wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2023 – 02:22 AM EDT

PDB ID	:	7KPF
Title	:	NME2 bound to myristoyl-CoA
Authors	:	Price, I.R.; Lin, H.
Deposited on	:	2020-11-11
Resolution	:	2.23 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.23 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.
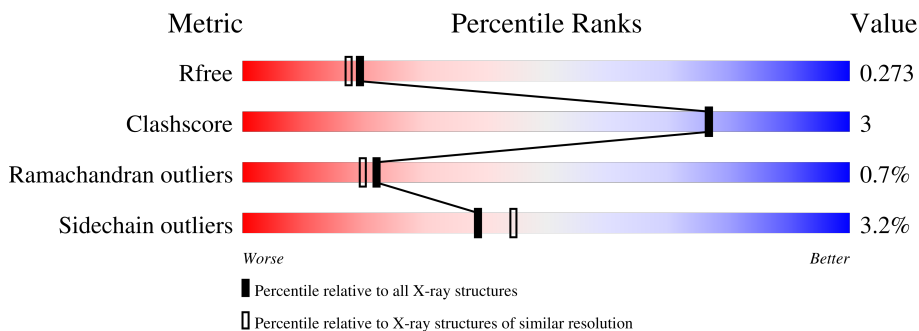
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)

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%

Mol	Chain	Length	Quality of chain
1	A	152	89% · 10% ·
1	B	152	95% · 5%
1	C	152	91% · 9% ·
1	D	152	83% · 10% · 7%
1	E	152	84% · 7% · 7%
1	F	152	76% · 12% · 11%

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
4	GOL	D	201	-	X	-	-

2   Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 14078 atoms, of which 6752 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 Nucleoside diphosphate kinase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	152	Total	C	H	N	O	S	0	1	0
			2429	783	1208	212	219	7			
1	B	152	Total	C	H	N	O	S	0	2	0
			2453	786	1227	213	220	7			
1	C	152	Total	C	H	N	O	S	0	2	0
			2453	786	1227	213	220	7			
1	D	142	Total	C	H	N	O	S	0	2	0
			2154	729	1011	199	208	7			
1	E	141	Total	C	H	N	O	S	0	1	0
			2115	713	995	196	204	7			
1	F	135	Total	C	H	N	O	S	0	1	0
			2095	675	1033	184	196	7			

- Molecule 2 is TETRADECANOYL-COA (three-letter code: MYA) (formula: $C_{35}H_{62}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).
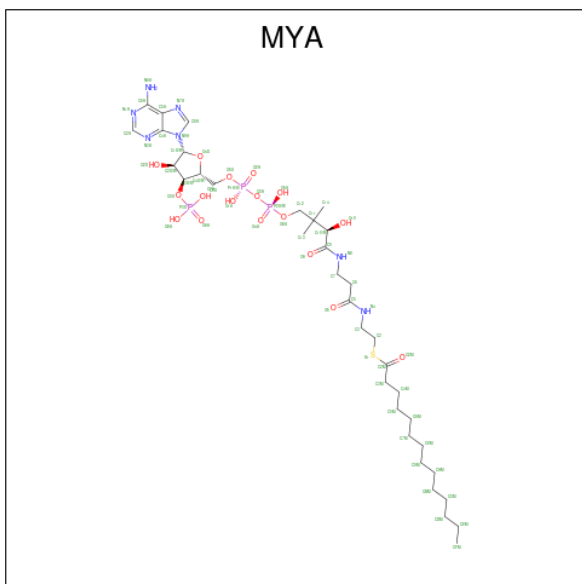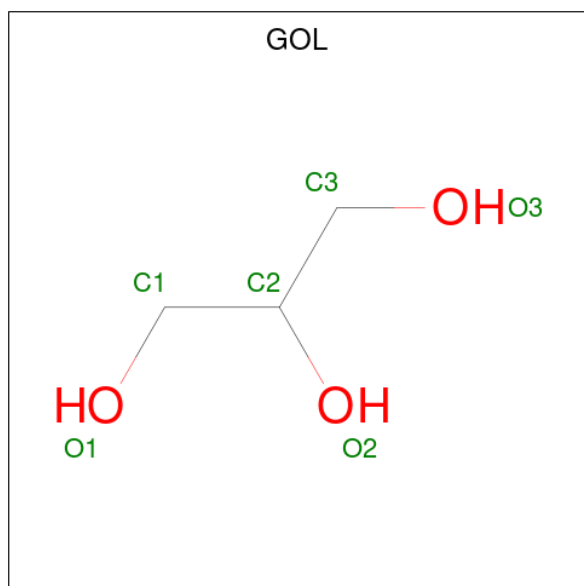
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			46	12	13	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			55	15	19	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			43	11	11	5	13	3		

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

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

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

GOL

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total 46	O 46	0	0
5	B	30	Total 30	O 30	0	0
5	C	37	Total 37	O 37	0	0
5	D	42	Total 42	O 42	0	0
5	E	39	Total 39	O 39	0	0
5	F	20	Total 20	O 20	0	0

3 Residue-property plots ⓘ

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. 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. 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.
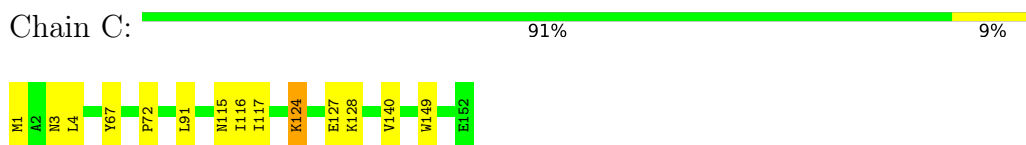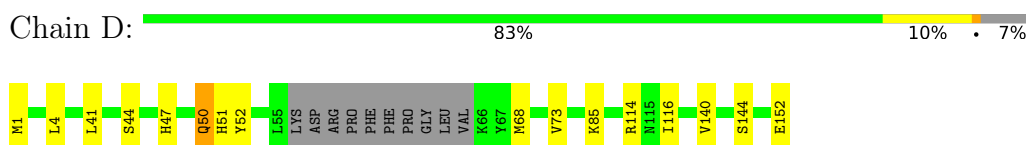
- Molecule 1: Nucleoside diphosphate kinase B
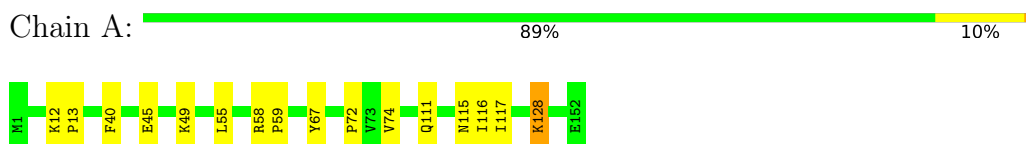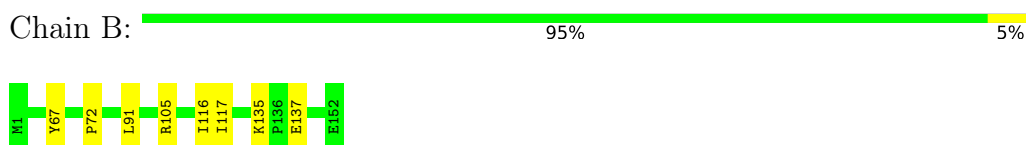
Chain A:

- Molecule 1: Nucleoside diphosphate kinase B
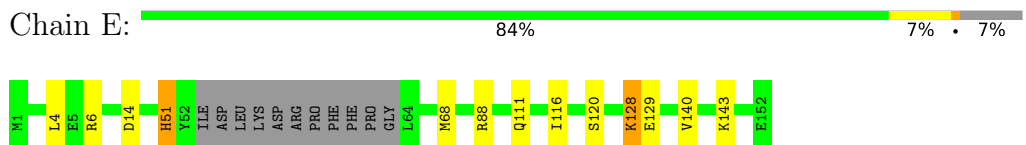
Chain B:

- Molecule 1: Nucleoside diphosphate kinase B

Chain C:

- Molecule 1: Nucleoside diphosphate kinase B

Chain D:

- Molecule 1: Nucleoside diphosphate kinase B

Chain E:

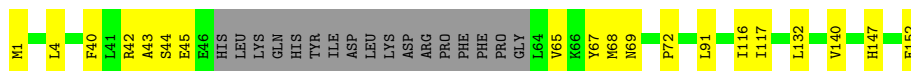- Molecule 1: Nucleoside diphosphate kinase B

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.73Å 107.52Å 115.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.56 – 2.23 78.56 – 2.24	Depositor EDS
% Data completeness (in resolution range)	96.2 (78.56-2.23) 88.4 (78.56-2.24)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.13-2998-0000	Depositor
R, R_{free}	0.190 , 0.229 0.243 , 0.273	Depositor DCC
R_{free} test set	2003 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å^2)	41.4	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 46.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14078	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MYA, GOL, 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	0.41	0/1252	0.60	0/1684
1	B	0.34	0/1260	0.58	0/1695
1	C	0.39	0/1260	0.58	0/1695
1	D	0.44	0/1172	0.65	0/1574
1	E	0.56	4/1146 (0.3%)	0.64	0/1540
1	F	0.40	0/1085	0.66	1/1458 (0.1%)
All	All	0.43	4/7175 (0.1%)	0.62	1/9646 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	120	SER	CB-OG	-5.90	1.34	1.42
1	E	129	GLU	CD-OE2	-5.50	1.19	1.25
1	E	129	GLU	CD-OE1	-5.25	1.19	1.25
1	E	129	GLU	C-O	-5.05	1.13	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	4	LEU	CB-CG-CD1	-5.10	102.34	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1221	1208	1233	10	0
1	B	1226	1227	1239	3	0
1	C	1226	1227	1239	11	0
1	D	1143	1011	1153	12	0
1	E	1120	995	1114	5	0
1	F	1062	1033	1059	9	0
2	A	33	13	13	1	0
2	B	36	19	19	1	0
2	C	32	11	11	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	3	0	0	0	0
4	D	6	8	8	0	0
5	A	46	0	0	0	0
5	B	30	0	0	0	0
5	C	37	0	0	0	0
5	D	42	0	0	0	0
5	E	39	0	0	0	0
5	F	20	0	0	0	0
All	All	7326	6752	7088	43	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.

The worst 5 of 43 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:F:45:GLU:HA	1:F:45:GLU:OE1	1.73	0.85
1:D:1:MET:HB3	1:D:4:LEU:HD23	1.62	0.78
1:C:1:MET:HB3	1:C:4:LEU:HD23	1.66	0.77
1:D:1:MET:HB3	1:D:4:LEU:CD2	2.19	0.72
1:D:50:GLN:NE2	1:D:51:HIS:NE2	2.49	0.61

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	151/152 (99%)	147 (97%)	3 (2%)	1 (1%)	22	20
1	B	152/152 (100%)	148 (97%)	3 (2%)	1 (1%)	22	20
1	C	152/152 (100%)	148 (97%)	3 (2%)	1 (1%)	22	20
1	D	140/152 (92%)	136 (97%)	3 (2%)	1 (1%)	22	20
1	E	138/152 (91%)	134 (97%)	3 (2%)	1 (1%)	22	20
1	F	132/152 (87%)	128 (97%)	3 (2%)	1 (1%)	19	16
All	All	865/912 (95%)	841 (97%)	18 (2%)	6 (1%)	22	20

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ILE
1	B	116	ILE
1	C	116	ILE
1	D	116	ILE
1	E	116	ILE

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	132/131 (101%)	130 (98%)	2 (2%)	65	72
1	B	133/131 (102%)	130 (98%)	3 (2%)	50	57
1	C	133/131 (102%)	131 (98%)	2 (2%)	65	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	124/131 (95%)	117 (94%)	7 (6%)	21	19
1	E	119/131 (91%)	113 (95%)	6 (5%)	24	24
1	F	113/131 (86%)	108 (96%)	5 (4%)	28	30
All	All	754/786 (96%)	729 (97%)	25 (3%)	39	43

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	LEU
1	E	88	ARG
1	F	147	HIS
1	E	51	HIS
1	E	128	LYS

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	50	GLN

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 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	MYA	B	201	-	33,38,65	3.24	9 (27%)	40,60,91	2.79	9 (22%)
2	MYA	C	201	-	29,34,65	3.40	8 (27%)	34,53,91	3.08	9 (26%)
4	GOL	D	201	-	5,5,5	2.16	3 (60%)	5,5,5	1.90	3 (60%)
2	MYA	A	201	-	30,35,65	3.33	9 (30%)	34,54,91	3.14	8 (23%)

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	201	-	-	10/24/44/80	0/3/3/3
2	MYA	C	201	-	-	3/20/40/80	0/3/3/3
4	GOL	D	201	-	-	4/4/4/4	-
2	MYA	A	201	-	-	6/21/41/80	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	MYA	O4X-C1X	12.75	1.58	1.41
2	C	201	MYA	O4X-C1X	12.39	1.58	1.41
2	A	201	MYA	O4X-C1X	12.27	1.58	1.41
2	C	201	MYA	C2X-C3X	-8.12	1.34	1.52
2	B	201	MYA	C2X-C3X	-8.07	1.34	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	MYA	C1X-N9A-C4A	13.25	149.93	126.64
2	C	201	MYA	C1X-N9A-C4A	12.89	149.29	126.64
2	B	201	MYA	C1X-N9A-C4A	12.28	148.22	126.64
2	A	201	MYA	C5A-C6A-N6A	7.14	131.21	120.35
2	C	201	MYA	C5A-C6A-N6A	6.93	130.88	120.35

There are no chirality outliers.
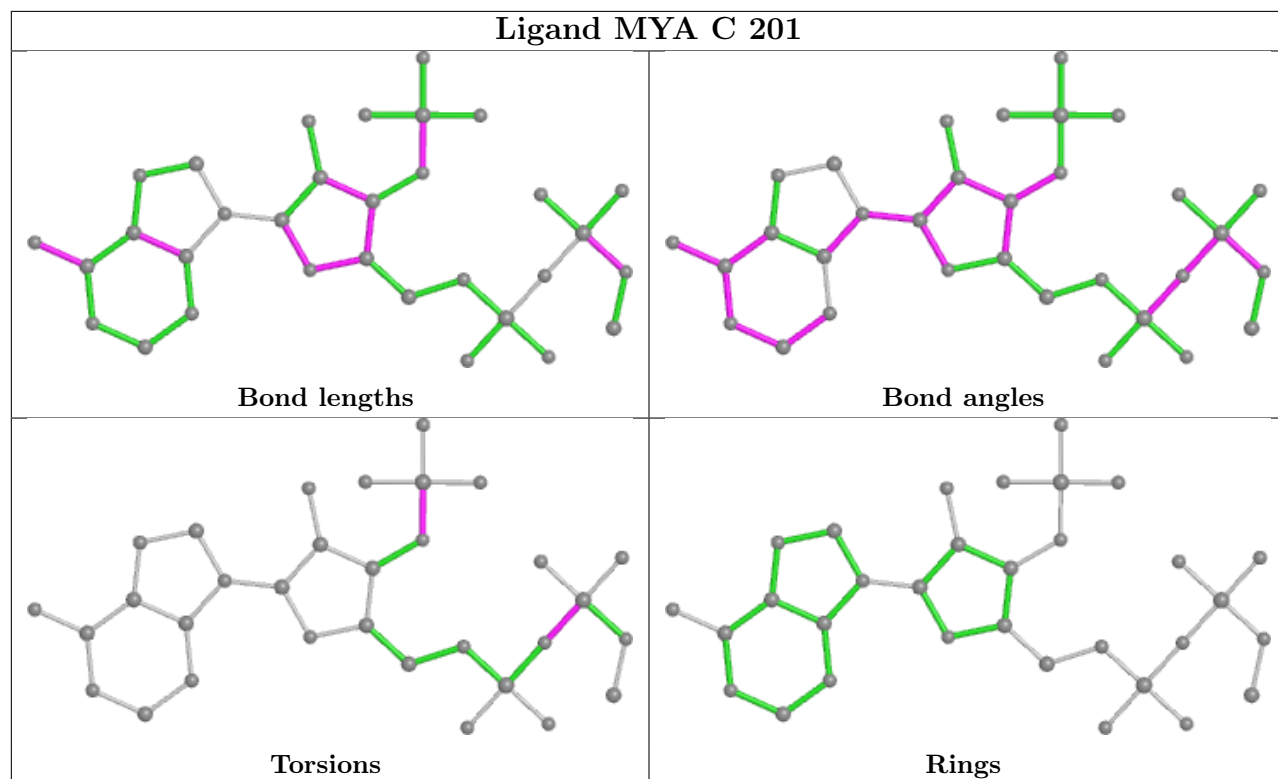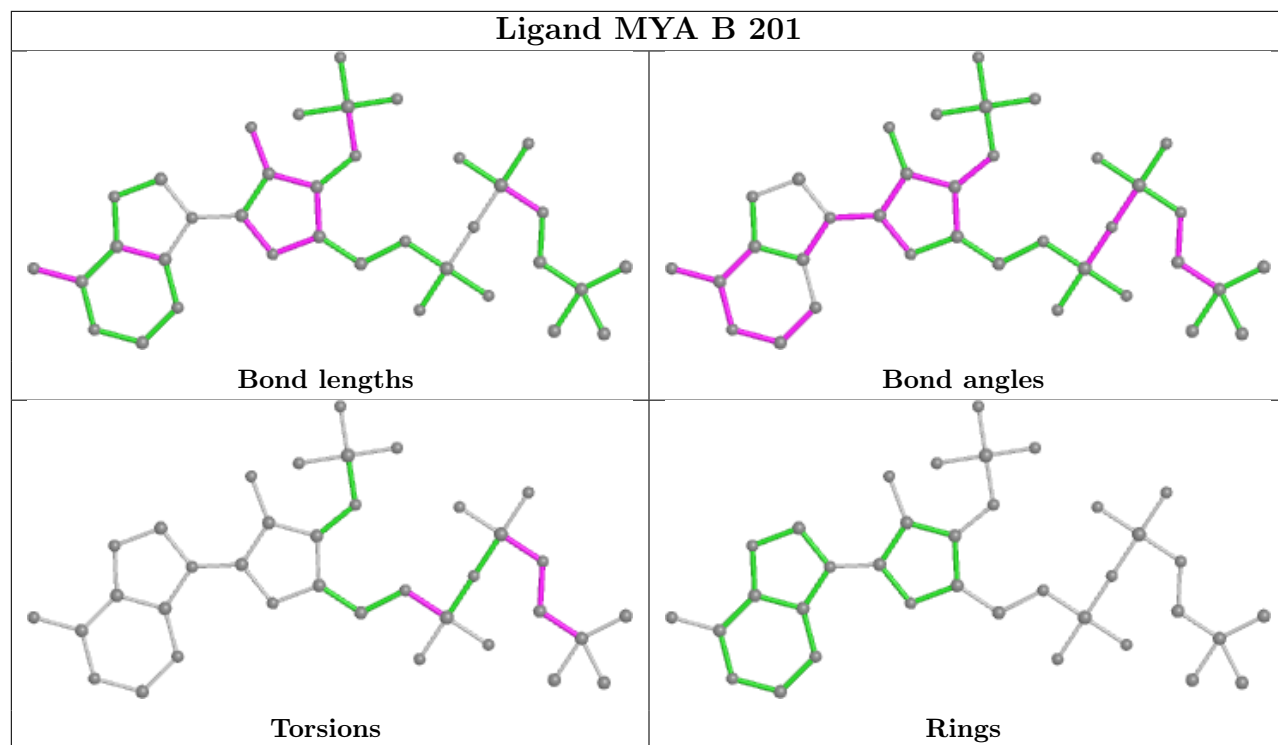
5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	MYA	C5X-O5X-P1A-O2A
2	A	201	MYA	C3X-O3X-P3X-O7A
2	B	201	MYA	C11-C12-O6A-P2A
2	B	201	MYA	C5X-O5X-P1A-O1A
2	B	201	MYA	C5X-O5X-P1A-O2A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	MYA	1	0
2	A	201	MYA	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 B 201

Bond lengths

Bond angles

Torsions

Rings

Ligand MYA C 201

Bond lengths

Bond angles

Torsions

Rings

Ligand MYA A 201

Bond lengths

Bond angles

Torsions

Rings
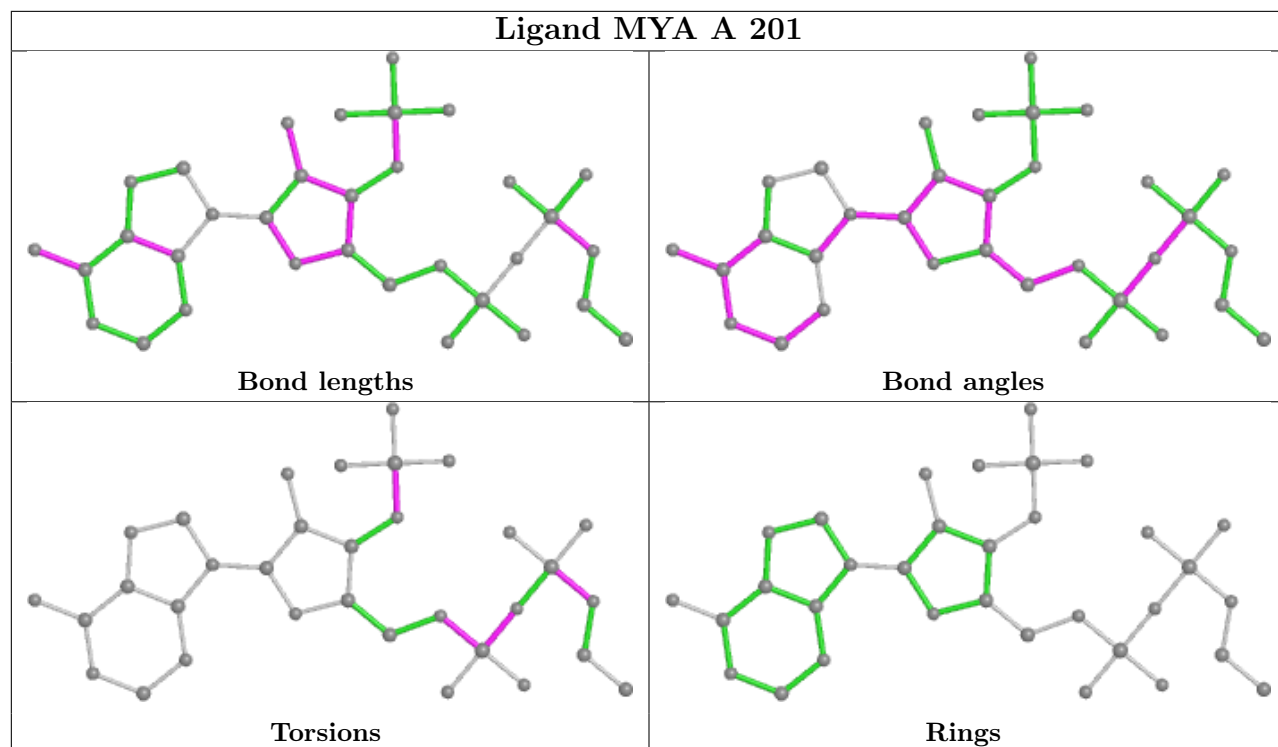
5.7 Other polymers (i)

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3   Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4   Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.
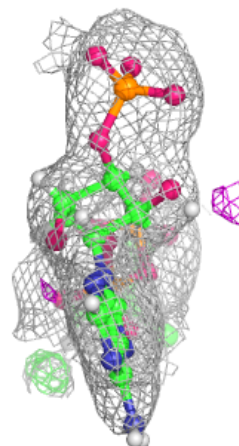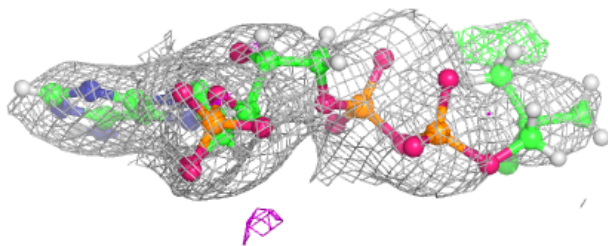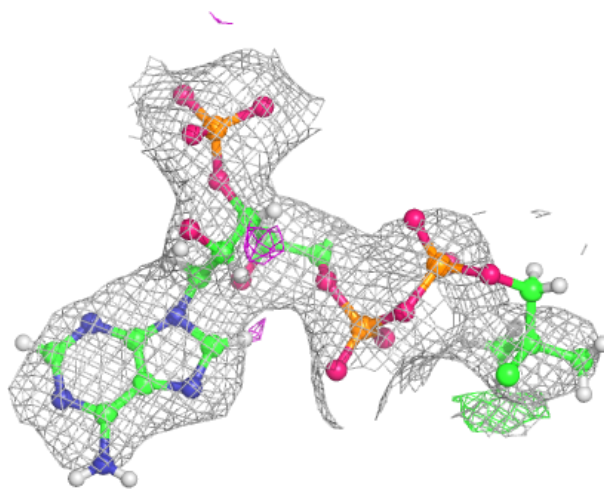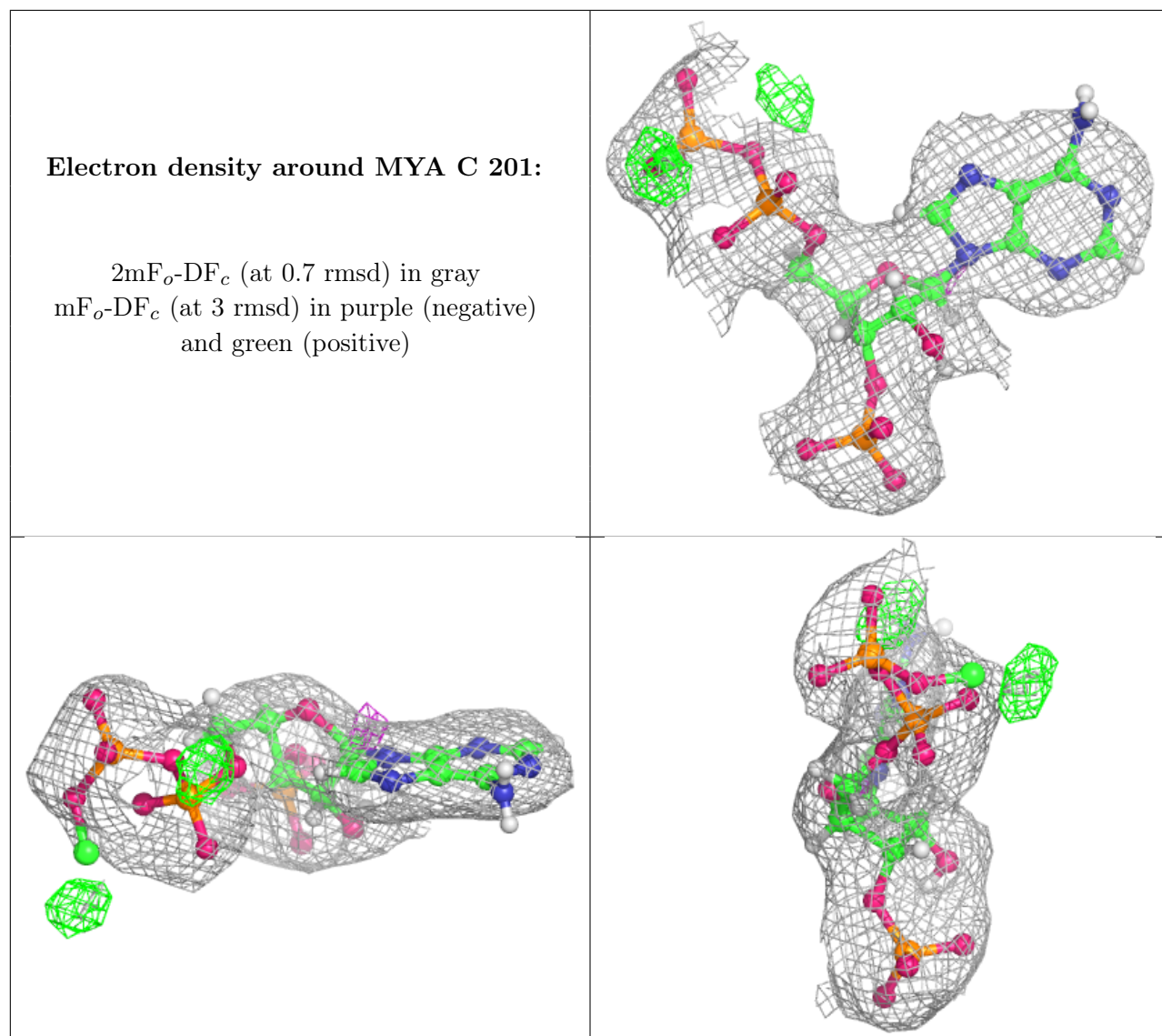
Electron density around MYA A 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
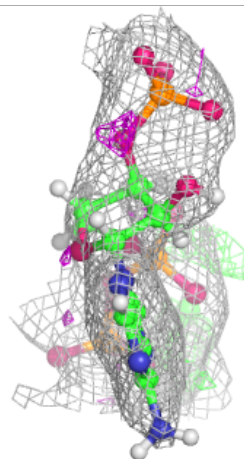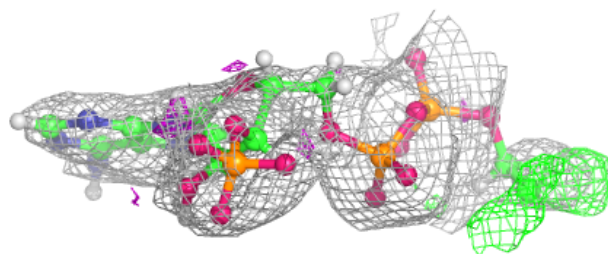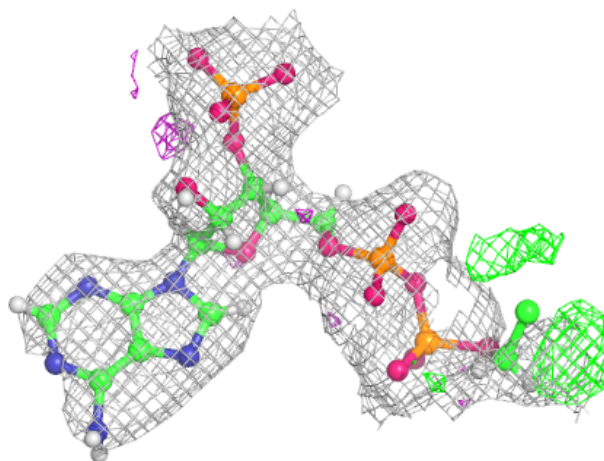
Electron density around MYA B 201:

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

Electron density around MYA C 201:

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

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.