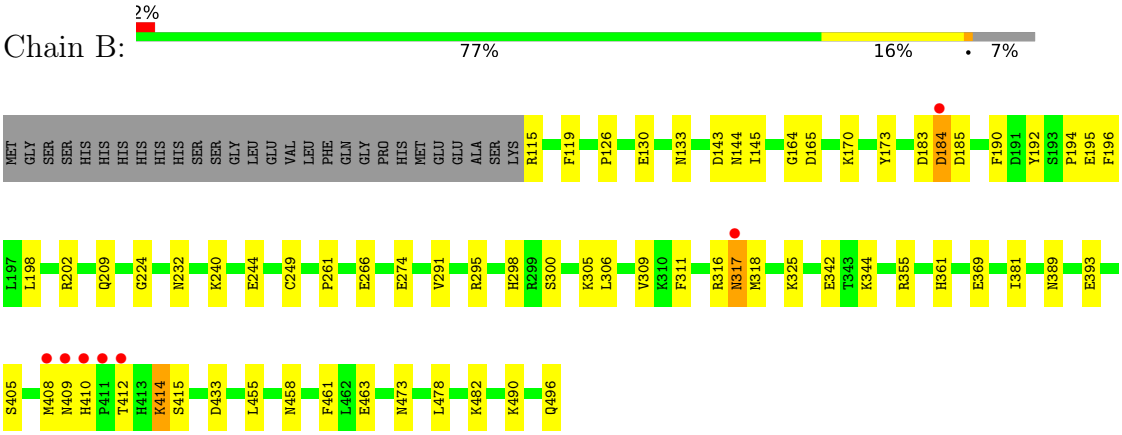
• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE 1

Chain A:



• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	78.63Å 179.12Å 58.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.56 – 2.08 89.56 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.9 (89.56-2.08) 100.0 (89.56-2.08)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.34 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.169 , 0.238 0.170 , 0.238	Depositor DCC
R_{free} test set	2515 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.848	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7221	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GOL, CIT, MYA, 646, CL, 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	A	0.81	0/3334	0.88	6/4524 (0.1%)
1	B	0.86	1/3362 (0.0%)	0.86	2/4563 (0.0%)
All	All	0.84	1/6696 (0.0%)	0.87	8/9087 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	266	GLU	CD-OE2	5.22	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	254[A]	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	254[B]	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	270	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	146	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	146	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	B	145	ILE	CG1-CB-CG2	-5.75	98.74	111.40
1	B	433	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	198	LEU	CA-CB-CG	5.09	127.02	115.30

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	3208	0	3245	45	0
1	B	3226	0	3255	53	0
2	A	63	0	58	0	0
2	B	63	0	58	0	0
3	A	32	0	24	5	0
3	B	32	0	24	10	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	13	0	5	1	0
5	B	13	0	5	2	0
6	A	12	0	16	3	0
6	B	12	0	16	8	0
7	A	3	0	0	0	0
7	B	5	0	0	0	0
8	A	283	0	0	7	0
8	B	254	0	0	7	0
All	All	7221	0	6706	102	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 8.

All (102) 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:A:494:VAL:O	6:A:1502:GOL:H31	1.48	1.11
1:B:173[B]:TYR:CD2	1:B:194:PRO:HG3	1.92	1.02
1:B:291[A]:VAL:CG1	6:B:1502:GOL:H2	1.92	0.99
1:B:291[A]:VAL:HG13	6:B:1502:GOL:H2	1.46	0.96
1:B:173[B]:TYR:CE2	1:B:194:PRO:HG3	2.04	0.91
1:A:187:MET:HE1	1:A:310:LYS:HE2	1.59	0.85
1:A:254[A]:LEU:CD2	1:A:259:VAL:HG21	2.08	0.83
1:B:291[B]:VAL:HG22	6:B:1502:GOL:H2	1.60	0.82
1:B:183:ASP:HA	3:B:1498:646:HABA	1.62	0.81
1:A:127[A]:LYS:HG3	1:A:130:GLU:OE2	1.92	0.70
5:B:1500:CIT:O6	8:B:2131:HOH:O	2.12	0.68
1:A:494:VAL:O	6:A:1502:GOL:C3	2.36	0.66
1:A:184:ASP:OD1	1:A:184:ASP:N	2.29	0.66
1:B:291[A]:VAL:HG13	6:B:1502:GOL:C2	2.25	0.66
1:A:410:HIS:HD2	1:A:412:THR:H	1.44	0.66
1:A:254[A]:LEU:HD23	1:A:259:VAL:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ARG:HD3	8:B:2147:HOH:O	1.98	0.62
1:A:496:GLN:HE22	6:A:1502:GOL:H2	1.64	0.62
1:A:145[A]:ILE:HD12	1:A:272:HIS:HB2	1.83	0.61
1:B:408:MET:O	1:B:409:ASN:HB2	2.01	0.61
1:B:496:GLN:HE22	6:B:1501:GOL:H11	1.69	0.58
1:B:317:ASN:HD22	1:B:317:ASN:N	2.02	0.58
1:B:298[A]:HIS:HE1	3:B:1498:646:OAD	1.86	0.57
3:B:1498:646:OAD	3:B:1498:646:CLG	2.59	0.57
5:B:1500:CIT:O4	5:B:1500:CIT:H22	2.05	0.56
1:A:303:PRO:HD2	8:A:2185:HOH:O	2.06	0.56
1:A:295[B]:ARG:HD2	1:A:473:ASN:OD1	2.05	0.56
1:B:291[B]:VAL:HG22	6:B:1502:GOL:C2	2.34	0.55
1:B:361:HIS:CD2	1:B:490[B]:LYS:HG2	2.41	0.54
1:A:351:GLN:NE2	1:B:144[A]:ASN:OD1	2.39	0.54
1:B:183:ASP:C	1:B:185:ASP:H	2.10	0.54
1:B:458:ASN:HA	1:B:461:PHE:CE2	2.42	0.54
1:B:295:ARG:HD2	1:B:473:ASN:OD1	2.07	0.54
1:A:454:ASP:HB2	1:A:459:LYS:HE3	1.90	0.53
1:A:195[B]:GLU:HG3	1:A:381:ILE:HD11	1.90	0.53
1:B:130:GLU:OE2	1:B:482:LYS:CE	2.57	0.53
1:B:126:PRO:HG3	1:B:482:LYS:HG3	1.91	0.53
1:B:291[A]:VAL:HG12	6:B:1502:GOL:H2	1.88	0.53
1:A:417[A]:LYS:HG2	8:A:2245:HOH:O	2.09	0.52
1:A:311:PHE:HE1	3:A:1498:646:HAA	1.75	0.51
1:A:166:ARG:HD3	8:A:2056:HOH:O	2.09	0.51
1:B:389:ASN:OD1	1:B:393[A]:GLU:HG2	2.11	0.50
1:A:322:ARG:NH1	1:A:325:LYS:HE3	2.26	0.50
5:A:1500:CIT:H22	5:A:1500:CIT:O4	2.11	0.50
1:A:355:ARG:NH2	1:B:143[A]:ASP:OD2	2.35	0.50
1:A:145[A]:ILE:HD12	1:A:272:HIS:CB	2.41	0.49
1:A:219:SER:O	1:A:220:ARG:HB2	2.12	0.49
1:B:209[A]:GLN:HG3	8:B:2092:HOH:O	2.11	0.49
1:A:244:GLU:HG2	1:A:280:VAL:CG1	2.43	0.49
1:B:414:LYS:HB2	1:B:414:LYS:HE3	1.60	0.48
1:B:355[B]:ARG:HD2	8:B:2109:HOH:O	2.12	0.48
1:B:170:LYS:HA	1:B:173[B]:TYR:CE2	2.49	0.48
1:B:164:GLY:H	1:B:202:ARG:NH2	2.11	0.48
1:B:190:PHE:CE1	3:B:1498:646:HACA	2.49	0.48
1:B:192:TYR:HD1	1:B:196:PHE:CD1	2.31	0.48
1:A:458:ASN:HA	1:A:461:PHE:CE2	2.49	0.48
1:A:475[A]:GLN:HB2	1:A:477:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1498:646:HAN	8:A:2087:HOH:O	2.13	0.47
1:A:145[A]:ILE:HD11	1:A:269:ARG:O	2.14	0.47
1:B:311:PHE:HE2	3:B:1498:646:HAA	1.78	0.47
1:A:147:GLN:NE2	8:A:2024:HOH:O	2.33	0.47
1:B:389:ASN:ND2	1:B:393[A]:GLU:HG2	2.29	0.46
1:A:190:PHE:CE1	3:A:1498:646:HACA	2.49	0.46
1:B:183:ASP:HA	3:B:1498:646:CAB	2.40	0.46
1:B:342:GLU:OE1	1:B:344:LYS:HE2	2.14	0.46
1:A:295[B]:ARG:NH2	1:A:470:GLY:O	2.46	0.46
1:A:244:GLU:HG2	1:A:280:VAL:HG13	1.98	0.46
1:B:119:PHE:CD1	1:B:261:PRO:HB3	2.51	0.46
1:B:305:LYS:O	1:B:309:VAL:HG22	2.16	0.45
1:B:300:SER:HB3	1:B:306:LEU:HD12	1.98	0.45
1:B:190:PHE:CD1	3:B:1498:646:HACA	2.52	0.45
1:A:253:LYS:HD3	1:A:253:LYS:HA	1.80	0.45
1:B:173[B]:TYR:CE2	1:B:194:PRO:CG	2.90	0.44
1:A:116:SER:HA	8:A:2001:HOH:O	2.17	0.44
1:A:410:HIS:CD2	1:A:412:THR:H	2.31	0.44
3:A:1498:646:OAE	3:A:1498:646:CLF	2.73	0.44
1:B:311:PHE:HE2	3:B:1498:646:CAA	2.30	0.44
1:B:389:ASN:CG	1:B:393[A]:GLU:HG2	2.38	0.44
1:B:165:ASP:OD1	1:B:165:ASP:C	2.56	0.43
1:A:274:GLU:OE2	1:B:369:GLU:HG3	2.19	0.43
1:A:326:LEU:HD12	1:A:466:LYS:HE3	2.00	0.43
1:B:482:LYS:HB3	8:B:2007:HOH:O	2.19	0.42
1:A:396:ASP:OD2	1:A:426:HIS:HA	2.20	0.42
1:B:389:ASN:HD21	1:B:393[A]:GLU:CG	2.32	0.42
1:A:234:HIS:CE1	1:A:236:TYR:O	2.72	0.42
1:B:244:GLU:OE2	6:B:1501:GOL:O3	2.33	0.42
1:B:195:GLU:HB3	1:B:381:ILE:HD11	2.02	0.42
1:B:291[B]:VAL:HG21	1:B:478:LEU:HG	2.02	0.42
1:A:326:LEU:CD1	1:A:466:LYS:HE3	2.50	0.42
1:B:405:SER:O	1:B:415:SER:HB2	2.20	0.42
3:B:1498:646:OAE	3:B:1498:646:CLF	2.75	0.42
3:B:1498:646:HAM	8:B:2139:HOH:O	2.20	0.42
1:A:322:ARG:HH11	1:A:325:LYS:HE3	1.85	0.41
1:A:471:ASP:O	3:A:1498:646:CLF	2.75	0.41
1:B:130:GLU:OE2	1:B:482:LYS:HE3	2.20	0.41
1:A:338:LEU:HD21	1:A:441:LEU:HD11	2.02	0.41
1:A:369:GLU:HG3	1:B:274:GLU:OE2	2.21	0.41
1:A:417[A]:LYS:CG	8:A:2245:HOH:O	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:GLU:HG3	8:B:2233:HOH:O	2.20	0.41
1:A:458:ASN:O	1:A:462:LEU:HG	2.21	0.40
1:B:224:GLY:HA2	1:B:249:CYS:O	2.21	0.40
1:A:410:HIS:CD2	1:A:413:HIS:H	2.39	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	392/410 (96%)	378 (96%)	14 (4%)	0	100 100
1	B	395/410 (96%)	380 (96%)	14 (4%)	1 (0%)	41 39
All	All	787/820 (96%)	758 (96%)	28 (4%)	1 (0%)	51 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	ASP

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	360/372 (97%)	343 (95%)	17 (5%)	26 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	363/372 (98%)	349 (96%)	14 (4%)	32 32
All	All	723/744 (97%)	692 (96%)	31 (4%)	31 28

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127[A]	LYS
1	A	127[B]	LYS
1	A	133	ASN
1	A	144	ASN
1	A	145[A]	ILE
1	A	145[B]	ILE
1	A	146	ARG
1	A	154	GLN
1	A	184	ASP
1	A	254[A]	LEU
1	A	254[B]	LEU
1	A	316	ARG
1	A	317	ASN
1	A	325	LYS
1	A	334	LYS
1	A	455	LEU
1	A	464	LYS
1	B	115	ARG
1	B	133	ASN
1	B	184	ASP
1	B	198	LEU
1	B	232	ASN
1	B	240	LYS
1	B	316	ARG
1	B	317	ASN
1	B	318	MET
1	B	325	LYS
1	B	410	HIS
1	B	412	THR
1	B	414	LYS
1	B	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	234	HIS
1	A	351	GLN
1	A	410	HIS
1	B	317	ASN
1	B	361	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	B	1497	4	57,65,65	0.85	0	68,91,91	1.85	12 (17%)
5	CIT	A	1500	-	12,12,12	1.06	0	17,17,17	1.46	3 (17%)
3	646	A	1498	-	30,35,35	2.03	7 (23%)	42,52,52	2.94	16 (38%)
6	GOL	B	1502	-	5,5,5	0.72	0	5,5,5	0.46	0
5	CIT	B	1500	-	12,12,12	1.19	1 (8%)	17,17,17	1.50	3 (17%)
6	GOL	A	1502	-	5,5,5	0.40	0	5,5,5	0.46	0
3	646	B	1498	-	30,35,35	2.57	6 (20%)	42,52,52	3.15	15 (35%)
6	GOL	A	1501	-	5,5,5	0.49	0	5,5,5	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MYA	A	1497	4	57,65,65	1.04	3 (5%)	68,91,91	1.56	11 (16%)
6	GOL	B	1501	-	5,5,5	0.66	0	5,5,5	0.92	0

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	B	1497	4	-	3/60/80/80	0/3/3/3
5	CIT	A	1500	-	-	2/16/16/16	-
3	646	A	1498	-	-	0/17/27/27	0/4/4/4
6	GOL	B	1502	-	-	0/4/4/4	-
5	CIT	B	1500	-	-	3/16/16/16	-
6	GOL	A	1502	-	-	2/4/4/4	-
3	646	B	1498	-	-	3/17/27/27	0/4/4/4
6	GOL	A	1501	-	-	0/4/4/4	-
2	MYA	A	1497	4	-	2/60/80/80	0/3/3/3
6	GOL	B	1501	-	-	4/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1498	646	CBC-SBF	-9.86	1.63	1.79
3	B	1498	646	CAV-NBE	7.19	1.47	1.37
3	A	1498	646	CBC-SBF	-6.93	1.68	1.79
3	A	1498	646	CAV-NBE	5.37	1.45	1.37
3	A	1498	646	OAD-SBF	3.07	1.47	1.43
2	A	1497	MYA	C2M-S1	-3.06	1.68	1.76
3	B	1498	646	CAX-CLG	2.76	1.80	1.73
2	A	1497	MYA	C2A-N3A	2.62	1.36	1.32
3	B	1498	646	CAU-NAR	2.54	1.38	1.33
3	B	1498	646	CBB-NAT	2.53	1.49	1.43
3	B	1498	646	CAW-CLF	2.53	1.79	1.73
3	A	1498	646	CBA-NBD	2.35	1.42	1.37
5	B	1500	CIT	O5-C6	2.24	1.29	1.22
2	A	1497	MYA	C9-N8	-2.23	1.28	1.33
3	A	1498	646	CAJ-CAW	2.18	1.42	1.38
3	A	1498	646	CAU-NAR	2.13	1.37	1.33
3	A	1498	646	CAW-CLF	2.01	1.78	1.73

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1498	646	OAE-SBF-OAD	-9.54	107.82	119.55
3	A	1498	646	OAD-SBF-CBC	8.44	121.29	108.74
3	B	1498	646	CAU-NAR-NBE	8.02	111.24	104.35
3	A	1498	646	CAY-CAL-CBA	7.42	120.87	118.25
3	A	1498	646	CAB-CAV-CBB	7.19	138.31	129.07
3	B	1498	646	CBC-SBF-NAT	6.95	114.52	106.68
2	B	1497	MYA	O2M-C2M-C3M	-6.75	116.02	123.99
3	B	1498	646	CAB-CAV-CBB	6.47	137.38	129.07
2	B	1497	MYA	N3A-C2A-N1A	-6.08	119.18	128.68
2	A	1497	MYA	N3A-C2A-N1A	-5.86	119.52	128.68
2	B	1497	MYA	C3M-C2M-S1	5.77	120.17	113.46
3	A	1498	646	OAE-SBF-OAD	-5.60	112.66	119.55
3	B	1498	646	CAC-NBE-CAV	-5.47	121.68	128.82
3	B	1498	646	CAX-CBC-SBF	-5.20	119.83	123.27
3	B	1498	646	CAY-CAL-CBA	4.52	119.85	118.25
3	B	1498	646	CAP-NBD-CAO	4.45	121.35	111.52
3	A	1498	646	CAP-NBD-CAO	4.20	120.80	111.52
3	A	1498	646	CAC-NBE-CAV	-4.18	123.35	128.82
2	B	1497	MYA	O4X-C1X-C2X	-4.17	100.83	106.93
2	A	1497	MYA	C6-C5-N4	4.14	123.40	116.42
2	A	1497	MYA	C3M-C2M-S1	4.04	118.16	113.46
3	A	1498	646	CAU-NAR-NBE	3.78	107.60	104.35
5	A	1500	CIT	O6-C6-C3	3.70	119.47	113.05
3	A	1498	646	CAH-NAQ-CBA	3.55	121.56	116.86
2	A	1497	MYA	O5-C5-C6	-3.42	115.76	122.02
3	A	1498	646	CAJ-CAW-CBC	3.40	124.79	121.37
3	A	1498	646	CAI-CAH-NAQ	-3.39	119.75	123.96
2	B	1497	MYA	C4M-C3M-C2M	-3.30	105.01	112.33
3	B	1498	646	CAH-NAQ-CBA	3.28	121.20	116.86
3	A	1498	646	CAK-CAX-CBC	3.21	124.60	121.37
2	A	1497	MYA	O2M-C2M-C3M	-3.17	120.24	123.99
3	B	1498	646	CAV-NBE-NAR	-3.09	108.33	112.10
2	B	1497	MYA	C6-C5-N4	2.89	121.29	116.42
5	B	1500	CIT	O7-C3-C6	2.88	112.90	108.86
2	B	1497	MYA	O3X-P3X-O9A	-2.85	98.40	109.39
3	A	1498	646	OAD-SBF-NAT	-2.78	99.79	106.73
3	B	1498	646	CAA-CAU-NAR	2.73	125.67	119.78
3	B	1498	646	CAI-CAY-CAZ	-2.71	116.66	121.36
3	A	1498	646	NAQ-CBA-NBD	2.68	120.81	116.79
3	B	1498	646	CBB-NAT-SBF	2.65	126.60	121.88
2	B	1497	MYA	P2A-O3A-P1A	-2.50	124.24	132.83
3	B	1498	646	CAI-CAH-NAQ	-2.48	120.88	123.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1497	MYA	O5X-C5X-C4X	-2.39	100.78	108.99
5	B	1500	CIT	C3-C4-C5	-2.37	108.07	113.81
3	B	1498	646	CAL-CAY-CAZ	2.32	124.70	120.86
2	B	1497	MYA	O5A-P2A-O4A	2.24	123.30	112.24
3	A	1498	646	CAX-CBC-SBF	2.23	124.74	123.27
5	A	1500	CIT	O5-C6-C3	-2.23	119.10	122.25
2	B	1497	MYA	C2A-N1A-C6A	2.21	122.53	118.75
2	A	1497	MYA	C2-S1-C2M	2.19	108.69	101.87
2	A	1497	MYA	C7-C6-C5	-2.16	108.76	112.36
2	B	1497	MYA	O6A-C12-C11	-2.15	107.09	110.55
5	A	1500	CIT	O4-C5-C4	2.13	121.20	114.35
2	A	1497	MYA	O7A-P3X-O9A	2.10	118.90	110.68
5	B	1500	CIT	O4-C5-C4	2.09	121.07	114.35
2	A	1497	MYA	P2A-O3A-P1A	-2.09	125.67	132.83
3	A	1498	646	CBB-NAT-SBF	-2.07	118.19	121.88
2	A	1497	MYA	O4X-C1X-C2X	-2.05	103.93	106.93
3	A	1498	646	CAL-CBA-NAQ	-2.04	119.19	122.73
2	B	1497	MYA	O8A-P3X-O7A	2.03	115.38	107.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1502	GOL	O1-C1-C2-C3
3	B	1498	646	CBB-NAT-SBF-OAD
3	B	1498	646	CBB-NAT-SBF-CBC
6	A	1502	GOL	O1-C1-C2-O2
6	B	1501	GOL	O1-C1-C2-C3
6	B	1501	GOL	C1-C2-C3-O3
6	B	1501	GOL	O2-C2-C3-O3
2	A	1497	MYA	C6-C7-N8-C9
2	A	1497	MYA	C8M-C9M-CAM-CBM
5	B	1500	CIT	C1-C2-C3-C6
6	B	1501	GOL	O1-C1-C2-O2
5	B	1500	CIT	C1-C2-C3-C4
2	B	1497	MYA	C8M-C9M-CAM-CBM
2	B	1497	MYA	C6-C7-N8-C9
3	B	1498	646	NAQ-CBA-NBD-CAO
2	B	1497	MYA	C3X-O3X-P3X-O7A
5	A	1500	CIT	C3-C4-C5-O3
5	A	1500	CIT	C3-C4-C5-O4
5	B	1500	CIT	C1-C2-C3-O7

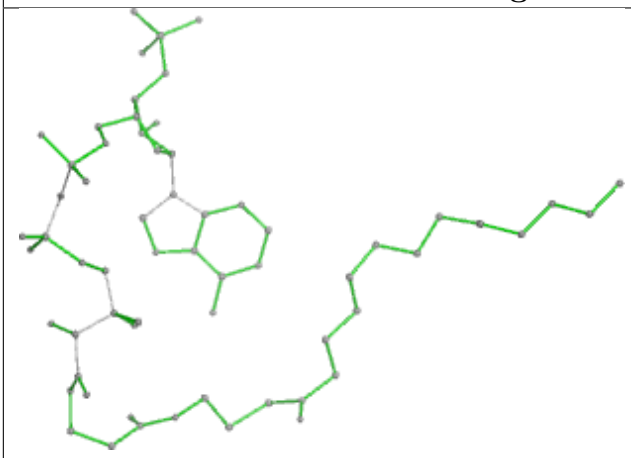
There are no ring outliers.

7 monomers are involved in 29 short contacts:

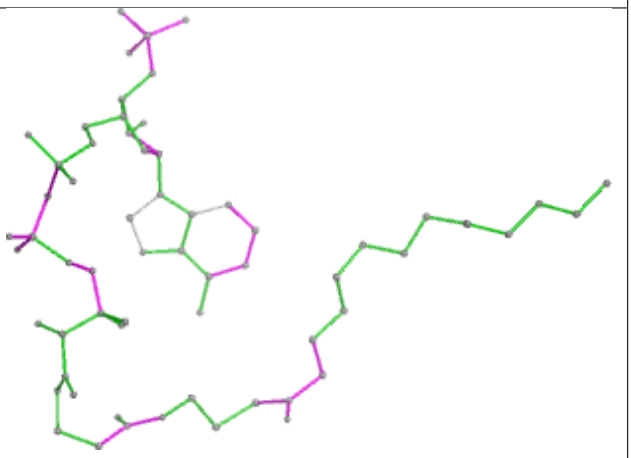
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1500	CIT	1	0
3	A	1498	646	5	0
6	B	1502	GOL	6	0
5	B	1500	CIT	2	0
6	A	1502	GOL	3	0
3	B	1498	646	10	0
6	B	1501	GOL	2	0

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.

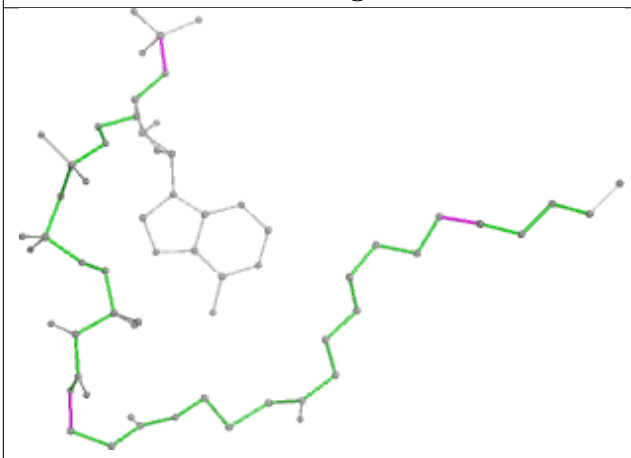
Ligand MYA B 1497



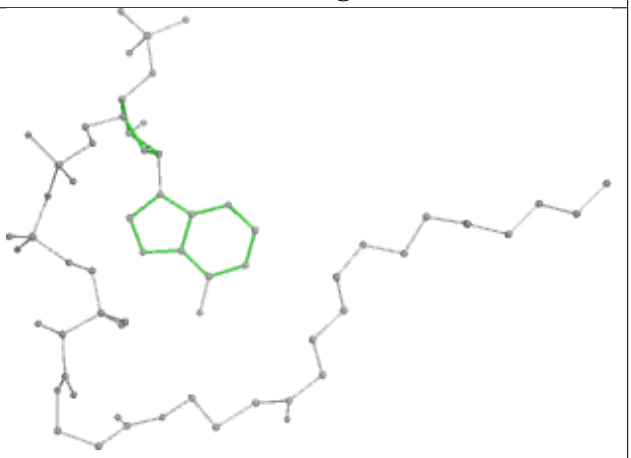
Bond lengths



Bond angles

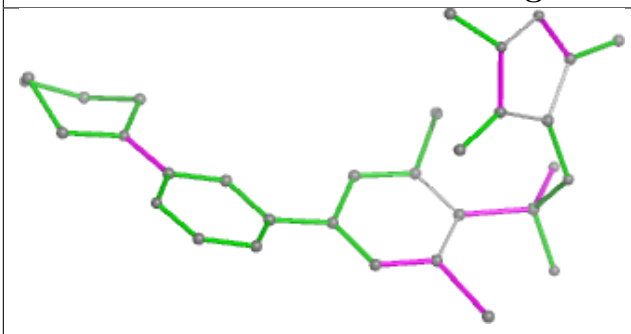


Torsions

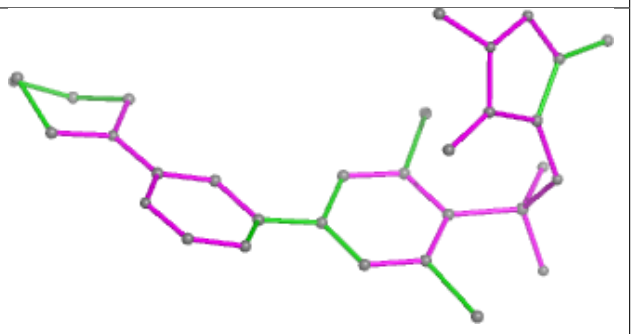


Rings

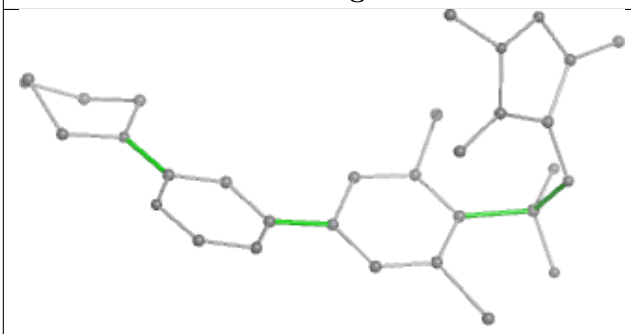
Ligand 646 A 1498



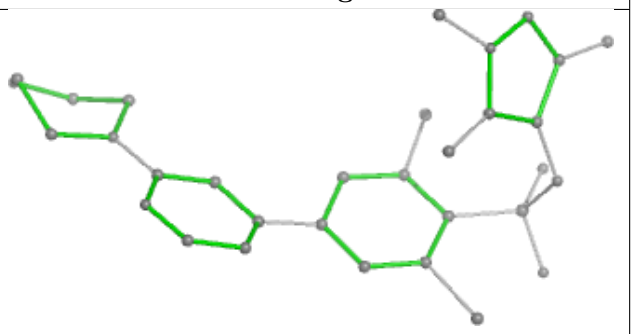
Bond lengths



Bond angles

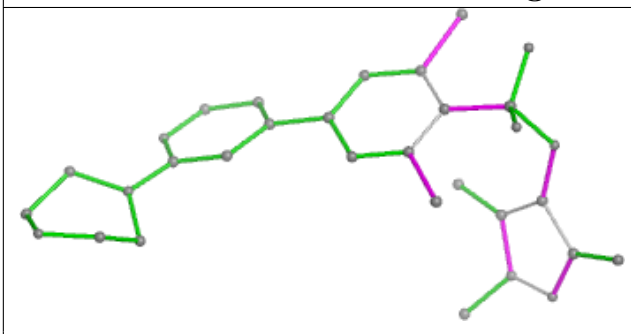


Torsions

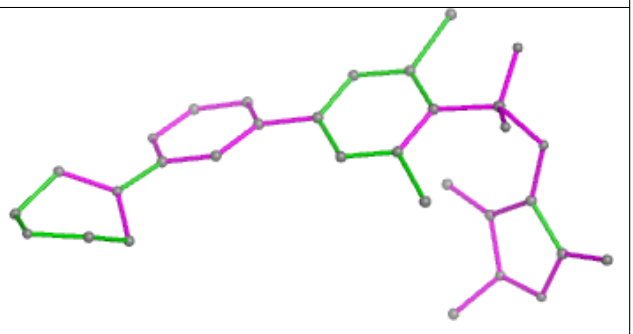


Rings

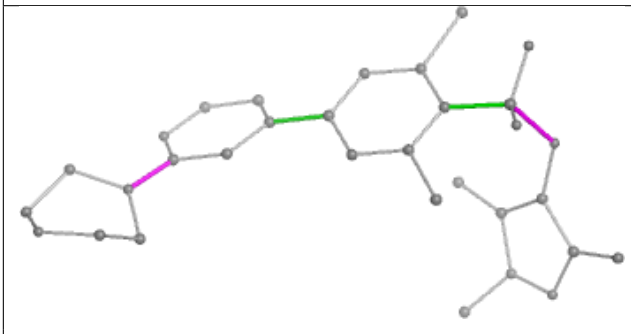
Ligand 646 B 1498



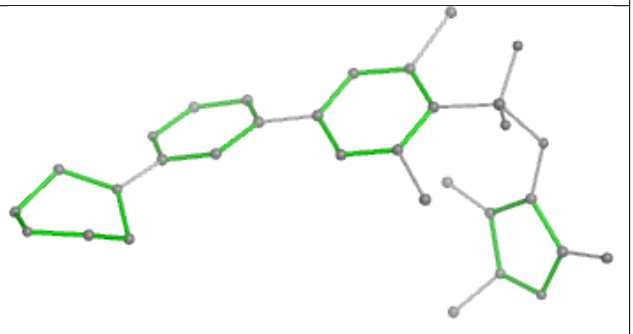
Bond lengths



Bond angles

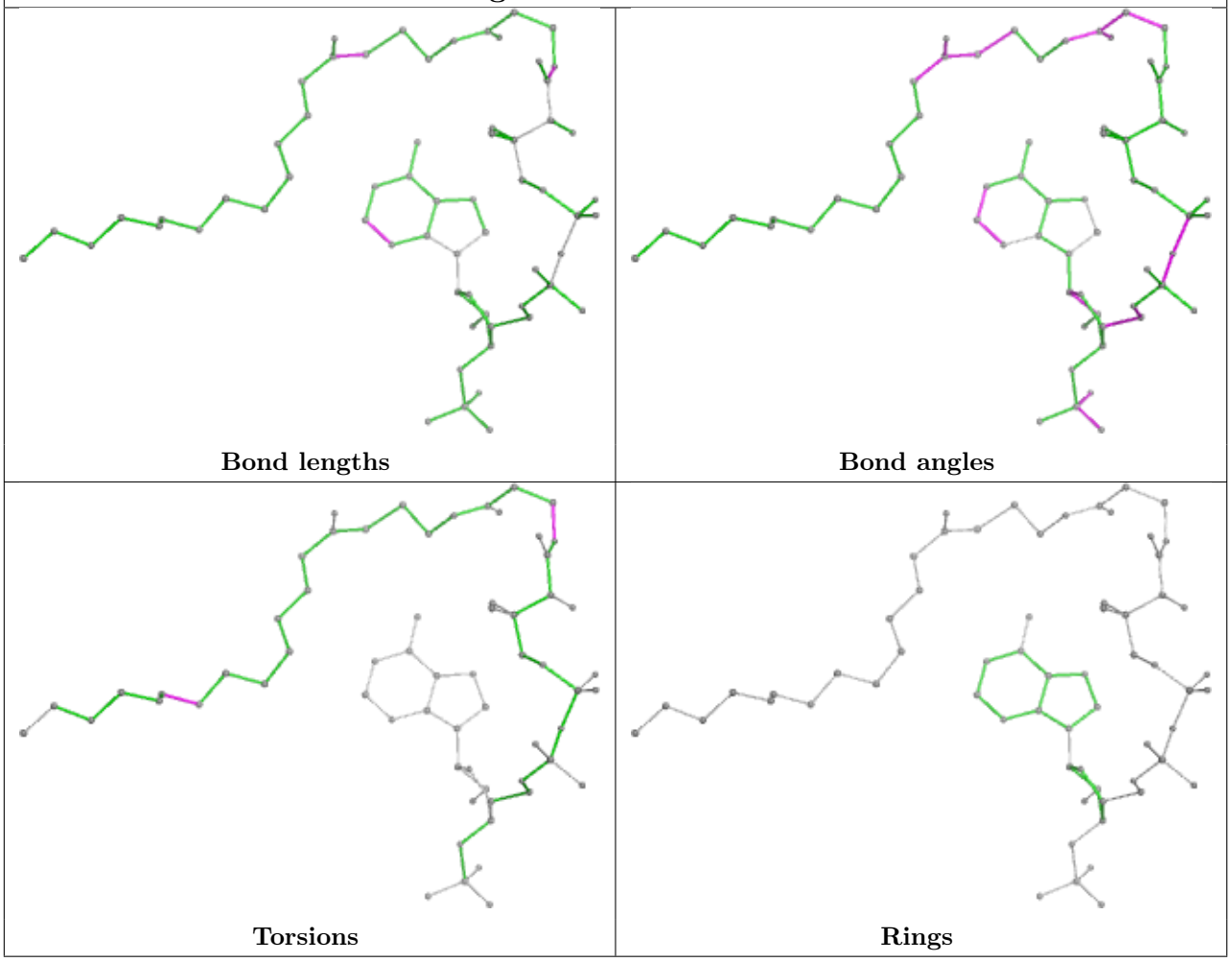


Torsions



Rings

Ligand MYA A 1497



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	382/410 (93%)	-0.68	4 (1%)	82	84	12, 21, 52, 89	0
1	B	382/410 (93%)	-0.67	7 (1%)	68	71	11, 20, 51, 129	1 (0%)
All	All	764/820 (93%)	-0.67	11 (1%)	75	78	11, 21, 52, 129	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	SER	5.7
1	B	411	PRO	5.0
1	A	316	ARG	4.1
1	B	412	THR	3.8
1	B	410	HIS	2.7
1	B	409	ASN	2.6
1	A	317	ASN	2.1
1	B	184	ASP	2.1
1	A	134	THR	2.1
1	B	317	ASN	2.0
1	B	408	MET	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 monosaccharides in this entry.

6.4 Ligands (i)

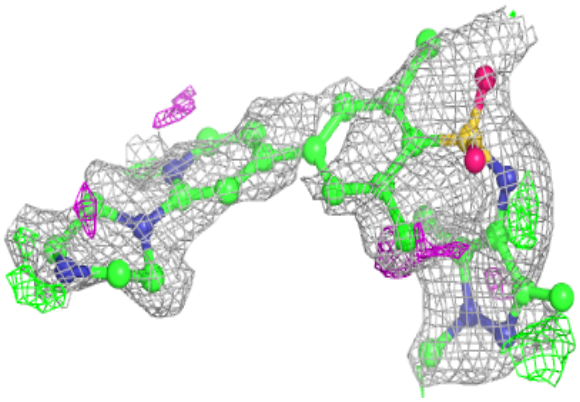
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

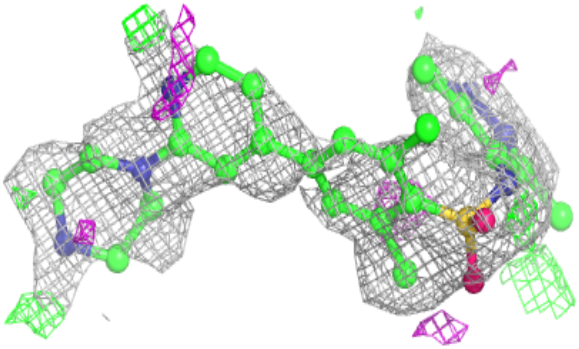
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	646	B	1498	32/32	0.77	0.22	55,71,102,119	0
6	GOL	B	1501	6/6	0.78	0.24	37,44,49,51	0
5	CIT	B	1500	13/13	0.88	0.15	35,41,44,46	0
3	646	A	1498	32/32	0.90	0.13	29,41,50,53	0
5	CIT	A	1500	13/13	0.90	0.15	33,46,56,62	0
6	GOL	A	1502	6/6	0.92	0.23	27,35,39,40	0
6	GOL	B	1502	6/6	0.94	0.16	22,27,31,37	0
4	MG	B	1499	1/1	0.96	0.17	27,27,27,27	0
7	CL	A	1503	1/1	0.96	0.05	31,31,31,31	0
7	CL	B	1506	1/1	0.97	0.05	35,35,35,35	0
2	MYA	B	1497	63/63	0.98	0.07	7,18,22,23	0
4	MG	A	1499	1/1	0.98	0.14	28,28,28,28	0
6	GOL	A	1501	6/6	0.98	0.10	27,30,31,32	0
7	CL	A	1504	1/1	0.98	0.12	21,21,21,21	0
7	CL	B	1505	1/1	0.98	0.09	24,24,24,24	0
2	MYA	A	1497	63/63	0.98	0.07	11,18,25,25	0
7	CL	B	1507	1/1	0.98	0.07	27,27,27,27	0
7	CL	A	1505	1/1	0.99	0.09	40,40,40,40	0
7	CL	B	1503	1/1	0.99	0.08	25,25,25,25	0
7	CL	B	1504	1/1	0.99	0.12	22,22,22,22	0

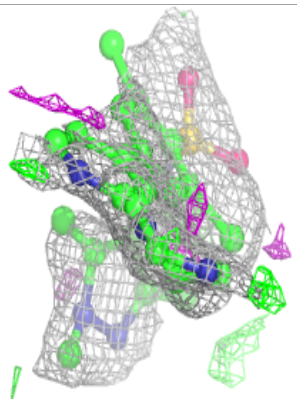
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 646 B 1498:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

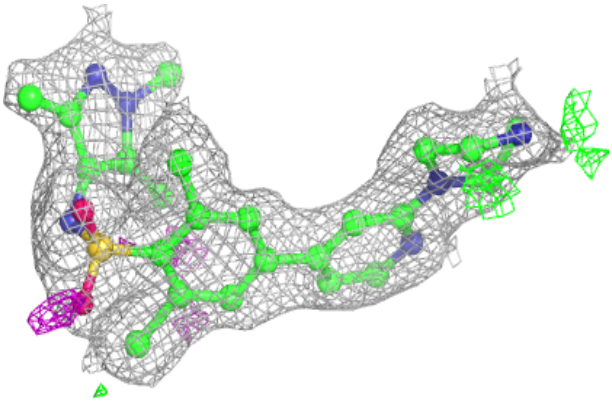


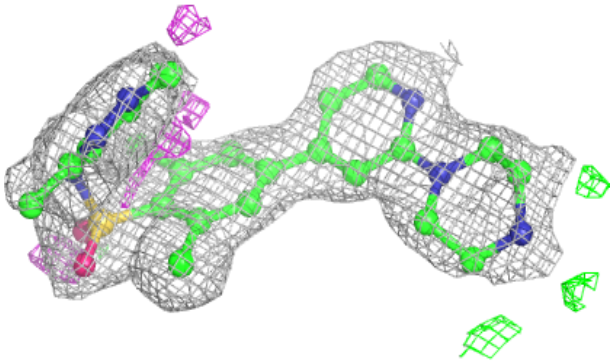


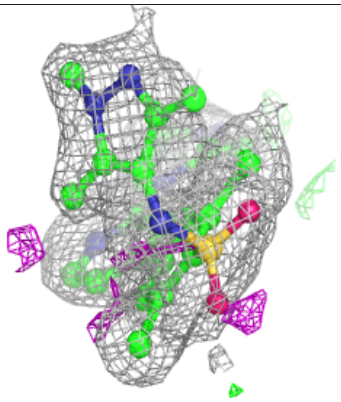


Electron density around 646 A 1498:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

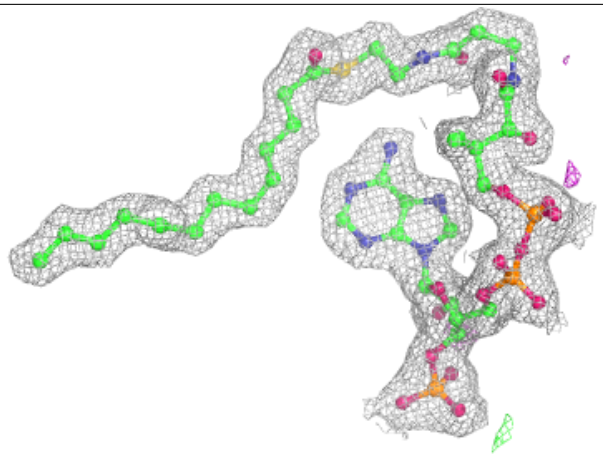


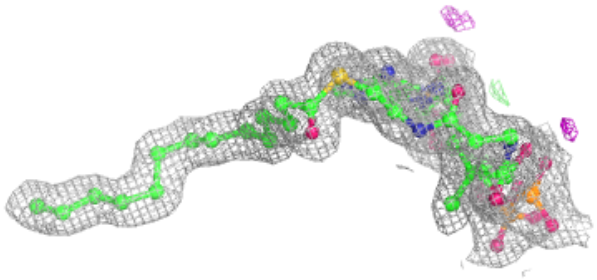


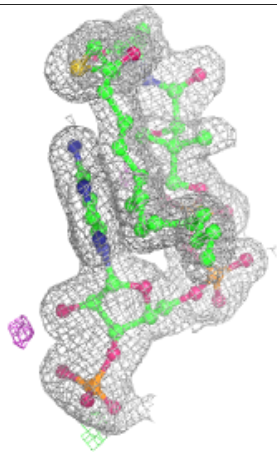


Electron density around MYA B 1497:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

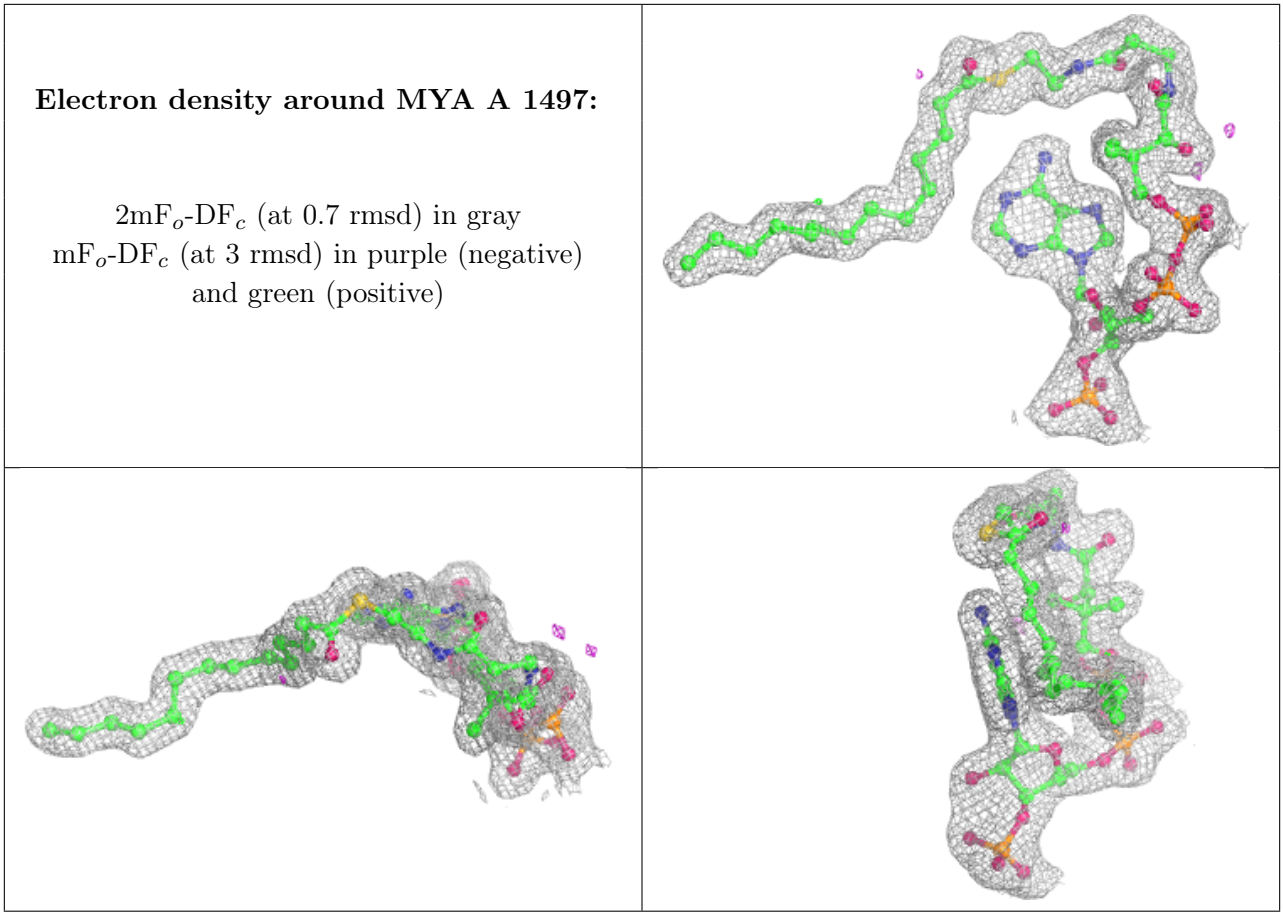






Electron density around MYA A 1497:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.