



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:23 AM UTC

PDB ID : 6SKJ / pdb_00006skj
Title : DeltaC2 C-terminal truncation of HsNMT1 in complex with MyrCoA and GNCFSKPR substrates
Authors : Dian, C.; Riviere, F.B.; Asensio, T.; Giglione, C.; Meinnel, T.
Deposited on : 2019-08-15
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

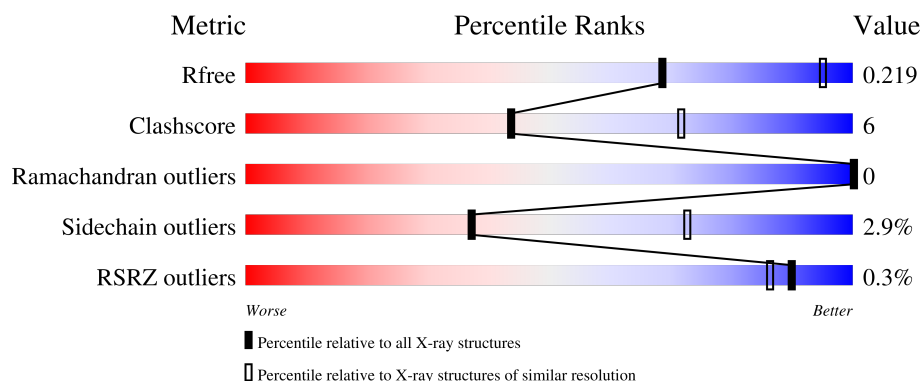
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	400	80% 16% .
1	B	400	81% 16% ..
2	C	8	88% 12%
2	D	8	50% 50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6773 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	387	Total	C	N	O	S	0	3	0
			3144	2035	525	567	17			
1	B	390	Total	C	N	O	S	0	1	0
			3140	2034	526	563	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLY	-	expression tag	UNP P30419
A	96	GLY	-	expression tag	UNP P30419
A	97	SER	-	expression tag	UNP P30419
A	98	GLU	-	expression tag	UNP P30419
B	95	GLY	-	expression tag	UNP P30419
B	96	GLY	-	expression tag	UNP P30419
B	97	SER	-	expression tag	UNP P30419
B	98	GLU	-	expression tag	UNP P30419

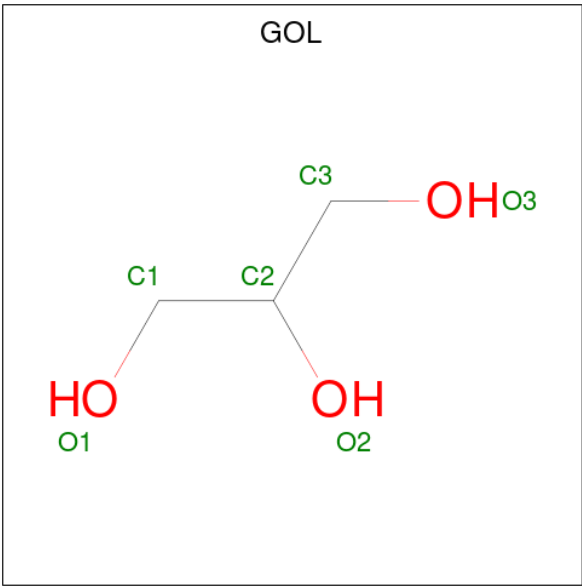
- Molecule 2 is a protein called Apoptosis-inducing factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	S	0	1	0
			61	37	11	12	1			
2	D	8	Total	C	N	O	S	0	1	0
			67	40	14	12	1			

There are 4 discrepancies between the modelled and reference sequences:

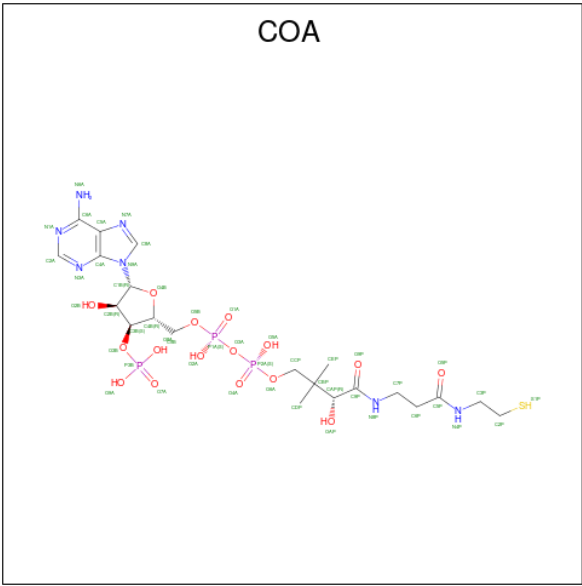
Chain	Residue	Modelled	Actual	Comment	Reference
C	3	ASN	GLY	engineered mutation	UNP Q96NN9
C	9	ARG	LYS	conflict	UNP Q96NN9
D	3	ASN	GLY	engineered mutation	UNP Q96NN9
D	9	ARG	LYS	conflict	UNP Q96NN9

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).

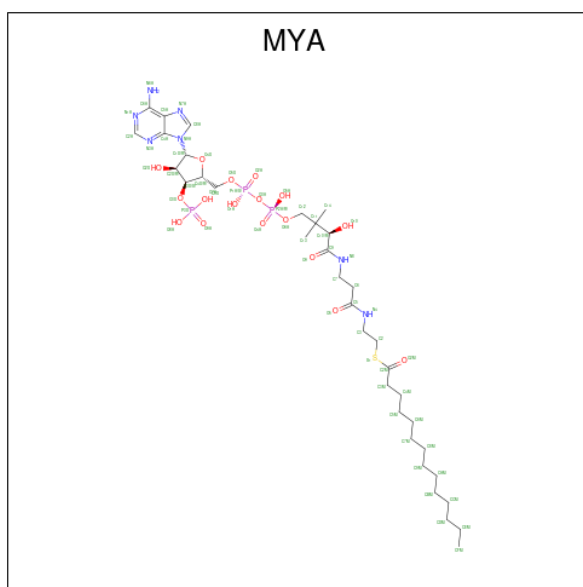


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	
								0	1

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

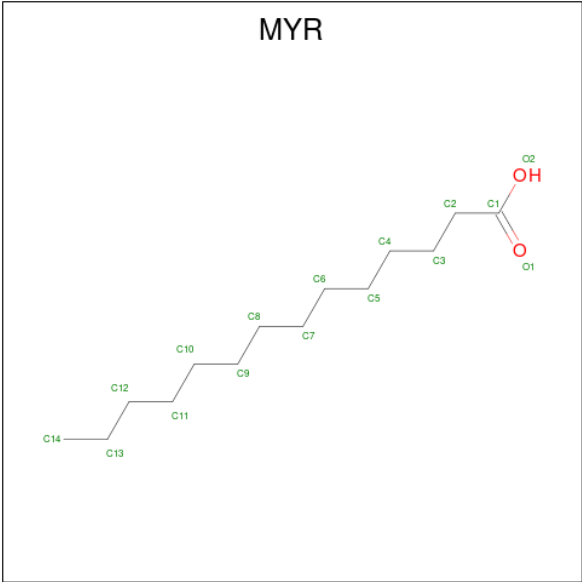
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg		
			1	1	0	0

- Molecule 6 is TETRADECANOYL-COA (CCD ID: MYA) (formula: C₃₅H₆₂N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	S	
			126	70	14	34	6	2	
6	D	1	Total	C	N	O	P	S	
			63	35	7	17	3	1	
								0	1

- Molecule 7 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	1
			15	14	1		

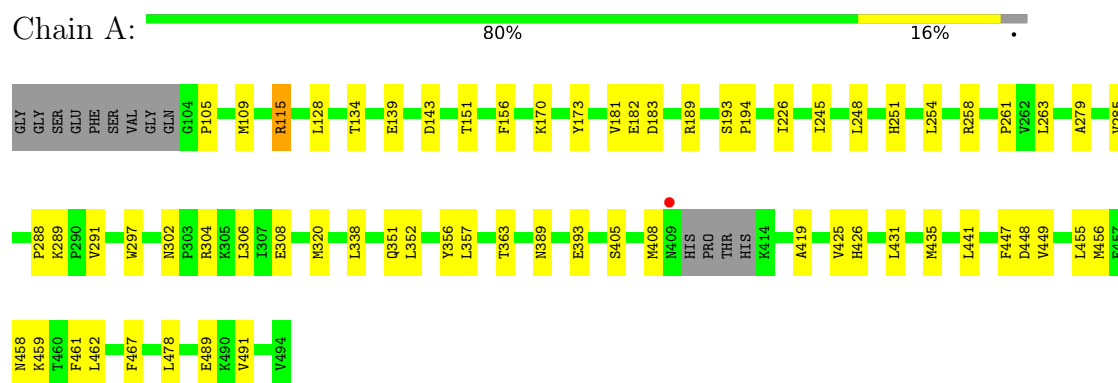
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	49	Total	O	0	1
			49	49		
8	B	37	Total	O	0	0
			37	37		
8	C	3	Total	O	0	0
			3	3		
8	D	1	Total	O	0	0
			1	1		

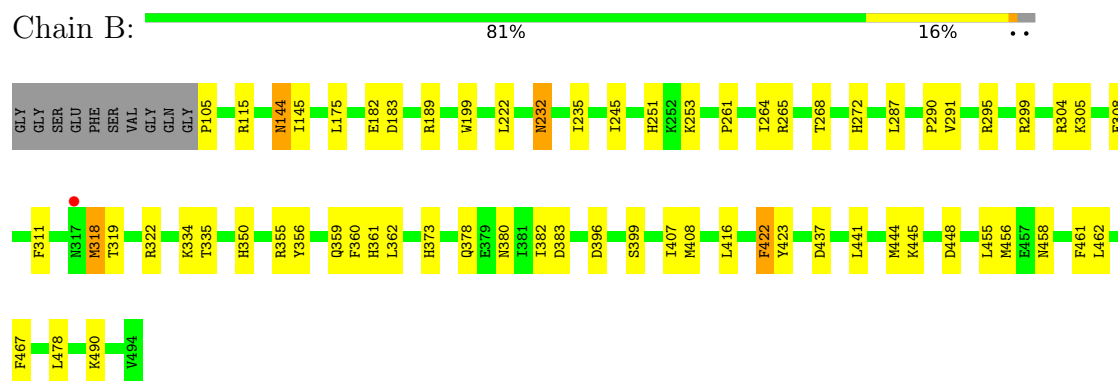
3 Residue-property plots

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 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.

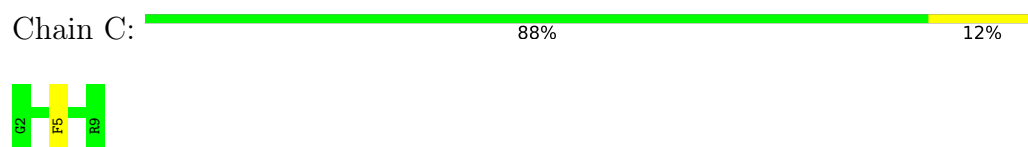
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1



• Molecule 2: Apoptosis-inducing factor 3



• Molecule 2: Apoptosis-inducing factor 3





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.97Å 58.27Å 154.13Å 90.00° 90.92° 90.00°	Depositor
Resolution (Å)	49.37 – 2.80 49.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.8 (49.37-2.80) 88.9 (49.37-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.189 , 0.219 0.191 , 0.219	Depositor DCC
R_{free} test set	1086 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 19.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6773	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MYA, COA, MYR, MG, GOL

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	0.16	0/3234	0.38	0/4397
1	B	0.17	0/3230	0.35	0/4397
2	C	0.16	0/62	0.44	0/80
2	D	0.15	0/68	0.42	0/87
All	All	0.16	0/6594	0.37	0/8961

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3144	0	3086	39	0
1	B	3140	0	3079	40	0
2	C	61	0	50	2	0
2	D	67	0	61	2	0
3	A	6	0	8	2	0
3	B	12	0	16	2	0
4	B	48	0	28	2	0
5	B	1	0	0	0	0
6	C	126	0	116	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	63	0	53	2	0
7	D	15	0	27	2	0
8	A	49	0	0	0	0
8	B	37	0	0	2	0
8	C	3	0	0	0	0
8	D	1	0	0	0	0
All	All	6773	0	6524	81	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 6.

All (81) 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)
4:B:503[B]:COA:O4B	4:B:503[B]:COA:C1B	1.66	1.26
1:B:251:HIS:HD2	1:B:253:LYS:H	1.27	0.83
1:A:291:VAL:HB	3:A:501:GOL:H11	1.70	0.71
1:B:245:ILE:HG13	6:D:202[A]:MYA:HAMA	1.72	0.70
1:A:351:GLN:NE2	1:B:144:ASN:OD1	2.25	0.69
1:A:115:ARG:HH11	1:A:115:ARG:HB3	1.59	0.68
1:A:338:LEU:HD21	1:A:441:LEU:HD11	1.75	0.67
1:A:143:ASP:O	1:B:350:HIS:ND1	2.26	0.65
1:A:459:LYS:NZ	1:A:489:GLU:OE1	2.26	0.64
1:B:291:VAL:HB	3:B:501:GOL:H11	1.80	0.64
1:A:302:ASN:HD22	1:A:448:ASP:HA	1.62	0.64
1:A:170:LYS:HA	1:A:173:TYR:CE2	2.35	0.62
1:B:182:GLU:OE2	1:B:189:ARG:NH1	2.33	0.61
1:B:183:ASP:OD2	2:D:7:LYS:NZ	2.33	0.61
1:B:441:LEU:HD23	1:B:444:MET:HE2	1.82	0.60
1:A:226:ILE:HD12	1:A:248:LEU:HD13	1.85	0.59
1:A:105:PRO:HB3	1:A:285:VAL:HG11	1.86	0.58
1:A:458:ASN:HA	1:A:461:PHE:CE2	2.39	0.58
1:B:251:HIS:CD2	1:B:253:LYS:H	2.15	0.57
1:B:305:LYS:NZ	1:B:448:ASP:OD2	2.38	0.56
1:B:380:ASN:ND2	8:B:601:HOH:O	2.37	0.56
1:B:478:LEU:HB2	3:B:501:GOL:H12	1.87	0.55
6:C:101[A]:MYA:H6MA	6:C:101[A]:MYA:H2AA	1.87	0.55
1:A:251:HIS:HB3	1:A:254:LEU:HD13	1.90	0.53
1:B:407:ILE:HD11	1:B:416:LEU:HB2	1.90	0.53
1:A:173:TYR:CE2	1:A:194:PRO:HG3	2.43	0.53
1:A:245:ILE:HG13	6:C:101[B]:MYA:HAMA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258[B]:ARG:HG2	1:A:261:PRO:HG2	1.90	0.52
1:A:389:ASN:HD21	1:A:393[B]:GLU:HG2	1.75	0.52
1:A:304:ARG:HD3	1:A:320:MET:HE3	1.92	0.51
1:B:268:THR:HG23	6:D:202[A]:MYA:HEMA	1.92	0.51
1:B:360:PHE:CE1	1:B:456:MET:HA	2.45	0.51
1:A:462:LEU:O	1:A:467:PHE:HB2	2.11	0.51
1:A:279:ALA:HB2	6:C:101[A]:MYA:HEM	1.92	0.51
1:A:182:GLU:OE2	1:A:189:ARG:NH2	2.38	0.50
1:B:264:ILE:HG23	7:D:201[B]:MYR:H72	1.93	0.50
1:A:426:HIS:CD2	1:A:431:LEU:HB2	2.47	0.50
1:A:435:MET:HG3	1:A:461:PHE:CE2	2.47	0.49
1:B:356:TYR:O	1:B:359:GLN:HG2	2.13	0.49
1:A:458:ASN:O	1:A:462:LEU:HG	2.13	0.48
1:B:458:ASN:HA	1:B:461:PHE:CE2	2.48	0.48
1:B:299:ARG:HB2	1:B:467:PHE:CE2	2.48	0.48
1:A:455:LEU:HB2	1:A:491:VAL:O	2.14	0.48
1:A:183:ASP:HB3	2:C:5:PHE:CD1	2.49	0.47
1:B:318:MET:HE3	1:B:318:MET:HB3	1.76	0.47
1:A:297:TRP:CG	1:A:462:LEU:HD13	2.49	0.47
1:B:264:ILE:O	1:B:268:THR:OG1	2.29	0.47
1:A:156:PHE:CE1	1:A:254:LEU:HD21	2.50	0.47
1:B:304:ARG:O	1:B:308:GLU:HG3	2.15	0.47
1:B:105:PRO:O	1:B:115[A]:ARG:NH1	2.49	0.46
6:C:101[A]:MYA:O6A	6:C:101[A]:MYA:O10	2.25	0.46
4:B:503[B]:COA:S1P	4:B:503[B]:COA:N6A	2.88	0.45
1:A:109:MET:HE3	1:A:128:LEU:HD22	1.99	0.45
1:B:399:SER:OG	1:B:422:PHE:HB3	2.16	0.45
1:B:235:ILE:HD13	1:B:362:LEU:HD13	1.98	0.44
1:B:145:ILE:HG12	1:B:272:HIS:HB3	2.00	0.44
1:B:199:TRP:O	1:B:373:HIS:NE2	2.46	0.43
1:A:304:ARG:O	1:A:308:GLU:HG3	2.18	0.43
1:A:357:LEU:O	1:A:363:THR:HG21	2.18	0.43
1:B:462:LEU:O	1:B:467:PHE:HB2	2.18	0.43
1:B:287:LEU:O	1:B:290:PRO:HD3	2.19	0.43
1:A:419:ALA:HB2	1:A:447:PHE:CD1	2.55	0.42
1:B:245:ILE:HG13	7:D:201[B]:MYR:H101	2.02	0.42
1:A:302:ASN:ND2	1:A:447:PHE:O	2.53	0.42
1:B:232:ASN:ND2	8:B:602:HOH:O	2.44	0.42
1:A:226:ILE:HG22	1:A:263:LEU:HD22	2.01	0.41
1:A:478:LEU:HB2	3:A:501:GOL:H12	2.01	0.41
1:B:335:THR:OG1	1:B:437:ASP:OD2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:PRO:HA	1:A:289:LYS:HA	1.87	0.41
1:B:383:ASP:OD1	1:B:445:LYS:NZ	2.33	0.41
1:B:311:PHE:O	2:D:8:PRO:HD2	2.20	0.41
1:A:356:TYR:HE2	1:A:456:MET:HE2	1.84	0.41
1:B:261:PRO:O	1:B:265:ARG:HG3	2.20	0.41
1:B:361:HIS:CE1	1:B:490:LYS:HD2	2.56	0.41
1:B:422:PHE:HB3	1:B:423:TYR:H	1.64	0.41
1:A:352:LEU:HB3	1:A:425:VAL:HG11	2.01	0.41
1:A:405:SER:OG	2:C:5:PHE:HE2	2.04	0.41
1:A:306:LEU:HD11	1:A:449:VAL:HB	2.02	0.41
1:B:318:MET:HE3	1:B:322:ARG:HB3	2.02	0.41
1:B:175:LEU:HD22	1:B:222:LEU:HG	2.03	0.41
1:B:378:GLN:H	1:B:382:ILE:HG23	1.86	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	386/400 (96%)	370 (96%)	16 (4%)	0	100	100
1	B	389/400 (97%)	368 (95%)	21 (5%)	0	100	100
2	C	6/8 (75%)	6 (100%)	0	0	100	100
2	D	6/8 (75%)	6 (100%)	0	0	100	100
All	All	787/816 (96%)	750 (95%)	37 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	342/360 (95%)	335 (98%)	7 (2%)	48	80
1	B	341/360 (95%)	330 (97%)	11 (3%)	34	70
2	C	6/7 (86%)	6 (100%)	0	100	100
2	D	7/7 (100%)	5 (71%)	2 (29%)	0	1
All	All	696/734 (95%)	676 (97%)	20 (3%)	37	73

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	134	THR
1	A	139	GLU
1	A	151	THR
1	A	181	VAL
1	A	193	SER
1	A	408	MET
1	B	144	ASN
1	B	232	ASN
1	B	295	ARG
1	B	318	MET
1	B	319	THR
1	B	334	LYS
1	B	355	ARG
1	B	396	ASP
1	B	408	MET
1	B	422	PHE
1	B	455	LEU
2	D	4	CYS
2	D	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	302	ASN
1	A	321	GLN
1	A	359	GLN
1	B	186	ASN
1	B	251	HIS
1	B	272	HIS
1	B	351	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
3	GOL	B	502	-	5,5,5	0.36	0	5,5,5	0.32	0
3	GOL	A	501	-	5,5,5	0.38	0	5,5,5	0.36	0
4	COA	B	503[B]	-	47,50,50	3.64	14 (29%)	69,75,75	1.94	17 (24%)
6	MYA	C	101[B]	2	63,65,65	2.20	10 (15%)	85,91,91	2.45	18 (21%)
7	MYR	D	201[B]	2	13,14,15	0.44	0	12,13,15	0.81	0
3	GOL	B	501	-	5,5,5	0.37	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MYA	D	202[A]	2	63,65,65	2.19	9 (14%)	85,91,91	2.44	18 (21%)
6	MYA	C	101[A]	-	63,65,65	1.27	8 (12%)	85,91,91	1.71	14 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	502	-	-	4/4/4/4	-
3	GOL	A	501	-	-	4/4/4/4	-
4	COA	B	503[B]	-	-	9/48/64/64	0/3/3/3
6	MYA	C	101[B]	2	-	19/64/80/80	0/3/3/3
7	MYR	D	201[B]	2	-	6/12/12/13	-
3	GOL	B	501	-	-	2/4/4/4	-
6	MYA	D	202[A]	2	-	9/64/80/80	0/3/3/3
6	MYA	C	101[A]	-	-	17/64/80/80	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	202[A]	MYA	O2M-C2M	14.48	1.43	1.21
6	C	101[B]	MYA	O2M-C2M	14.33	1.43	1.21
4	B	503[B]	COA	P2A-O3A	11.03	1.71	1.59
4	B	503[B]	COA	O4B-C1B	10.68	1.66	1.42
4	B	503[B]	COA	P1A-O3A	9.45	1.69	1.59
4	B	503[B]	COA	C2B-C1B	-6.64	1.32	1.53
4	B	503[B]	COA	C6A-N6A	6.59	1.51	1.34
4	B	503[B]	COA	C9P-N8P	6.26	1.48	1.33
4	B	503[B]	COA	C5P-N4P	6.19	1.48	1.33
4	B	503[B]	COA	O4B-C4B	-6.10	1.31	1.45
4	B	503[B]	COA	P3B-O3B	4.69	1.67	1.59
6	C	101[A]	MYA	C2A-N3A	3.65	1.40	1.33
6	D	202[A]	MYA	C2A-N3A	3.49	1.40	1.33
6	C	101[B]	MYA	C2A-N3A	3.46	1.40	1.33
6	C	101[A]	MYA	C2A-N1A	3.42	1.40	1.33
6	C	101[B]	MYA	C2A-N1A	3.30	1.39	1.33
6	D	202[A]	MYA	C2A-N1A	3.26	1.39	1.33
6	D	202[A]	MYA	C5A-N7A	-3.22	1.33	1.39
6	C	101[B]	MYA	C5A-N7A	-3.15	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	101[A]	MYA	C5A-N7A	-3.06	1.33	1.39
6	D	202[A]	MYA	C5A-C4A	-2.97	1.33	1.39
6	C	101[B]	MYA	C5A-C4A	-2.95	1.33	1.39
4	B	503[B]	COA	O3B-C3B	-2.89	1.34	1.44
6	C	101[A]	MYA	C5A-C4A	-2.85	1.34	1.39
6	C	101[B]	MYA	C3M-C2M	2.79	1.53	1.50
6	C	101[B]	MYA	C5A-C6A	-2.68	1.33	1.41
4	B	503[B]	COA	O9P-C9P	-2.68	1.18	1.23
6	D	202[A]	MYA	C5A-C6A	-2.65	1.33	1.41
6	C	101[A]	MYA	C5A-C6A	-2.54	1.33	1.41
6	C	101[B]	MYA	C8A-N9A	-2.52	1.33	1.37
6	D	202[A]	MYA	C8A-N9A	-2.47	1.33	1.37
6	D	202[A]	MYA	C3M-C2M	2.42	1.53	1.50
6	C	101[A]	MYA	C8A-N9A	-2.41	1.33	1.37
4	B	503[B]	COA	C8A-N7A	2.31	1.36	1.31
4	B	503[B]	COA	C3B-C4B	2.23	1.58	1.52
4	B	503[B]	COA	P2A-O6A	2.17	1.67	1.59
6	C	101[B]	MYA	O4X-C1X	2.12	1.46	1.42
6	C	101[A]	MYA	O4X-C1X	2.03	1.46	1.42
6	C	101[A]	MYA	C3M-C2M	2.02	1.52	1.50
6	D	202[A]	MYA	P3X-O8A	-2.02	1.47	1.54
6	C	101[B]	MYA	P3X-O8A	-2.02	1.47	1.54

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	202[A]	MYA	O2M-C2M-C3M	-11.63	110.56	123.98
6	C	101[B]	MYA	O2M-C2M-S1	-11.34	108.26	122.68
6	C	101[B]	MYA	O2M-C2M-C3M	-10.76	111.56	123.98
6	D	202[A]	MYA	O2M-C2M-S1	-10.21	109.69	122.68
6	D	202[A]	MYA	N3A-C2A-N1A	-6.99	118.00	128.58
6	C	101[B]	MYA	N3A-C2A-N1A	-6.92	118.11	128.58
6	C	101[A]	MYA	N3A-C2A-N1A	-6.76	118.36	128.58
4	B	503[B]	COA	N6A-C6A-N1A	-5.53	106.05	118.38
4	B	503[B]	COA	N3A-C2A-N1A	-5.52	120.22	128.58
4	B	503[B]	COA	C5A-C4A-N3A	-5.08	119.72	126.72
6	D	202[A]	MYA	C5A-C4A-N3A	-4.76	120.16	126.72
6	D	202[A]	MYA	C3M-C2M-S1	-4.67	107.84	113.40
6	C	101[B]	MYA	C5A-C4A-N3A	-4.66	120.29	126.72
6	C	101[A]	MYA	C5A-C4A-N3A	-4.58	120.40	126.72
4	B	503[B]	COA	N9A-C8A-N7A	-4.39	107.70	113.94
6	D	202[A]	MYA	N9A-C8A-N7A	-4.32	107.81	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503[B]	COA	C5A-C6A-N6A	4.27	133.86	123.29
6	C	101[B]	MYA	N9A-C8A-N7A	-4.19	107.99	113.94
6	C	101[A]	MYA	N9A-C8A-N7A	-3.94	108.34	113.94
6	C	101[B]	MYA	C3M-C2M-S1	-3.90	108.75	113.40
6	C	101[B]	MYA	C2X-C3X-C4X	-3.89	96.43	103.24
4	B	503[B]	COA	O6A-CCP-CBP	-3.88	104.31	110.55
6	C	101[A]	MYA	C2X-C3X-C4X	-3.82	96.55	103.24
6	C	101[B]	MYA	O4X-C1X-N9A	3.70	115.20	108.09
6	C	101[A]	MYA	O4X-C1X-N9A	3.67	115.13	108.09
4	B	503[B]	COA	C2A-N3A-C4A	3.49	120.35	111.83
6	D	202[A]	MYA	C2A-N3A-C4A	3.39	120.11	111.83
6	C	101[B]	MYA	C2A-N3A-C4A	3.33	119.97	111.83
6	C	101[A]	MYA	C2A-N3A-C4A	3.26	119.80	111.83
6	D	202[A]	MYA	C5A-N7A-C8A	3.19	108.47	103.45
4	B	503[B]	COA	C5A-N7A-C8A	3.15	108.39	103.45
6	C	101[A]	MYA	O2M-C2M-C3M	-3.12	120.38	123.98
6	D	202[A]	MYA	O6A-C12-C11	-3.08	105.60	110.55
6	C	101[B]	MYA	C5A-N7A-C8A	3.05	108.25	103.45
4	B	503[B]	COA	N3A-C4A-N9A	3.04	132.33	127.17
6	C	101[B]	MYA	O6A-C12-C11	-2.93	105.84	110.55
6	D	202[A]	MYA	C6A-C5A-C4A	2.88	121.11	117.18
6	C	101[A]	MYA	C5A-N7A-C8A	2.87	107.95	103.45
6	C	101[B]	MYA	C6A-C5A-C4A	2.83	121.05	117.18
6	D	202[A]	MYA	N3A-C4A-N9A	2.83	131.98	127.17
6	C	101[A]	MYA	C5A-C6A-N6A	-2.76	116.44	123.29
6	C	101[B]	MYA	N3A-C4A-N9A	2.76	131.86	127.17
6	D	202[A]	MYA	C5A-C6A-N6A	-2.75	116.48	123.29
6	C	101[A]	MYA	C6A-C5A-C4A	2.74	120.92	117.18
6	C	101[B]	MYA	C5A-C6A-N6A	-2.70	116.59	123.29
4	B	503[B]	COA	C4A-C5A-N7A	-2.70	107.49	110.58
4	B	503[B]	COA	C4A-N9A-C8A	2.59	108.46	105.74
6	D	202[A]	MYA	P3X-O3X-C3X	-2.59	116.51	123.43
6	C	101[A]	MYA	N3A-C4A-N9A	2.59	131.57	127.17
6	D	202[A]	MYA	O4X-C1X-C2X	-2.56	101.14	106.62
6	C	101[A]	MYA	C3M-C2M-S1	2.50	116.38	113.40
6	D	202[A]	MYA	C4A-C5A-N7A	-2.47	107.75	110.58
4	B	503[B]	COA	C5B-C4B-C3B	-2.43	106.30	114.38
6	C	101[B]	MYA	C4A-C5A-N7A	-2.41	107.83	110.58
4	B	503[B]	COA	CEP-CBP-CAP	2.36	112.79	108.77
6	D	202[A]	MYA	C2X-C3X-C4X	-2.35	99.13	103.24
6	C	101[A]	MYA	C4A-C5A-N7A	-2.35	107.90	110.58
6	C	101[B]	MYA	C1X-N9A-C8A	-2.27	122.07	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	202[A]	MYA	C4A-N9A-C8A	2.26	108.11	105.74
6	C	101[B]	MYA	C4A-N9A-C8A	2.24	108.09	105.74
4	B	503[B]	COA	CDP-CBP-CAP	2.15	112.44	108.77
4	B	503[B]	COA	P3B-O3B-C3B	-2.12	117.78	123.43
4	B	503[B]	COA	C6P-C7P-N8P	-2.11	107.52	112.00
6	C	101[B]	MYA	P3X-O3X-C3X	-2.03	118.01	123.43
6	C	101[A]	MYA	C5A-C4A-N9A	2.03	108.02	105.81
6	D	202[A]	MYA	C1X-N9A-C8A	-2.01	122.62	127.09
4	B	503[B]	COA	C6P-C5P-N4P	2.01	120.01	116.34

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	GOL	C1-C2-C3-O3
4	B	503[B]	COA	CCP-O6A-P2A-O4A
6	C	101[A]	MYA	C10-C11-C12-O6A
6	C	101[A]	MYA	C13-C11-C12-O6A
6	C	101[A]	MYA	C14-C11-C12-O6A
6	C	101[B]	MYA	C3-C2-S1-C2M
6	C	101[B]	MYA	C10-C11-C12-O6A
6	C	101[B]	MYA	C13-C11-C12-O6A
6	C	101[B]	MYA	C14-C11-C12-O6A
6	C	101[B]	MYA	C12-O6A-P2A-O3A
6	C	101[B]	MYA	C12-O6A-P2A-O4A
6	C	101[B]	MYA	C12-O6A-P2A-O5A
6	D	202[A]	MYA	O2M-C2M-S1-C2
6	C	101[B]	MYA	C3X-C4X-C5X-O5X
3	B	501	GOL	O1-C1-C2-O2
3	A	501	GOL	O1-C1-C2-C3
3	A	501	GOL	C1-C2-C3-O3
3	B	501	GOL	O1-C1-C2-C3
3	B	502	GOL	O1-C1-C2-C3
3	B	502	GOL	O2-C2-C3-O3
6	C	101[A]	MYA	C3X-C4X-C5X-O5X
6	D	202[A]	MYA	C8M-C9M-CAM-CBM
7	D	201[B]	MYR	C4-C5-C6-C7
4	B	503[B]	COA	C3B-C4B-C5B-O5B
6	C	101[B]	MYA	O4X-C4X-C5X-O5X
6	C	101[B]	MYA	C8M-C9M-CAM-CBM
3	A	501	GOL	O1-C1-C2-O2
3	A	501	GOL	O2-C2-C3-O3

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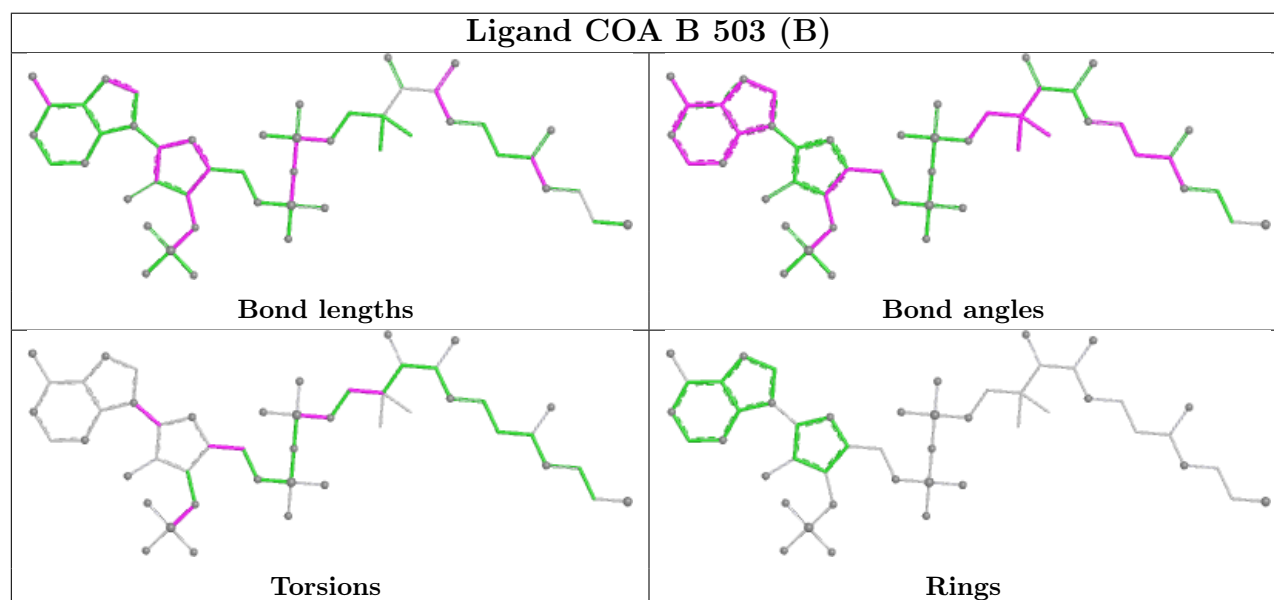
Mol	Chain	Res	Type	Atoms
6	C	101[A]	MYA	O4X-C4X-C5X-O5X
4	B	503[B]	COA	O4B-C4B-C5B-O5B
6	C	101[A]	MYA	CAM-CBM-CCM-CDM
6	C	101[B]	MYA	O2M-C2M-S1-C2
7	D	201[B]	MYR	C5-C6-C7-C8
6	C	101[A]	MYA	S1-C2M-C3M-C4M
6	C	101[A]	MYA	O2M-C2M-C3M-C4M
6	C	101[B]	MYA	S1-C2M-C3M-C4M
6	D	202[A]	MYA	S1-C2M-C3M-C4M
6	D	202[A]	MYA	CBM-CCM-CDM-CEM
3	B	502	GOL	O1-C1-C2-O2
6	C	101[A]	MYA	C2X-C1X-N9A-C8A
6	C	101[B]	MYA	C3M-C2M-S1-C2
7	D	201[B]	MYR	C9-C10-C11-C12
7	D	201[B]	MYR	C6-C7-C8-C9
6	C	101[A]	MYA	C8M-C9M-CAM-CBM
6	C	101[B]	MYA	C2X-C1X-N9A-C8A
4	B	503[B]	COA	CEP-CBP-CCP-O6A
6	D	202[A]	MYA	C14-C11-C12-O6A
4	B	503[B]	COA	CAP-CBP-CCP-O6A
6	D	202[A]	MYA	C10-C11-C12-O6A
6	C	101[A]	MYA	C12-O6A-P2A-O3A
6	C	101[A]	MYA	C12-O6A-P2A-O4A
6	C	101[A]	MYA	C12-O6A-P2A-O5A
6	C	101[B]	MYA	C5X-O5X-P1A-O2A
6	D	202[A]	MYA	C12-O6A-P2A-O4A
7	D	201[B]	MYR	C10-C11-C12-C13
6	C	101[B]	MYA	CAM-CBM-CCM-CDM
6	C	101[A]	MYA	C2X-C1X-N9A-C4A
6	C	101[B]	MYA	C2X-C1X-N9A-C4A
4	B	503[B]	COA	C3B-O3B-P3B-O8A
6	D	202[A]	MYA	C2X-C1X-N9A-C8A
4	B	503[B]	COA	C3B-O3B-P3B-O7A
6	C	101[B]	MYA	O4X-C1X-N9A-C8A
6	C	101[A]	MYA	C6-C7-N8-C9
6	C	101[A]	MYA	O4X-C1X-N9A-C8A
6	C	101[B]	MYA	C6-C7-N8-C9
4	B	503[B]	COA	CDP-CBP-CCP-O6A
6	D	202[A]	MYA	C13-C11-C12-O6A
7	D	201[B]	MYR	C7-C8-C9-C10
6	C	101[A]	MYA	C3-C2-S1-C2M
4	B	503[B]	COA	C2B-C1B-N9A-C8A

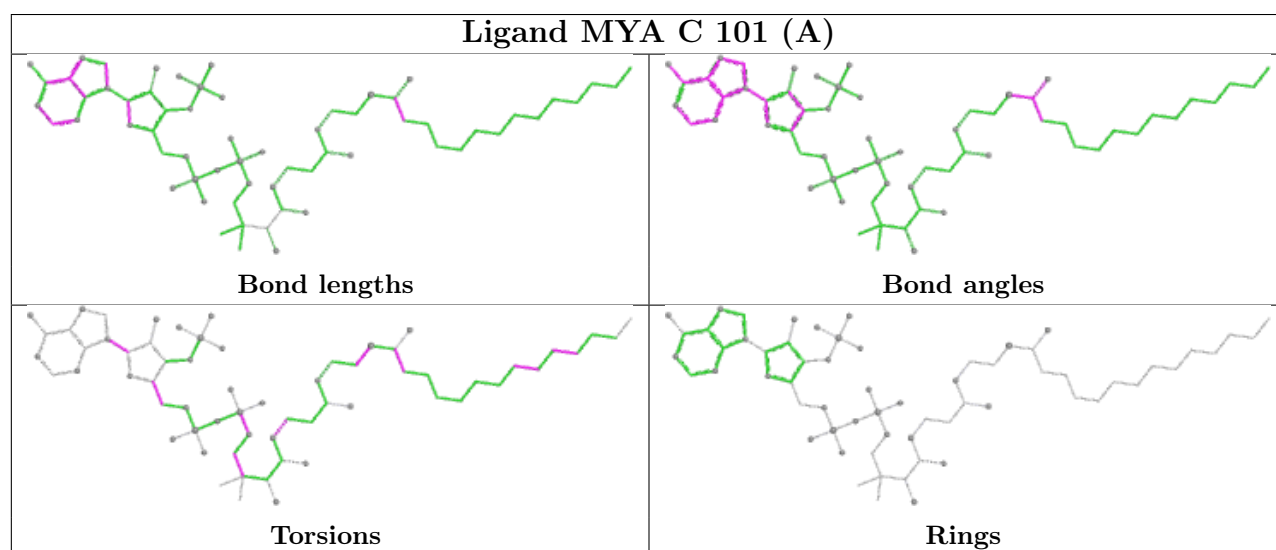
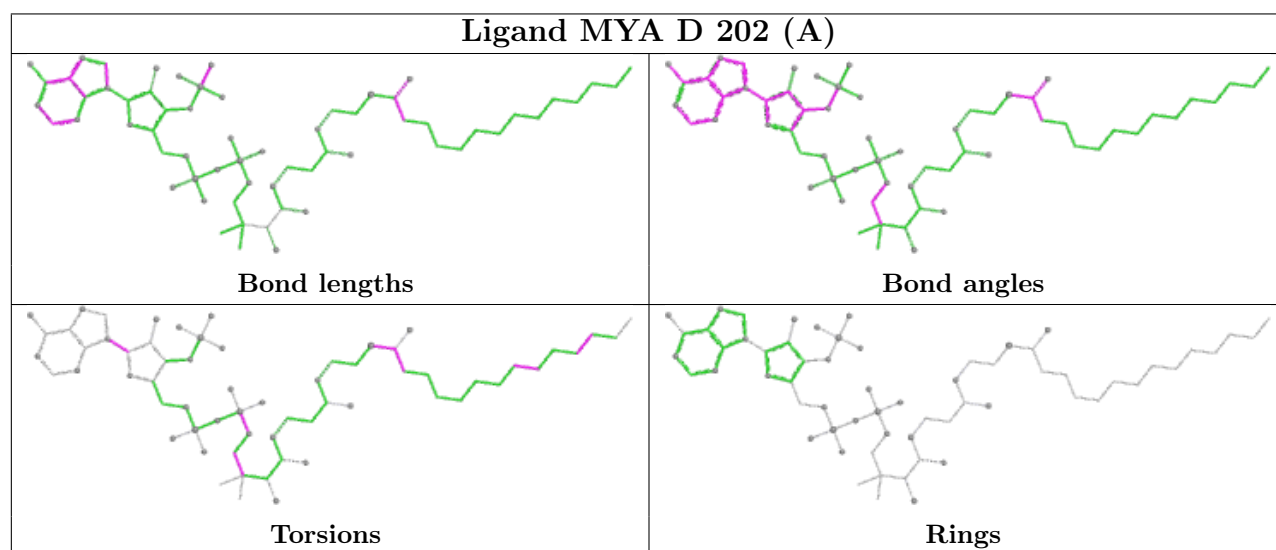
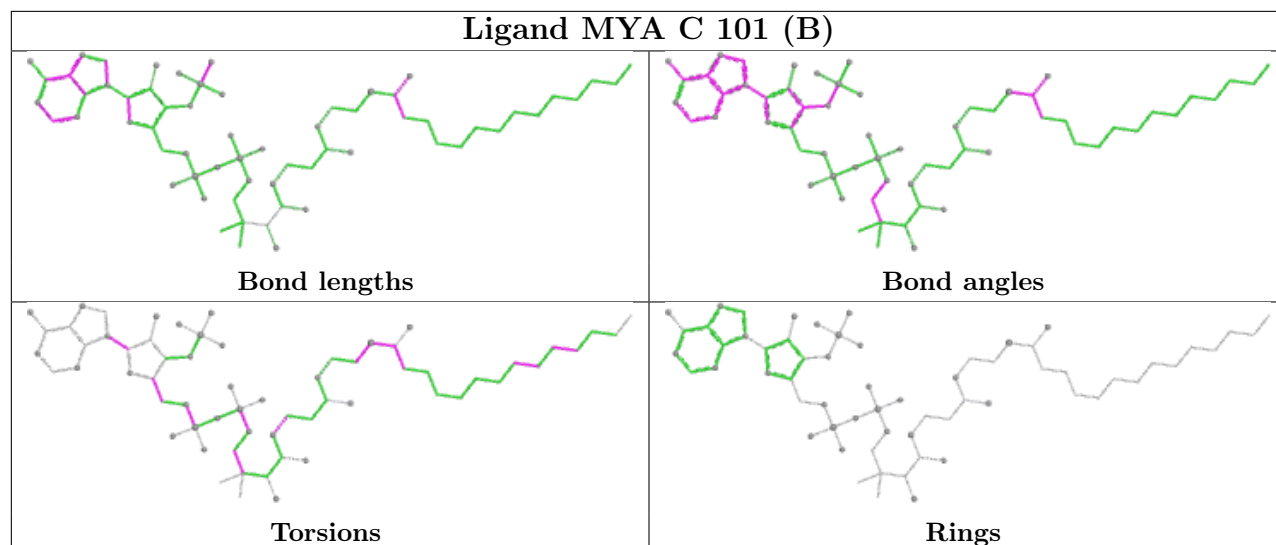
There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GOL	2	0
4	B	503[B]	COA	2	0
6	C	101[B]	MYA	1	0
7	D	201[B]	MYR	2	0
3	B	501	GOL	2	0
6	D	202[A]	MYA	2	0
6	C	101[A]	MYA	3	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 than 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.





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	387/400 (96%)	-0.49	1 (0%) 90 86	12, 23, 45, 53	3 (0%)
1	B	390/400 (97%)	-0.44	1 (0%) 90 86	13, 26, 53, 72	1 (0%)
2	C	8/8 (100%)	-0.11	0 100 100	13, 30, 31, 34	1 (12%)
2	D	8/8 (100%)	-0.17	0 100 100	15, 32, 36, 42	1 (12%)
All	All	793/816 (97%)	-0.46	2 (0%) 90 86	12, 25, 48, 72	6 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	ASN	2.6
1	B	317	ASN	2.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

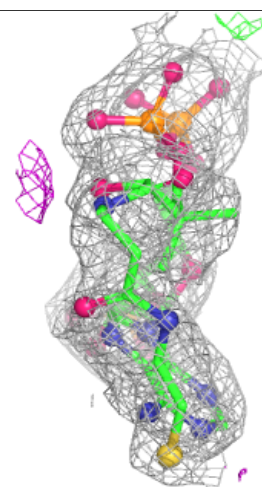
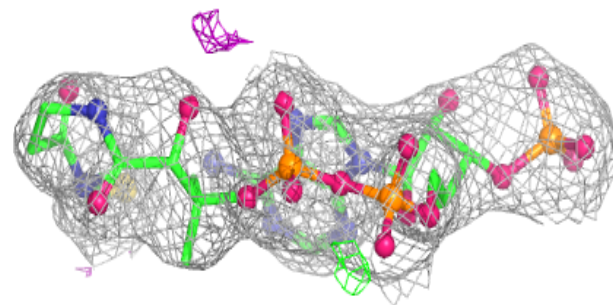
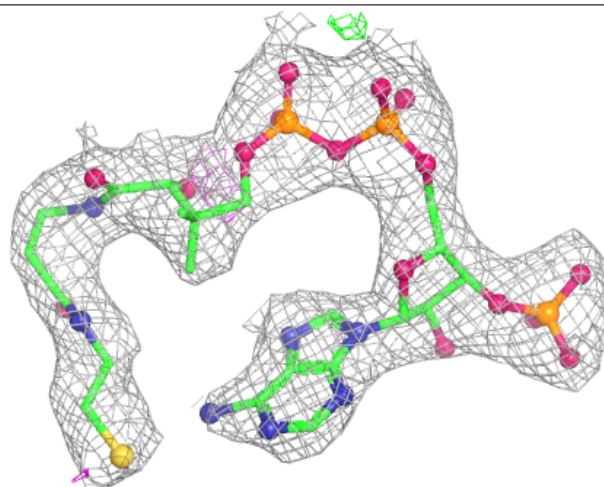
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	502	6/6	0.73	0.14	25,33,39,42	0
4	COA	B	503[B]	48/48	0.92	0.09	31,36,39,41	48
6	MYA	D	202[A]	63/63	0.92	0.09	16,35,39,40	63
6	MYA	C	101[B]	63/63	0.93	0.09	15,24,28,31	63
6	MYA	C	101[A]	63/63	0.93	0.09	15,24,28,31	63
3	GOL	A	501	6/6	0.94	0.09	23,26,27,28	0
7	MYR	D	201[B]	15/16	0.94	0.11	16,20,26,28	15
5	MG	B	504	1/1	0.95	0.12	24,24,24,24	0
3	GOL	B	501	6/6	0.96	0.07	23,24,26,28	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.

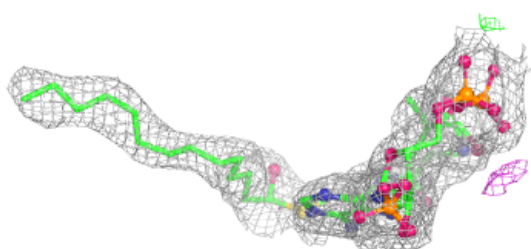
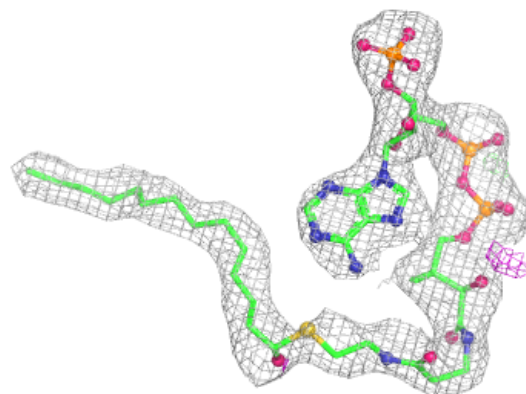
Electron density around COA B 503 (B):

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

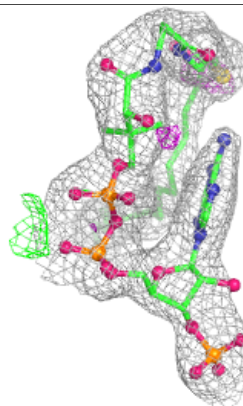
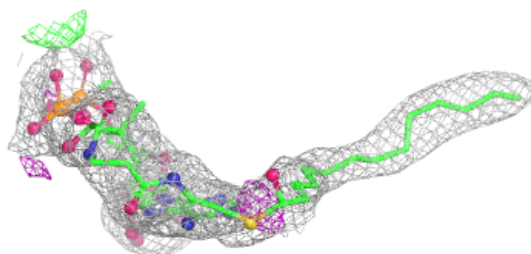
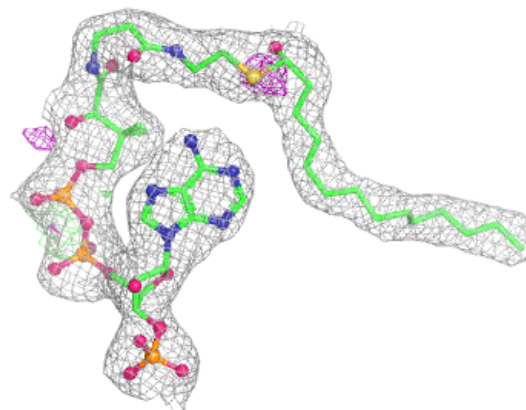


Electron density around MYA D 202 (A):

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

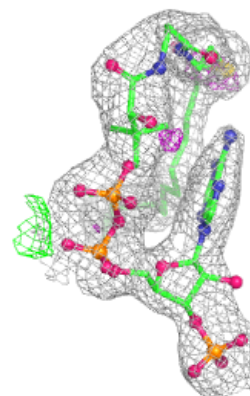
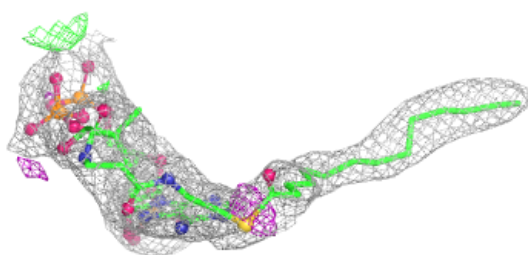
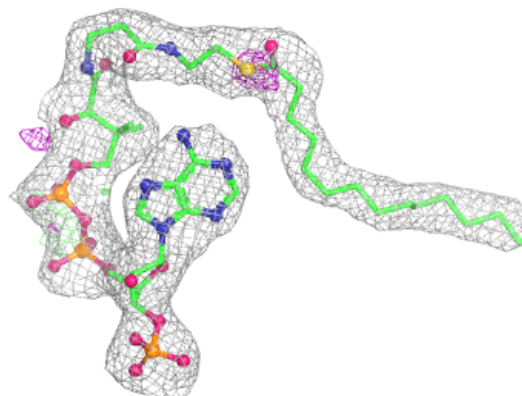
**Electron density around MYA C 101 (B):**

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



Electron density around MYA C 101 (A):

$2mF_o-DF_c$ (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.