Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 02:23 pm GMT

PDB ID	:	6F56
Title	:	Mutant of Human N-myristoyltransferase with bound myristoyl-CoA
Authors	:	Brenk, R.; Kehrein, J.; Kersten, C.
Deposited on	:	2017-11-30
Resolution	:	1.94 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:

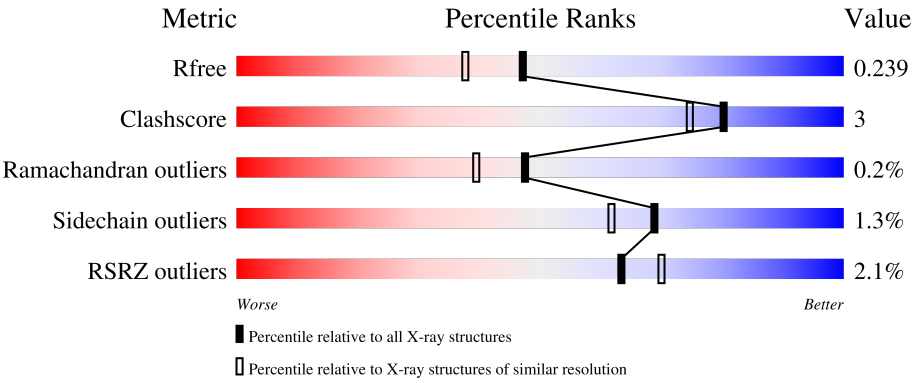
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	86% 7% 7%
1	B	410	3% 86% 6% 7%
1	C	410	3% 84% 9% 7%
1	D	410	2% 86% 7% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13363 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycylpeptide N-tetradecanoyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	152	7	0
			3168	2053	535	562	18			
1	B	382	Total	C	N	O	S	155	2	0
			3142	2036	531	557	18			
1	C	382	Total	C	N	O	S	177	2	0
			3139	2034	530	557	18			
1	D	382	Total	C	N	O	S	338	2	0
			3141	2035	531	557	18			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	MET	-	initiating methionine	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	108	HIS	-	expression tag	UNP P30419
A	295	GLN	ARG	engineered mutation	UNP P30419
A	297	PHE	TRP	engineered mutation	UNP P30419
A	452	MET	ALA	engineered mutation	UNP P30419
A	453	VAL	LEU	engineered mutation	UNP P30419
A	462	VAL	LEU	engineered mutation	UNP P30419
A	473	HIS	ASN	engineered mutation	UNP P30419
A	495	MET	LEU	engineered mutation	UNP P30419
A	496	LEU	GLN	engineered mutation	UNP P30419
B	87	MET	-	initiating methionine	UNP P30419
B	88	GLY	-	expression tag	UNP P30419
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
B	295	GLN	ARG	engineered mutation	UNP P30419
B	297	PHE	TRP	engineered mutation	UNP P30419
B	452	MET	ALA	engineered mutation	UNP P30419
B	453	VAL	LEU	engineered mutation	UNP P30419
B	462	VAL	LEU	engineered mutation	UNP P30419
B	473	HIS	ASN	engineered mutation	UNP P30419
B	495	MET	LEU	engineered mutation	UNP P30419
B	496	LEU	GLN	engineered mutation	UNP P30419
C	87	MET	-	initiating methionine	UNP P30419
C	88	GLY	-	expression tag	UNP P30419
C	89	SER	-	expression tag	UNP P30419

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Chain	Residue	Modelled	Actual	Comment	Reference
C	90	SER	-	expression tag	UNP P30419
C	91	HIS	-	expression tag	UNP P30419
C	92	HIS	-	expression tag	UNP P30419
C	93	HIS	-	expression tag	UNP P30419
C	94	HIS	-	expression tag	UNP P30419
C	95	HIS	-	expression tag	UNP P30419
C	96	HIS	-	expression tag	UNP P30419
C	97	SER	-	expression tag	UNP P30419
C	98	SER	-	expression tag	UNP P30419
C	99	GLY	-	expression tag	UNP P30419
C	100	LEU	-	expression tag	UNP P30419
C	101	GLU	-	expression tag	UNP P30419
C	102	VAL	-	expression tag	UNP P30419
C	103	LEU	-	expression tag	UNP P30419
C	104	PHE	-	expression tag	UNP P30419
C	105	GLN	-	expression tag	UNP P30419
C	106	GLY	-	expression tag	UNP P30419
C	107	PRO	-	expression tag	UNP P30419
C	108	HIS	-	expression tag	UNP P30419
C	295	GLN	ARG	engineered mutation	UNP P30419
C	297	PHE	TRP	engineered mutation	UNP P30419
C	452	MET	ALA	engineered mutation	UNP P30419
C	453	VAL	LEU	engineered mutation	UNP P30419
C	462	VAL	LEU	engineered mutation	UNP P30419
C	473	HIS	ASN	engineered mutation	UNP P30419
C	495	MET	LEU	engineered mutation	UNP P30419
C	496	LEU	GLN	engineered mutation	UNP P30419
D	87	MET	-	initiating methionine	UNP P30419
D	88	GLY	-	expression tag	UNP P30419
D	89	SER	-	expression tag	UNP P30419
D	90	SER	-	expression tag	UNP P30419
D	91	HIS	-	expression tag	UNP P30419
D	92	HIS	-	expression tag	UNP P30419
D	93	HIS	-	expression tag	UNP P30419
D	94	HIS	-	expression tag	UNP P30419
D	95	HIS	-	expression tag	UNP P30419
D	96	HIS	-	expression tag	UNP P30419
D	97	SER	-	expression tag	UNP P30419
D	98	SER	-	expression tag	UNP P30419
D	99	GLY	-	expression tag	UNP P30419
D	100	LEU	-	expression tag	UNP P30419
D	101	GLU	-	expression tag	UNP P30419

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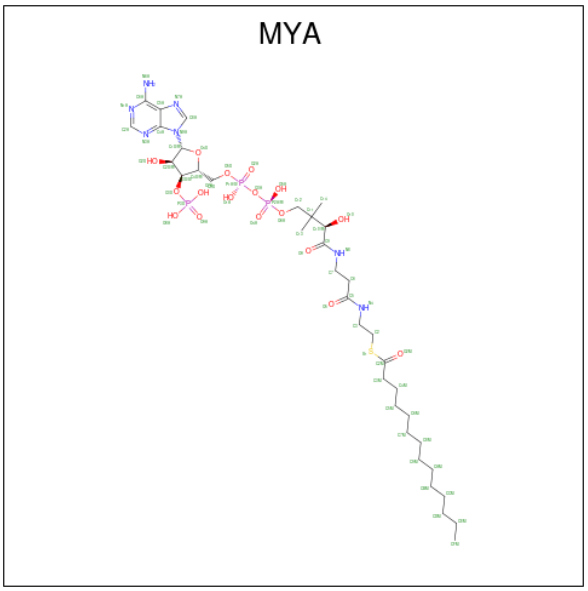
Chain	Residue	Modelled	Actual	Comment	Reference
D	102	VAL	-	expression tag	UNP P30419
D	103	LEU	-	expression tag	UNP P30419
D	104	PHE	-	expression tag	UNP P30419
D	105	GLN	-	expression tag	UNP P30419
D	106	GLY	-	expression tag	UNP P30419
D	107	PRO	-	expression tag	UNP P30419
D	108	HIS	-	expression tag	UNP P30419
D	295	GLN	ARG	engineered mutation	UNP P30419
D	297	PHE	TRP	engineered mutation	UNP P30419
D	452	MET	ALA	engineered mutation	UNP P30419
D	453	VAL	LEU	engineered mutation	UNP P30419
D	462	VAL	LEU	engineered mutation	UNP P30419
D	473	HIS	ASN	engineered mutation	UNP P30419
D	495	MET	LEU	engineered mutation	UNP P30419
D	496	LEU	GLN	engineered mutation	UNP P30419

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

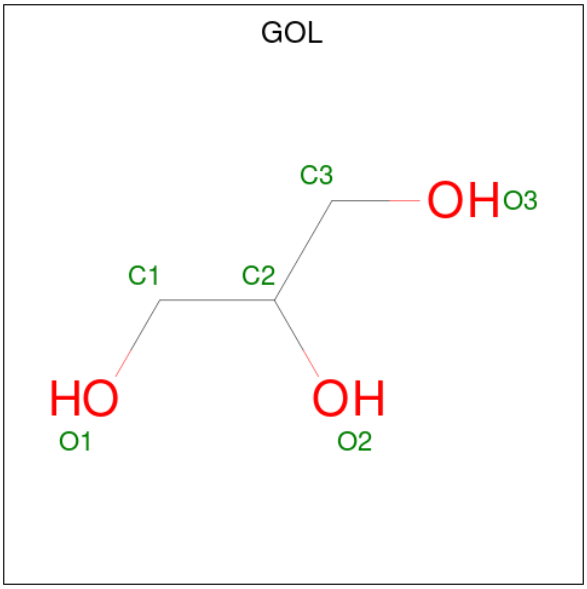


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 5 is water.

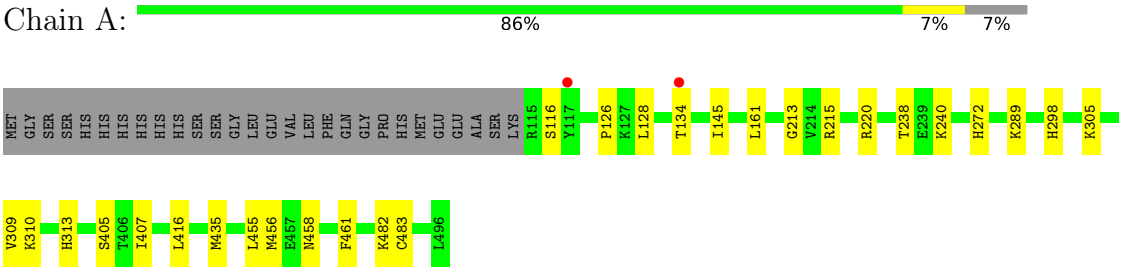
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	135	Total O 135 135	0	0
5	B	139	Total O 139 139	0	0
5	C	92	Total O 92 92	0	0
5	D	97	Total O 97 97	0	0

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.

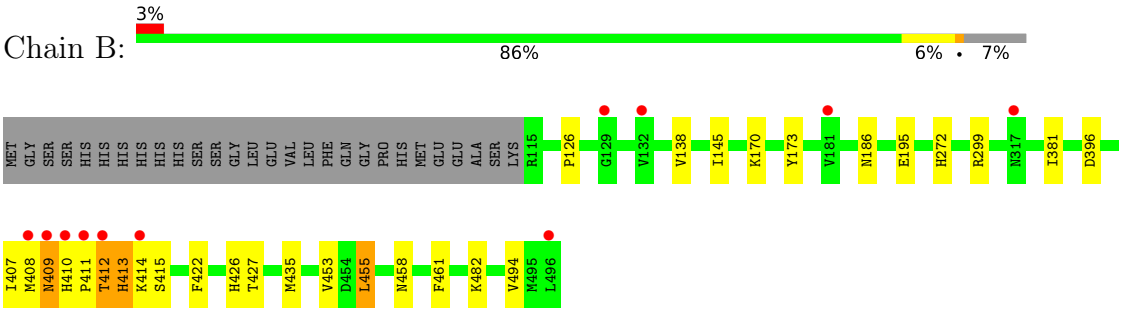
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1

Chain A:



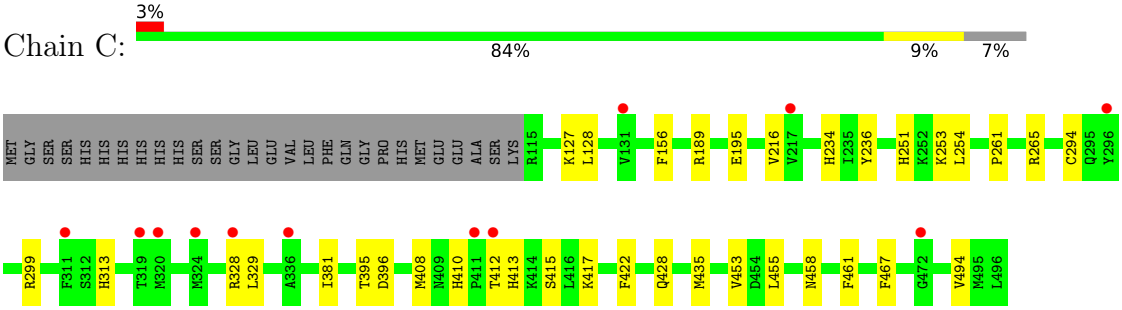
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1

Chain B:



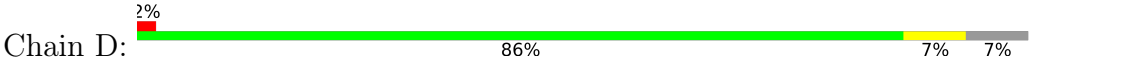
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1

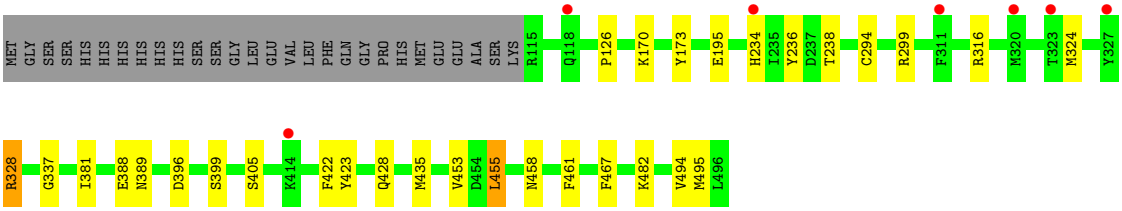
Chain C:



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1

Chain D:




MET
GLY
SER
SER
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
LEU
GLU
GLU
VAL
LEU
PHE
GLN
GLY
PRO
HIS
MET
GLU
GLU
ALA
SER
LYS
R115
Q118
P126
K170
Y173
E195
H234
I235
Y236
D237
T238
C294
R299
F311
R316
M320
T323
M324
Y327
R328
G337
I381
E388
N389
D396
S399
S405
K414
F422
Y423
Q428
M435
V453
D454
L455
N458
F461
F467
K482
V494
M495
L496

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.19Å 159.13Å 174.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.50 – 1.94 87.50 – 1.94	Depositor EDS
% Data completeness (in resolution range)	92.7 (87.50-1.94) 88.2 (87.50-1.94)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.200 , 0.239 0.200 , 0.239	Depositor DCC
R_{free} test set	5517 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.844	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13363	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.74% 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: MG, GOL, 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	0.27	0/3278	0.47	0/4449
1	B	0.27	0/3237	0.51	3/4395 (0.1%)
1	C	0.27	0/3234	0.47	0/4391
1	D	0.26	0/3236	0.46	0/4394
All	All	0.27	0/12985	0.48	3/17629 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	413	HIS	N-CA-C	7.45	131.12	111.00
1	B	413	HIS	CB-CA-C	-6.83	96.75	110.40
1	B	414	LYS	N-CA-C	5.33	125.39	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	411	PRO	Peptide

5.2 Too-close contacts (i)

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	3168	0	3179	14	0
1	B	3142	0	3142	15	0
1	C	3139	0	3139	19	0
1	D	3141	0	3140	15	0
2	A	63	0	58	0	0
2	B	63	0	58	0	0
2	C	63	0	58	0	0
2	D	63	0	58	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
4	C	12	0	16	1	0
4	D	18	0	24	2	0
5	A	135	0	0	1	0
5	B	139	0	0	0	0
5	C	92	0	0	0	0
5	D	97	0	0	0	0
All	All	13363	0	12904	65	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 3.

All (65) 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:407:ILE:HD12	1:B:413:HIS:O	1.92	0.69
1:D:126:PRO:HG3	1:D:482:LYS:HG3	1.75	0.68
1:D:195:GLU:HB3	1:D:381:ILE:HD11	1.78	0.65
1:B:396:ASP:OD2	1:B:426:HIS:HA	1.97	0.65
1:B:422:PHE:O	1:B:494:VAL:HG21	1.98	0.63
1:D:453:VAL:HG12	1:D:455:LEU:HG	1.87	0.57
1:D:234:HIS:NE2	1:D:236:TYR:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:HIS:NE2	1:C:236:TYR:O	2.40	0.54
1:A:126:PRO:HG3	1:A:482:LYS:HG3	1.88	0.54
1:A:161:LEU:HD21	1:A:213:GLY:HA3	1.90	0.54
1:C:299:ARG:NH1	1:C:329:LEU:HD11	2.24	0.53
1:D:234:HIS:HD2	1:D:238:THR:O	1.92	0.52
1:D:389:ASN:HB3	1:D:428:GLN:HE22	1.73	0.52
1:A:455:LEU:HD13	1:A:456:MET:HG3	1.91	0.52
1:A:145:ILE:HD12	1:A:272:HIS:HB3	1.91	0.52
1:A:458:ASN:HA	1:A:461:PHE:CE2	2.46	0.51
4:D:503:GOL:O1	4:D:503:GOL:O3	2.21	0.51
1:B:195:GLU:HB3	1:B:381:ILE:HD11	1.93	0.51
1:C:195:GLU:HB3	1:C:381:ILE:HD11	1.92	0.50
1:C:251:HIS:HB3	1:C:254:LEU:HD13	1.92	0.50
1:D:337:GLY:HA3	1:D:388:GLU:O	2.13	0.49
1:C:156:PHE:CE1	1:C:216:VAL:HG12	2.47	0.49
1:B:170:LYS:HA	1:B:173:TYR:CE2	2.49	0.48
1:B:458:ASN:HA	1:B:461:PHE:CE2	2.48	0.48
1:C:294:CYS:HB3	1:C:453:VAL:HG12	1.95	0.48
1:C:412:THR:OG1	1:C:413:HIS:N	2.47	0.48
1:A:298:HIS:ND1	5:A:604:HOH:O	2.35	0.48
1:C:410:HIS:CD2	1:C:413:HIS:H	2.32	0.47
1:D:458:ASN:HA	1:D:461:PHE:CE2	2.49	0.47
1:B:126:PRO:HG3	1:B:482:LYS:HG2	1.96	0.47
1:C:415:SER:HB3	1:C:417:LYS:HE2	1.97	0.47
1:B:453:VAL:HG12	1:B:455:LEU:HG	1.96	0.47
1:B:408:MET:O	1:B:409:ASN:HB2	2.15	0.47
1:A:309:VAL:HG11	1:A:407:ILE:HD13	1.97	0.46
1:C:458:ASN:HA	1:C:461:PHE:CE2	2.49	0.46
1:D:422:PHE:O	1:D:494:VAL:HG21	2.15	0.46
1:B:145:ILE:HD12	1:B:272:HIS:HB3	1.97	0.46
1:D:170:LYS:HA	1:D:173:TYR:CE2	2.51	0.45
1:D:399:SER:OG	1:D:423:TYR:O	2.32	0.45
1:B:138:VAL:HG22	1:B:482:LYS:HG3	1.99	0.45
1:C:422:PHE:O	1:C:494:VAL:HG21	2.18	0.44
1:D:294:CYS:HB3	1:D:453:VAL:HG13	1.99	0.44
1:C:494:VAL:O	4:C:503:GOL:H32	2.17	0.44
1:C:261:PRO:O	1:C:265:ARG:HG3	2.18	0.43
1:B:435:MET:HG3	1:B:461:PHE:CZ	2.54	0.43
1:B:396:ASP:OD2	1:B:427:THR:N	2.50	0.43
1:D:299:ARG:HB2	1:D:467:PHE:CE2	2.54	0.43
1:A:238:THR:HG22	1:A:240:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:HIS:C	1:B:412:THR:H	2.22	0.42
1:A:416:LEU:HD12	1:A:416:LEU:HA	1.84	0.42
1:A:305:LYS:O	1:A:309:VAL:HG22	2.20	0.42
1:D:324:MET:O	1:D:328:ARG:HB2	2.20	0.41
1:C:189:ARG:NH2	1:C:408:MET:SD	2.93	0.41
1:A:435:MET:HG3	1:A:461:PHE:CZ	2.54	0.41
1:C:127:LYS:HD2	1:C:127:LYS:HA	1.60	0.41
1:D:435:MET:HG3	1:D:461:PHE:CE2	2.55	0.41
1:A:215:ARG:NH1	1:A:220:ARG:O	2.47	0.41
1:C:395:THR:OG1	1:C:396:ASP:OD1	2.21	0.41
4:D:503:GOL:HO3	4:D:503:GOL:HO1	1.62	0.41
1:A:128:LEU:HD12	1:A:289:LYS:HG3	2.03	0.41
1:A:134:THR:O	1:A:483:CYS:HA	2.21	0.41
1:C:299:ARG:HB2	1:C:467:PHE:CE2	2.56	0.41
1:B:412:THR:HG23	1:B:413:HIS:ND1	2.36	0.40
1:C:127:LYS:HE3	1:C:128:LEU:H	1.86	0.40
1:C:435:MET:HG3	1:C:461:PHE:CZ	2.56	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	387/410 (94%)	376 (97%)	11 (3%)	0	100 100
1	B	382/410 (93%)	369 (97%)	10 (3%)	3 (1%)	19 9
1	C	382/410 (93%)	374 (98%)	8 (2%)	0	100 100
1	D	382/410 (93%)	371 (97%)	11 (3%)	0	100 100
All	All	1533/1640 (94%)	1490 (97%)	40 (3%)	3 (0%)	47 39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	412	THR
1	B	409	ASN
1	B	186	ASN

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	356/373 (95%)	352 (99%)	4 (1%)	73	67
1	B	351/373 (94%)	348 (99%)	3 (1%)	78	75
1	C	351/373 (94%)	346 (99%)	5 (1%)	67	58
1	D	351/373 (94%)	345 (98%)	6 (2%)	60	49
All	All	1409/1492 (94%)	1391 (99%)	18 (1%)	69	62

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	SER
1	A	310	LYS
1	A	313	HIS
1	A	405	SER
1	B	299	ARG
1	B	415	SER
1	B	455	LEU
1	C	253	LYS
1	C	313	HIS
1	C	328	ARG
1	C	428	GLN
1	C	455	LEU
1	D	316	ARG
1	D	328	ARG
1	D	396	ASP
1	D	405	SER
1	D	455	LEU
1	D	495	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	234	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
4	GOL	A	504	-	5,5,5	0.51	0	5,5,5	0.25	0
4	GOL	B	504	-	5,5,5	0.54	0	5,5,5	0.65	0
4	GOL	D	503	-	5,5,5	0.54	0	5,5,5	0.50	0
2	MYA	A	501	3	57,65,65	1.20	6 (10%)	68,91,91	1.74	11 (16%)
2	MYA	B	501	3	57,65,65	1.18	6 (10%)	68,91,91	1.73	11 (16%)
4	GOL	A	503	-	5,5,5	0.56	0	5,5,5	0.15	0
2	MYA	D	501	-	57,65,65	1.20	5 (8%)	68,91,91	1.71	11 (16%)
2	MYA	C	501	3	57,65,65	1.20	5 (8%)	68,91,91	1.76	12 (17%)
4	GOL	D	504	-	5,5,5	0.54	0	5,5,5	0.23	0
4	GOL	B	503	-	5,5,5	0.54	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	D	505	-	5,5,5	0.52	0	5,5,5	0.26	0
4	GOL	C	503	-	5,5,5	0.55	0	5,5,5	0.58	0
4	GOL	C	504	-	5,5,5	0.54	0	5,5,5	0.25	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
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	B	504	-	-	0/4/4/4	-
4	GOL	D	503	-	-	0/4/4/4	-
2	MYA	A	501	3	-	2/60/80/80	0/3/3/3
2	MYA	B	501	3	-	1/60/80/80	0/3/3/3
4	GOL	A	503	-	-	0/4/4/4	-
2	MYA	D	501	-	-	1/60/80/80	0/3/3/3
2	MYA	C	501	3	-	1/60/80/80	0/3/3/3
4	GOL	D	504	-	-	0/4/4/4	-
4	GOL	B	503	-	-	0/4/4/4	-
4	GOL	D	505	-	-	0/4/4/4	-
4	GOL	C	503	-	-	2/4/4/4	-
4	GOL	C	504	-	-	0/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MYA	C2A-N3A	3.72	1.38	1.32
2	D	501	MYA	C2A-N3A	3.70	1.38	1.32
2	C	501	MYA	C2A-N3A	3.64	1.38	1.32
2	B	501	MYA	C2A-N3A	3.32	1.37	1.32
2	C	501	MYA	O4X-C1X	3.07	1.45	1.41
2	A	501	MYA	O4X-C1X	3.02	1.45	1.41
2	D	501	MYA	O4X-C1X	3.01	1.45	1.41
2	B	501	MYA	O4X-C1X	2.86	1.45	1.41
2	B	501	MYA	C4A-N3A	-2.39	1.32	1.35
2	C	501	MYA	C4A-N3A	-2.38	1.32	1.35
2	D	501	MYA	C4A-N3A	-2.38	1.32	1.35
2	B	501	MYA	O10-C10	2.26	1.46	1.42
2	C	501	MYA	O10-C10	2.20	1.46	1.42
2	A	501	MYA	C4A-N3A	-2.18	1.32	1.35
2	A	501	MYA	O5-C5	2.16	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	MYA	O9-C9	2.06	1.27	1.23
2	D	501	MYA	O2M-C2M	2.06	1.24	1.21
2	C	501	MYA	O2M-C2M	2.06	1.24	1.21
2	B	501	MYA	O2M-C2M	2.05	1.24	1.21
2	A	501	MYA	O9-C9	2.04	1.27	1.23
2	B	501	MYA	O5-C5	2.04	1.27	1.23
2	A	501	MYA	P3X-O7A	-2.02	1.47	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	MYA	C3M-C2M-S1	6.92	121.51	113.46
2	C	501	MYA	C3M-C2M-S1	6.90	121.49	113.46
2	D	501	MYA	C3M-C2M-S1	6.80	121.38	113.46
2	A	501	MYA	C3M-C2M-S1	6.75	121.31	113.46
2	B	501	MYA	N3A-C2A-N1A	-6.04	119.24	128.68
2	A	501	MYA	N3A-C2A-N1A	-6.03	119.26	128.68
2	C	501	MYA	N3A-C2A-N1A	-5.91	119.44	128.68
2	D	501	MYA	N3A-C2A-N1A	-5.89	119.47	128.68
2	D	501	MYA	O2M-C2M-C3M	-4.69	118.46	123.99
2	C	501	MYA	O2M-C2M-C3M	-4.58	118.58	123.99
2	B	501	MYA	O2M-C2M-C3M	-4.45	118.74	123.99
2	A	501	MYA	O2M-C2M-C3M	-4.35	118.86	123.99
2	A	501	MYA	O2M-C2M-S1	-3.16	118.51	122.61
2	B	501	MYA	C1X-N9A-C4A	-3.02	121.33	126.64
2	A	501	MYA	C13-C11-C10	2.90	113.85	108.82
2	C	501	MYA	C13-C11-C10	2.83	113.73	108.82
2	B	501	MYA	C4M-C3M-C2M	-2.71	106.33	112.33
2	B	501	MYA	C2A-N1A-C6A	2.68	123.34	118.75
2	D	501	MYA	C13-C11-C10	2.64	113.40	108.82
2	B	501	MYA	C13-C11-C10	2.61	113.35	108.82
2	C	501	MYA	C1X-N9A-C4A	-2.57	122.12	126.64
2	A	501	MYA	C2A-N1A-C6A	2.55	123.12	118.75
2	C	501	MYA	C2A-N1A-C6A	2.53	123.09	118.75
2	C	501	MYA	C13-C11-C12	-2.53	104.10	108.23
2	A	501	MYA	O8A-P3X-O7A	2.52	117.26	107.64
2	C	501	MYA	O2M-C2M-S1	-2.51	119.36	122.61
2	C	501	MYA	O8A-P3X-O7A	2.47	117.09	107.64
2	D	501	MYA	C2A-N1A-C6A	2.47	122.98	118.75
2	B	501	MYA	O8A-P3X-O7A	2.38	116.74	107.64
2	A	501	MYA	C13-C11-C12	-2.38	104.36	108.23
2	A	501	MYA	P2A-O3A-P1A	-2.31	124.90	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	MYA	C1X-N9A-C4A	-2.29	122.61	126.64
2	C	501	MYA	C4M-C3M-C2M	-2.28	107.27	112.33
2	C	501	MYA	C6-C5-N4	-2.28	112.58	116.42
2	D	501	MYA	C6-C7-N8	-2.28	107.29	111.90
2	D	501	MYA	O8A-P3X-O7A	2.26	116.28	107.64
2	B	501	MYA	O2M-C2M-S1	-2.23	119.72	122.61
2	C	501	MYA	C5A-C6A-N6A	2.19	123.68	120.35
2	D	501	MYA	C4M-C3M-C2M	-2.19	107.48	112.33
2	D	501	MYA	O4X-C1X-C2X	-2.11	103.84	106.93
2	D	501	MYA	C13-C11-C12	-2.11	104.79	108.23
2	A	501	MYA	C6-C5-N4	-2.03	113.00	116.42
2	D	501	MYA	C1X-N9A-C4A	-2.02	123.09	126.64
2	B	501	MYA	C7-C6-C5	2.01	115.71	112.36
2	B	501	MYA	C6-C5-N4	-2.01	113.04	116.42

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	MYA	C3X-O3X-P3X-O8A
4	C	503	GOL	C1-C2-C3-O3
4	C	503	GOL	O2-C2-C3-O3
2	C	501	MYA	C3X-O3X-P3X-O8A
2	B	501	MYA	C8M-C9M-CAM-CBM
2	D	501	MYA	O2M-C2M-S1-C2
2	A	501	MYA	C3X-O3X-P3X-O7A

There are no ring outliers.

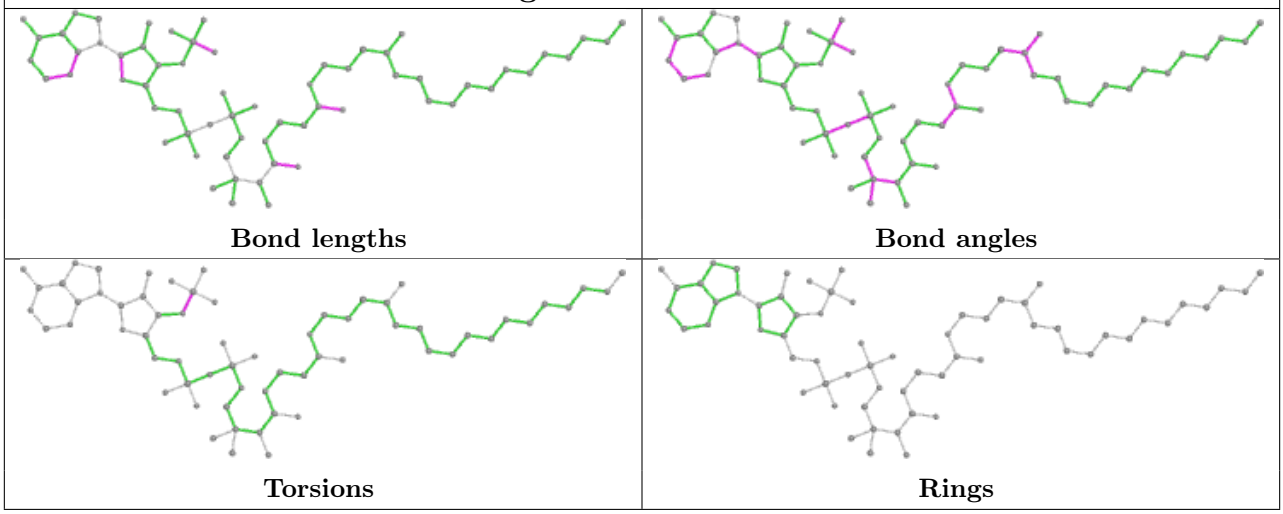
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	503	GOL	2	0
4	C	503	GOL	1	0

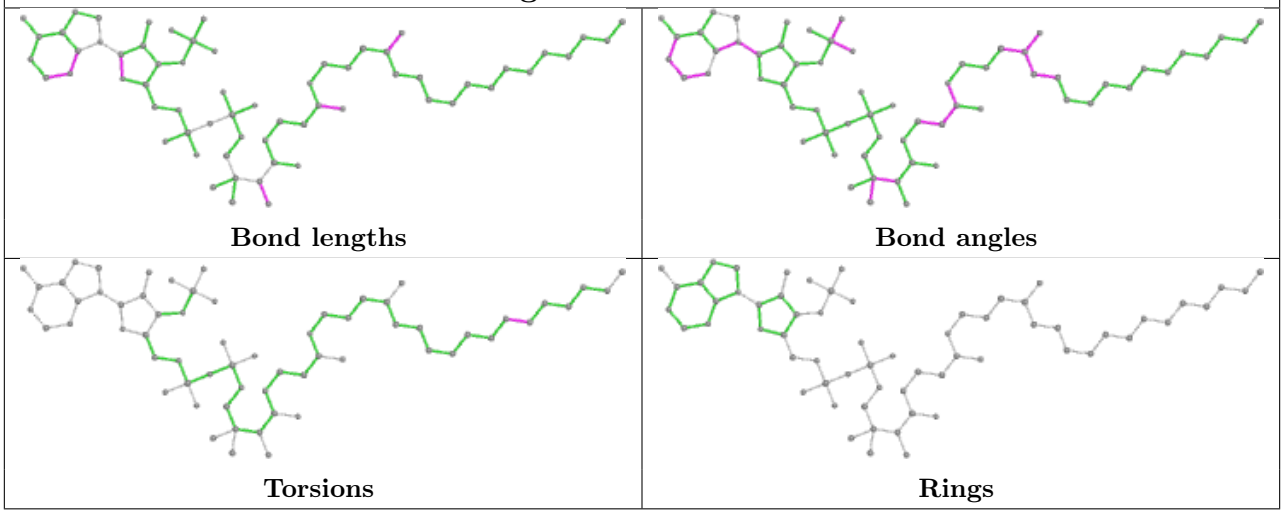
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

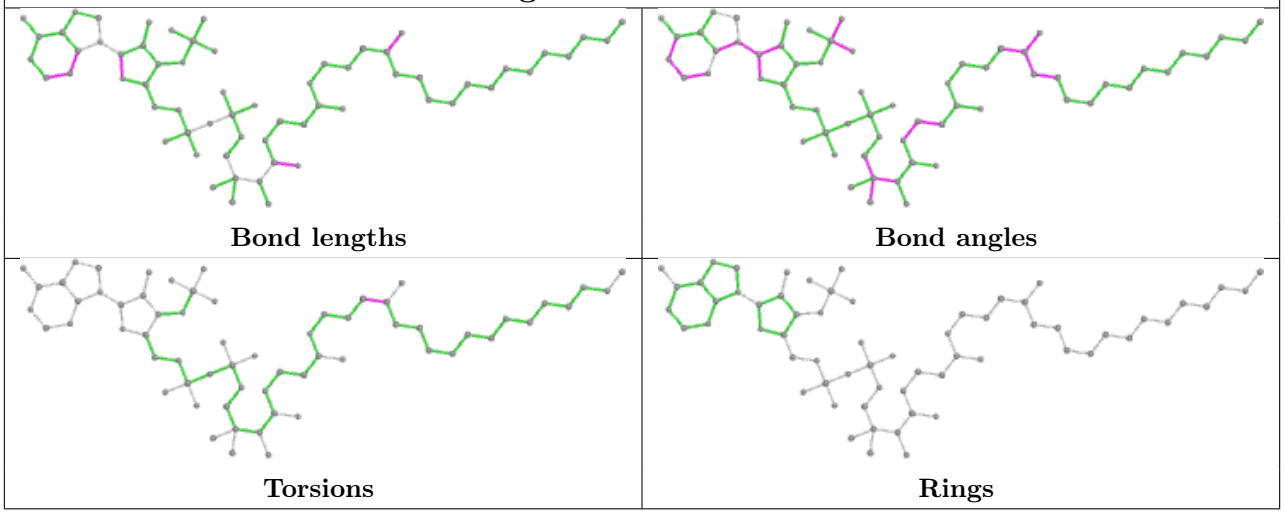
Ligand MYA A 501



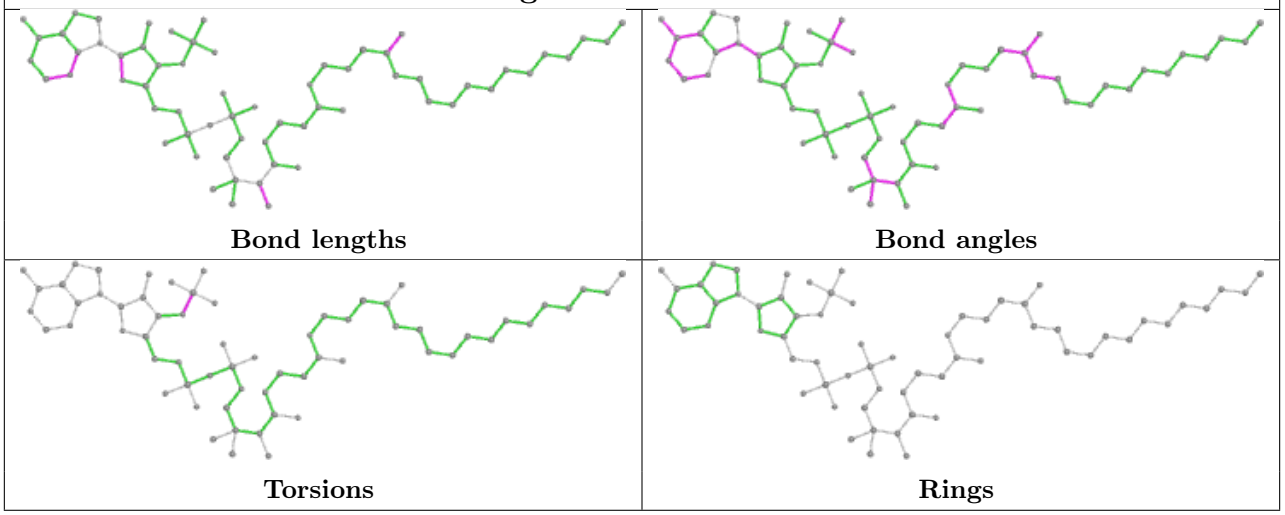
Ligand MYA B 501



Ligand MYA D 501



Ligand MYA C 501



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	379/410 (92%)	0.08	2 (0%)	91	93	19, 31, 48, 58	41 (10%)
1	B	376/410 (91%)	0.21	11 (2%)	51	59	18, 28, 48, 86	29 (7%)
1	C	377/410 (91%)	0.25	12 (3%)	47	55	22, 36, 57, 69	38 (10%)
1	D	358/410 (87%)	0.23	7 (1%)	65	71	22, 34, 56, 70	33 (9%)
All	All	1490/1640 (90%)	0.19	32 (2%)	63	70	18, 32, 53, 86	141 (9%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	411	PRO	12.4
1	B	410	HIS	7.1
1	B	409	ASN	5.7
1	D	327	TYR	4.6
1	B	181	VAL	3.8
1	C	472	GLY	3.5
1	D	323	THR	3.1
1	B	412	THR	3.1
1	C	131	VAL	3.0
1	C	296	TYR	3.0
1	B	408	MET	3.0
1	D	311	PHE	2.9
1	C	336	ALA	2.9
1	C	411	PRO	2.8
1	B	317	ASN	2.8
1	C	217	VAL	2.5
1	D	414	LYS	2.4
1	B	129	GLY	2.4
1	C	328	ARG	2.4
1	B	132	VAL	2.4
1	C	412	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	117	TYR	2.3
1	C	319	THR	2.2
1	D	118	GLN	2.2
1	C	311	PHE	2.2
1	C	320	MET	2.1
1	B	414	LYS	2.1
1	C	324	MET	2.1
1	A	134	THR	2.0
1	B	496	LEU	2.0
1	D	234	HIS	2.0
1	D	320	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	D	505	6/6	0.68	0.16	47,52,55,58	0
4	GOL	D	503	6/6	0.83	0.18	35,39,44,47	0
4	GOL	C	503	6/6	0.86	0.18	38,39,42,43	0
4	GOL	A	504	6/6	0.88	0.16	33,39,42,45	0
3	MG	B	502	1/1	0.90	0.16	40,40,40,40	0
4	GOL	B	504	6/6	0.92	0.14	30,36,39,41	0
3	MG	A	502	1/1	0.93	0.24	42,42,42,42	0
3	MG	D	502	1/1	0.94	0.18	47,47,47,47	0
4	GOL	D	504	6/6	0.94	0.11	30,32,36,38	0
2	MYA	C	501	63/63	0.94	0.12	23,35,44,50	0
2	MYA	A	501	63/63	0.95	0.11	14,30,37,41	0
4	GOL	C	504	6/6	0.95	0.15	32,39,40,43	0

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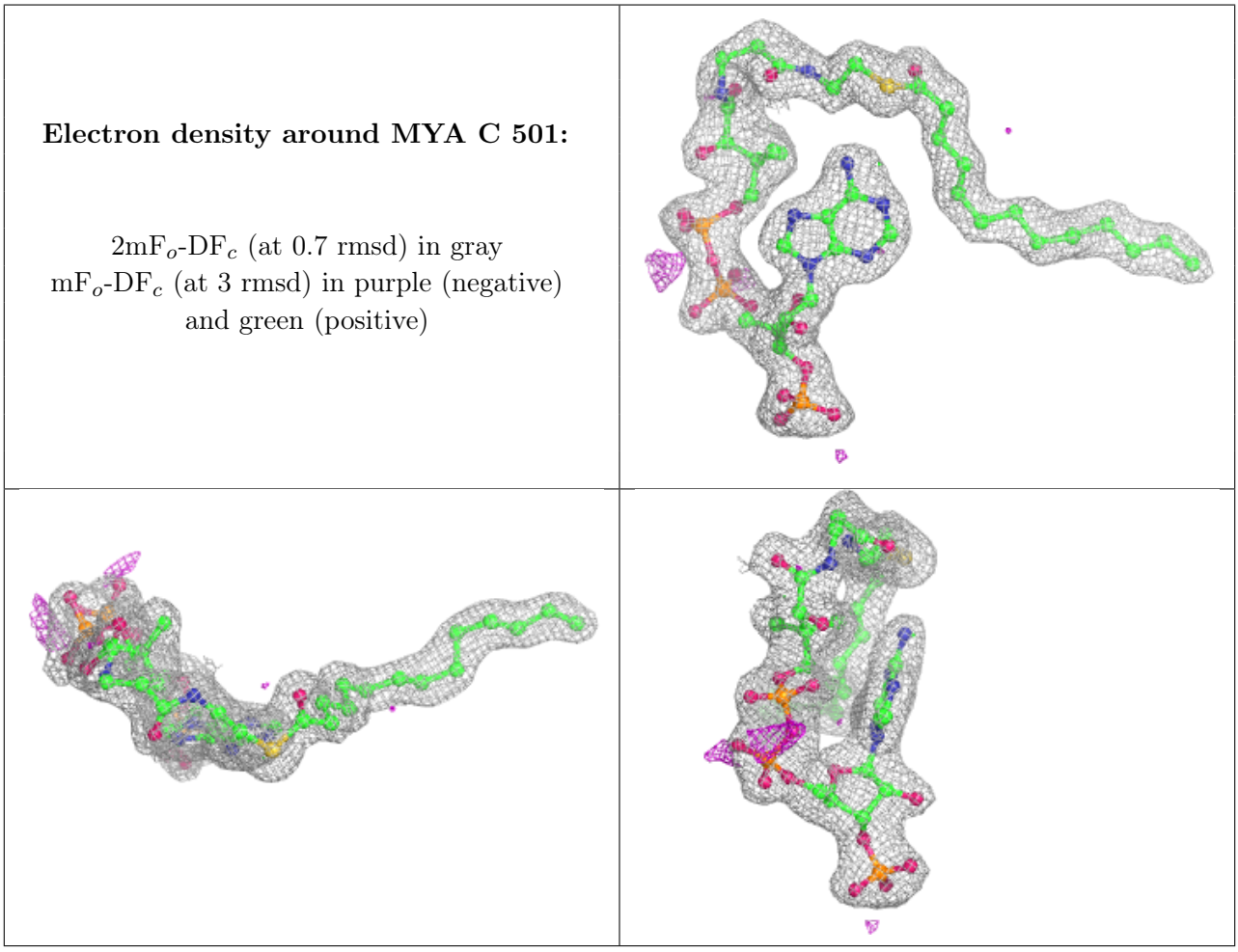
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MYA	D	501	63/63	0.95	0.12	20,34,40,43	0
4	GOL	B	503	6/6	0.95	0.13	28,30,33,36	0
3	MG	C	502	1/1	0.95	0.37	50,50,50,50	0
2	MYA	B	501	63/63	0.96	0.11	15,28,34,36	0
4	GOL	A	503	6/6	0.96	0.09	25,28,33,33	0

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.

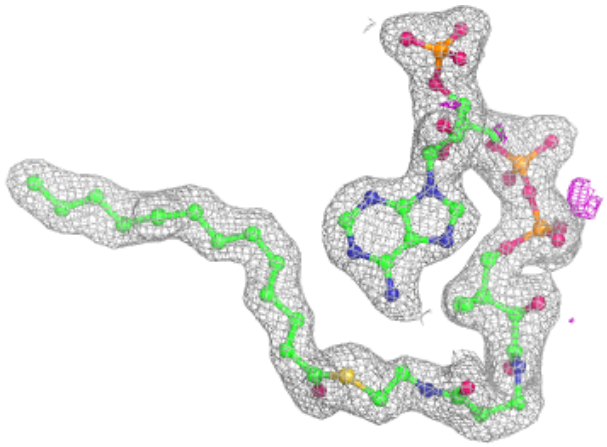
Electron density around MYA C 501:

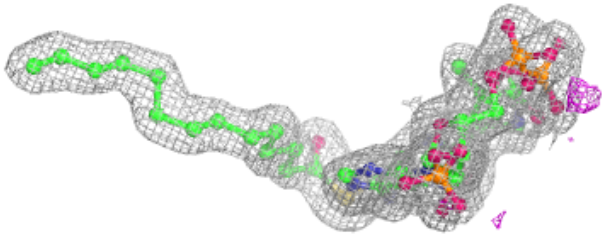
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

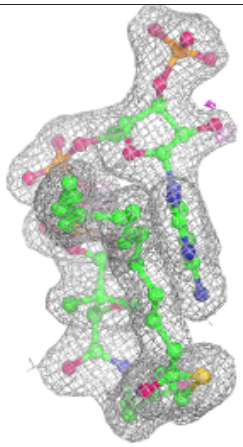


Electron density around MYA A 501:

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

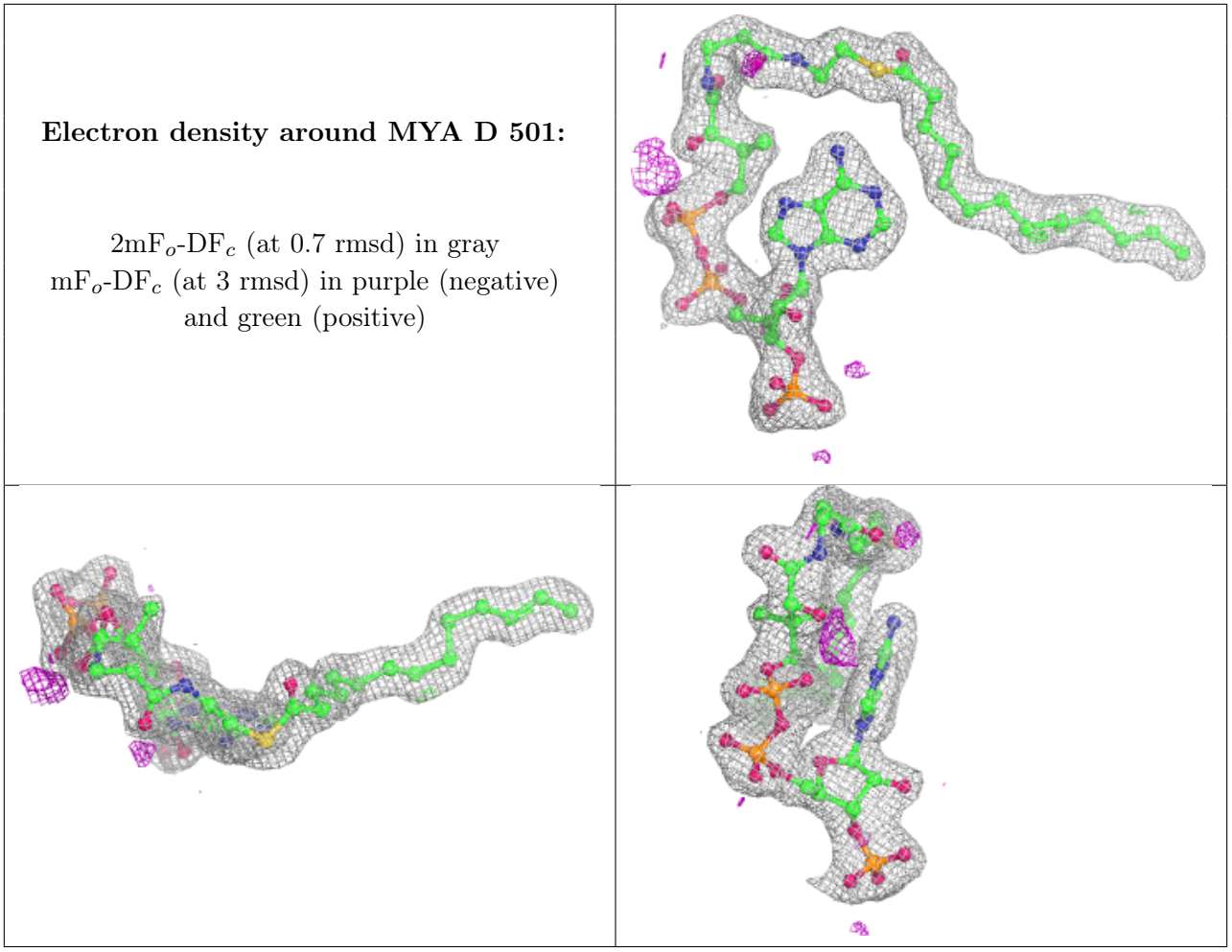






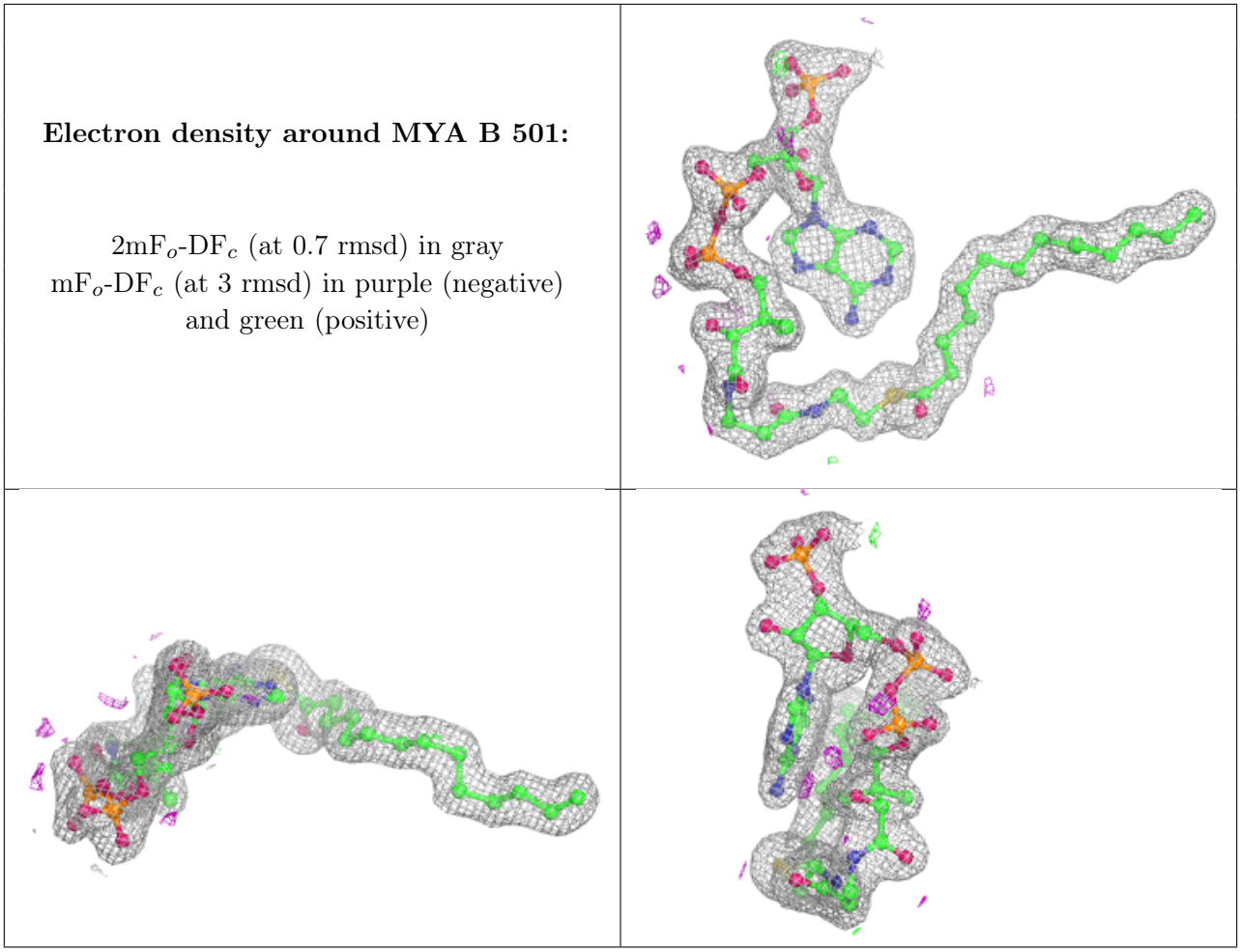
Electron density around MYA D 501:

$2mF_o$-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 501:

$2mF_o$-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 (i)

There are no such residues in this entry.