



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:54 PM UTC

PDB ID : 4C2Y / pdb_00004c2y
Title : Human N-myristoyltransferase (NMT1) with Myristoyl-CoA co-factor
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 : 1.64 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

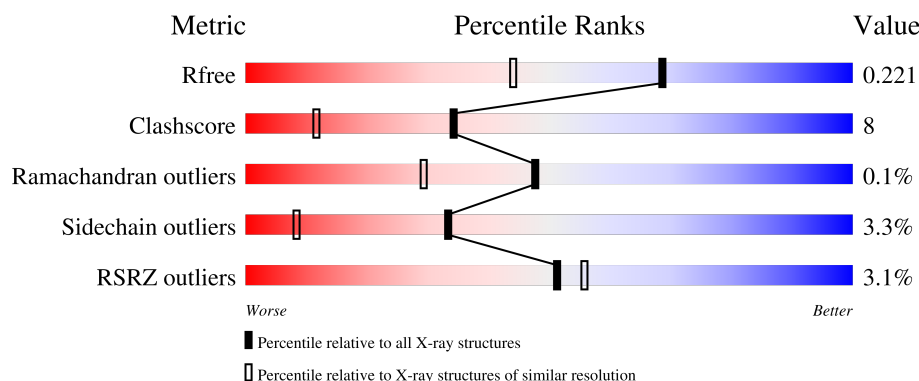
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

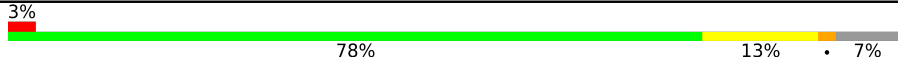
The reported resolution of this entry is 1.64 Å.

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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	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
5	GOL	B	1500	-	-	X	-
5	GOL	B	1503	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7569 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	0	27	0
			3286	2137	553	579	17			
1	B	382	Total	C	N	O	S	0	25	0
			3285	2138	547	583	17			

There are 44 discrepancies between the modelled and reference sequences:

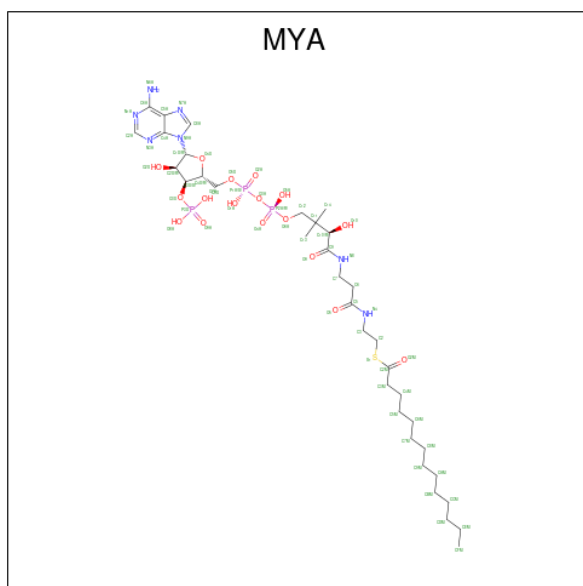
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	MET	-	expression tag	UNP P30419
A	88	GLY	-	expression tag	UNP P30419
A	89	SER	-	expression tag	UNP P30419
A	90	SER	-	expression tag	UNP P30419
A	91	HIS	-	expression tag	UNP P30419
A	92	HIS	-	expression tag	UNP P30419
A	93	HIS	-	expression tag	UNP P30419
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 (CCD ID: 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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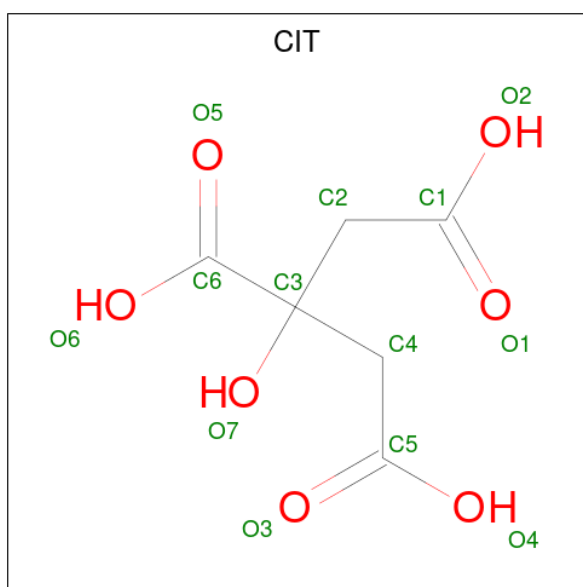
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

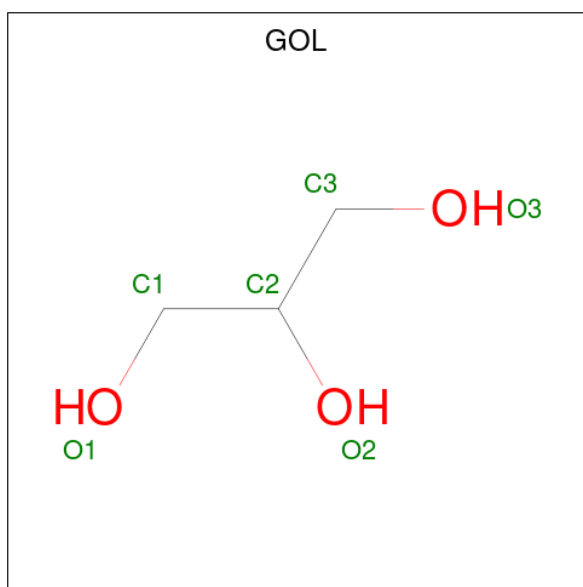
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

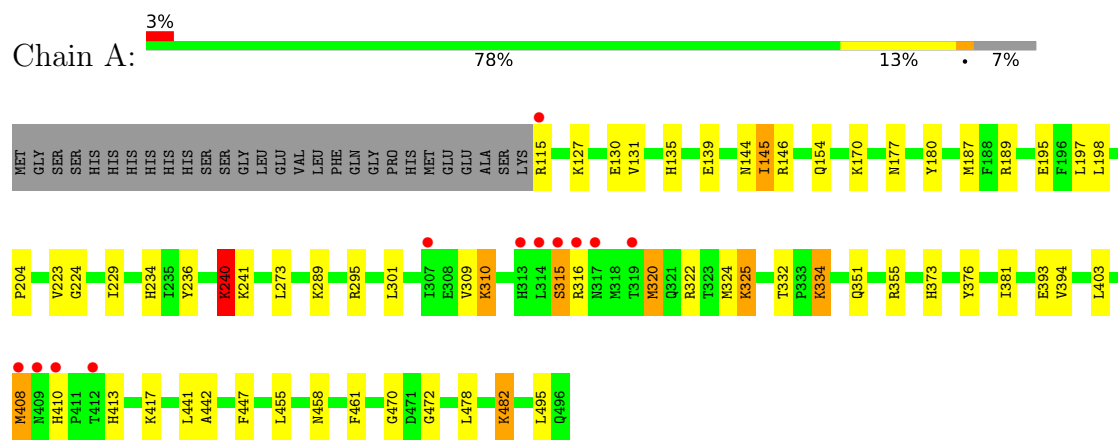
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	389	Total	O	0	0
			389	389		
6	B	413	Total	O	0	0
			413	413		

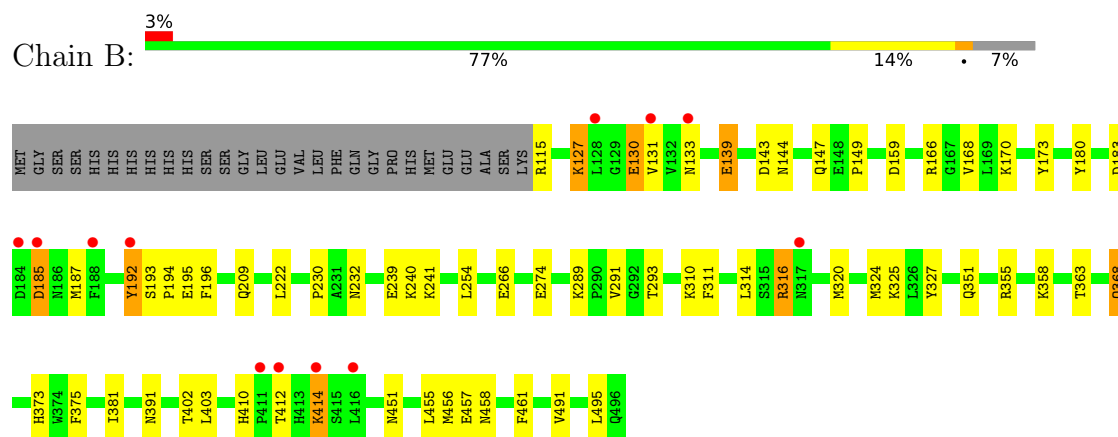
3 Residue-property plots [i](#)

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



• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.74Å 178.48Å 58.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.24 – 1.64 89.24 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.9 (89.24-1.64) 97.9 (89.24-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.170 , 0.222 0.169 , 0.221	Depositor DCC
R_{free} test set	4944 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7569	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.53% 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: GOL, MG, MYA, CIT

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	1.33	12/3454 (0.3%)	1.23	14/4684 (0.3%)
1	B	1.43	20/3446 (0.6%)	1.25	13/4679 (0.3%)
All	All	1.38	32/6900 (0.5%)	1.24	27/9363 (0.3%)

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	A	0	1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	THR	C-O	7.42	1.32	1.24
1	B	327	TYR	N-CA	7.33	1.55	1.46
1	B	139	GLU	N-CA	7.18	1.52	1.45
1	B	168	VAL	N-CA	6.59	1.54	1.46
1	A	224	GLY	N-CA	6.50	1.51	1.45
1	B	193	SER	CA-C	6.34	1.60	1.52
1	A	180	TYR	N-CA	6.33	1.52	1.46
1	B	456	MET	CA-C	6.18	1.59	1.53
1	A	441	LEU	N-CA	-6.17	1.38	1.46
1	B	266	GLU	N-CA	6.15	1.53	1.46
1	B	222	LEU	N-CA	6.09	1.53	1.46
1	A	495	LEU	N-CA	6.05	1.53	1.45
1	A	139	GLU	N-CA	6.03	1.50	1.45
1	B	159	ASP	N-CA	6.01	1.53	1.46
1	B	391	ASN	CA-C	-5.87	1.44	1.52
1	A	478	LEU	C-O	5.71	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	TYR	C-O	-5.71	1.17	1.23
1	B	368	GLN	N-CA	5.57	1.53	1.46
1	A	240[A]	LYS	C-O	-5.46	1.17	1.23
1	A	240[B]	LYS	C-O	-5.46	1.17	1.23
1	B	491	VAL	N-CA	5.41	1.52	1.46
1	B	180	TYR	N-CA	5.39	1.51	1.46
1	A	154	GLN	CA-C	5.39	1.59	1.52
1	B	358	LYS	N-CA	5.37	1.53	1.46
1	A	373	HIS	C-O	5.34	1.30	1.24
1	B	147	GLN	CA-C	-5.21	1.45	1.52
1	B	495	LEU	N-CA	5.20	1.52	1.45
1	A	154	GLN	C-O	-5.19	1.17	1.23
1	B	457	GLU	N-CA	5.17	1.52	1.46
1	B	375	PHE	N-CA	5.16	1.52	1.45
1	B	451	ASN	CA-C	-5.12	1.46	1.52
1	A	394	VAL	C-O	5.06	1.29	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	LEU	O-C-N	8.86	126.59	121.27
1	B	131	VAL	CB-CA-C	8.63	123.16	110.98
1	A	139	GLU	CA-C-N	-7.27	113.19	120.31
1	A	139	GLU	C-N-CA	-7.27	113.19	120.31
1	A	320	MET	N-CA-C	-6.52	104.25	111.36
1	A	441	LEU	N-CA-C	6.06	117.88	111.28
1	B	403	LEU	O-C-N	5.88	125.35	121.23
1	B	373	HIS	N-CA-C	5.72	117.19	111.07
1	B	410	HIS	CA-C-N	5.72	125.34	119.56
1	B	410	HIS	C-N-CA	5.72	125.34	119.56
1	B	363	THR	CA-C-N	-5.71	114.72	120.31
1	B	363	THR	C-N-CA	-5.71	114.72	120.31
1	A	301	LEU	N-CA-C	-5.67	106.40	113.55
1	B	130	GLU	N-CA-C	-5.61	101.35	109.59
1	B	311	PHE	N-CA-C	-5.57	105.29	111.36
1	A	408	MET	CB-CG-SD	-5.55	96.04	112.70
1	A	197	LEU	N-CA-C	-5.44	105.50	111.82
1	B	254	LEU	CA-CB-CG	5.35	135.03	116.30
1	B	402	THR	CA-C-N	-5.29	116.28	122.00
1	B	402	THR	C-N-CA	-5.29	116.28	122.00
1	A	442	ALA	N-CA-C	-5.17	105.72	111.36
1	A	223	VAL	CA-C-N	-5.14	114.49	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	VAL	C-N-CA	-5.14	114.49	121.27
1	B	391	ASN	CB-CA-C	-5.07	101.63	110.09
1	A	376	TYR	CA-C-N	-5.06	114.70	119.76
1	A	376	TYR	C-N-CA	-5.06	114.70	119.76
1	A	229	ILE	N-CA-C	-5.05	105.05	109.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	315	SER	Peptide

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	3286	0	3359	48	2
1	B	3285	0	3324	59	0
2	A	63	0	58	0	0
2	B	63	0	58	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	5	0	0
4	B	13	0	5	2	0
5	A	18	0	24	0	0
5	B	24	0	32	22	0
6	A	389	0	0	8	2
6	B	413	0	0	10	0
All	All	7569	0	6865	104	2

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 (104) 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:355[B]:ARG:HH11	1:B:355[B]:ARG:CG	1.48	1.25
1:B:291[A]:VAL:CG1	5:B:1500:GOL:H2	1.73	1.16
1:B:355[B]:ARG:NH1	1:B:355[B]:ARG:HG2	1.37	1.15
1:B:274:GLU:OE1	5:B:1503:GOL:H31	1.51	1.11
1:A:295[B]:ARG:NH1	1:A:470:GLY:O	1.87	1.08
1:B:291[B]:VAL:HG22	5:B:1500:GOL:C2	1.85	1.07
1:B:291[B]:VAL:HG22	5:B:1500:GOL:H2	1.31	1.06
1:B:173[B]:TYR:CD2	1:B:194:PRO:HG3	1.90	1.05
1:A:240[B]:LYS:HE3	1:A:240[B]:LYS:CA	1.88	1.03
1:B:291[A]:VAL:HG12	5:B:1500:GOL:H2	1.39	1.03
1:A:240[B]:LYS:HE3	1:A:240[B]:LYS:HA	1.04	1.02
1:B:316:ARG:H	1:B:316:ARG:HD2	1.18	1.02
1:A:240[B]:LYS:HA	1:A:240[B]:LYS:CE	1.90	1.02
1:A:145[A]:ILE:HG21	1:A:273:LEU:HD23	1.54	0.90
1:B:291[B]:VAL:CG2	5:B:1500:GOL:H2	2.02	0.89
1:B:149:PRO:HG2	5:B:1501:GOL:H2	1.57	0.86
1:B:232[B]:ASN:ND2	1:B:239[B]:GLU:OE2	2.09	0.85
1:A:240[B]:LYS:CA	1:A:240[B]:LYS:CE	2.53	0.79
1:B:173[B]:TYR:CE2	1:B:194:PRO:HG3	2.17	0.79
1:B:291[B]:VAL:HG22	5:B:1500:GOL:C3	2.15	0.77
1:A:204:PRO:HB3	5:B:1503:GOL:H2	1.66	0.77
1:B:291[A]:VAL:CG1	5:B:1500:GOL:C2	2.61	0.74
1:B:355[B]:ARG:HH11	1:B:355[B]:ARG:HG2	0.63	0.74
1:A:145[A]:ILE:CG2	1:A:273:LEU:HD23	2.19	0.73
1:B:316:ARG:H	1:B:316:ARG:CD	1.98	0.73
1:B:274:GLU:OE1	5:B:1503:GOL:C3	2.35	0.71
1:A:295[B]:ARG:HD3	1:A:472:GLY:O	1.92	0.70
1:A:320:MET:HG3	1:A:324[A]:MET:HE2	1.74	0.69
1:B:291[A]:VAL:HG12	5:B:1500:GOL:C2	2.19	0.68
1:A:145[A]:ILE:HD13	1:A:273:LEU:HG	1.75	0.68
5:B:1501:GOL:C3	6:B:2066:HOH:O	2.44	0.66
1:A:234[B]:HIS:CE1	1:A:236:TYR:O	2.48	0.66
1:B:320:MET:HG3	1:B:324:MET:HE2	1.77	0.65
1:B:291[B]:VAL:CG2	5:B:1500:GOL:O1	2.45	0.65
1:B:170:LYS:HA	1:B:173[B]:TYR:CE2	2.30	0.65
5:B:1501:GOL:H32	6:B:2066:HOH:O	1.97	0.64
1:B:173[B]:TYR:CE2	1:B:194:PRO:CG	2.81	0.63
1:A:289[B]:LYS:HE3	6:A:2243:HOH:O	1.97	0.63
1:A:334[A]:LYS:HD2	6:A:2269:HOH:O	1.98	0.62
1:B:291[A]:VAL:HG13	5:B:1500:GOL:C2	2.30	0.61
1:B:289:LYS:NZ	6:B:2254:HOH:O	2.34	0.60
1:A:355:ARG:NH2	1:B:143[B]:ASP:OD2	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LYS:HG3	6:B:2208:HOH:O	2.02	0.59
1:B:291[B]:VAL:CG2	5:B:1500:GOL:C2	2.69	0.59
1:A:240[B]:LYS:HE2	1:A:241:LYS:N	2.18	0.59
1:A:417:LYS:HG2	1:A:447:PHE:CD1	2.39	0.58
1:A:240[A]:LYS:NZ	6:A:2199:HOH:O	2.33	0.58
1:A:351:GLN:NE2	1:B:144[A]:ASN:OD1	2.37	0.58
1:A:195[B]:GLU:H	1:A:195[B]:GLU:CD	2.13	0.57
1:B:291[B]:VAL:HG23	5:B:1500:GOL:O1	2.04	0.56
1:A:144[B]:ASN:HD21	1:B:351:GLN:NE2	2.03	0.56
1:B:240:LYS:CG	6:B:2208:HOH:O	2.53	0.56
1:A:145[A]:ILE:HG12	1:A:146:ARG:N	2.19	0.55
1:A:145[A]:ILE:HG22	1:B:368:GLN:CD	2.32	0.55
1:A:458:ASN:HA	1:A:461:PHE:CE2	2.42	0.55
1:A:195[A]:GLU:HG3	1:A:381:ILE:HD11	1.88	0.55
1:B:316:ARG:HD2	1:B:316:ARG:N	2.03	0.54
1:B:187[A]:MET:HE1	1:B:310:LYS:HB2	1.88	0.54
1:A:145[A]:ILE:HG21	1:A:273:LEU:CD2	2.34	0.54
1:A:187:MET:HE1	1:A:310:LYS:HB2	1.90	0.54
1:B:230:PRO:HB2	1:B:241[A]:LYS:HE3	1.90	0.53
1:A:170[A]:LYS:HD3	6:A:2076:HOH:O	2.08	0.53
1:A:145[A]:ILE:HG22	1:B:368:GLN:OE1	2.10	0.52
1:A:127[B]:LYS:CD	1:A:130:GLU:OE1	2.59	0.51
1:A:145[A]:ILE:CG2	1:A:273:LEU:CD2	2.87	0.51
1:B:170:LYS:HA	1:B:173[B]:TYR:CD2	2.46	0.51
1:B:291[A]:VAL:HG12	5:B:1500:GOL:O3	2.10	0.50
1:A:240[B]:LYS:CA	1:A:240[B]:LYS:HE2	2.39	0.50
1:B:139:GLU:OE1	4:B:1499:CIT:O3	2.29	0.50
1:A:410:HIS:HD2	1:A:413:HIS:H	1.59	0.49
1:B:458:ASN:HA	1:B:461:PHE:CE2	2.48	0.49
1:A:135:HIS:HA	1:A:482:LYS:O	2.13	0.49
1:A:240[B]:LYS:CE	1:A:241:LYS:H	2.26	0.48
1:B:127[A]:LYS:HG2	1:B:130:GLU:HB2	1.94	0.48
1:B:209[A]:GLN:HG3	6:B:2166:HOH:O	2.14	0.48
4:B:1499:CIT:O4	4:B:1499:CIT:H22	2.14	0.47
1:A:144[B]:ASN:HD21	1:B:351:GLN:CD	2.23	0.47
1:B:274:GLU:CD	5:B:1503:GOL:H31	2.34	0.46
1:B:185:ASP:HB3	1:B:187[A]:MET:HG3	1.98	0.46
1:A:417:LYS:HG3	6:A:2334:HOH:O	2.16	0.46
1:B:192:TYR:HD1	1:B:196:PHE:CD1	2.34	0.46
1:B:127[B]:LYS:HD3	6:B:2010:HOH:O	2.16	0.45
1:B:355[B]:ARG:CG	1:B:355[B]:ARG:NH1	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:C	1:A:310:LYS:HG2	2.41	0.44
1:A:240[B]:LYS:CE	1:A:241:LYS:N	2.79	0.44
1:B:170:LYS:HG2	6:B:2107:HOH:O	2.17	0.44
1:B:291[A]:VAL:HG12	5:B:1500:GOL:C3	2.47	0.44
1:B:144[B]:ASN:O	1:B:144[B]:ASN:CG	2.60	0.44
1:A:127[B]:LYS:HD3	1:A:130:GLU:OE1	2.17	0.44
1:A:177:ASN:O	1:A:189[A]:ARG:HD2	2.17	0.44
1:B:355[B]:ARG:NH1	6:B:2307:HOH:O	2.49	0.44
1:A:204:PRO:CB	5:B:1503:GOL:H2	2.43	0.44
1:B:232[B]:ASN:CG	1:B:239[B]:GLU:OE2	2.60	0.43
1:B:414:LYS:HE3	1:B:414:LYS:HB2	1.57	0.43
1:B:241[B]:LYS:HB2	1:B:241[B]:LYS:HE3	1.85	0.42
1:A:332[B]:THR:HG22	6:A:2267:HOH:O	2.18	0.42
1:A:322:ARG:NH1	1:A:325:LYS:HE3	2.34	0.42
1:B:314:LEU:HD23	1:B:314:LEU:HA	1.86	0.42
1:B:195:GLU:HB3	1:B:381:ILE:HD11	2.01	0.42
1:A:295[A]:ARG:NH1	6:A:2248:HOH:O	2.41	0.41
1:A:324[B]:MET:CE	6:A:2257:HOH:O	2.68	0.41
1:A:240[B]:LYS:HE2	1:A:241:LYS:H	1.85	0.41
1:B:240:LYS:HG2	6:B:2208:HOH:O	2.19	0.40
1:A:170[B]:LYS:HA	1:A:170[B]:LYS:HD3	1.84	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393[B]:GLU:OE2	6:A:2022:HOH:O[1_554]	1.92	0.28
1:A:393[B]:GLU:CD	6:A:2022:HOH:O[1_554]	2.17	0.03

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	407/410 (99%)	395 (97%)	12 (3%)	0	100	100
1	B	405/410 (99%)	392 (97%)	11 (3%)	2 (0%)	24	9
All	All	812/820 (99%)	787 (97%)	23 (3%)	2 (0%)	48	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183[A]	ASP
1	B	183[B]	ASP

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	375/372 (101%)	359 (96%)	16 (4%)	26	4
1	B	373/372 (100%)	362 (97%)	11 (3%)	37	11
All	All	748/744 (100%)	721 (96%)	27 (4%)	33	6

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	131	VAL
1	A	145[A]	ILE
1	A	145[B]	ILE
1	A	198	LEU
1	A	240[A]	LYS
1	A	240[B]	LYS
1	A	310	LYS
1	A	315	SER
1	A	316	ARG
1	A	325	LYS
1	A	334[A]	LYS
1	A	334[B]	LYS
1	A	408	MET

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Mol	Chain	Res	Type
1	A	455	LEU
1	A	482	LYS
1	B	115	ARG
1	B	127[A]	LYS
1	B	127[B]	LYS
1	B	133	ASN
1	B	166	ARG
1	B	185	ASP
1	B	316	ARG
1	B	325	LYS
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
1	A	351	GLN
1	A	410	HIS
1	A	413	HIS
1	B	133	ASN
1	B	147	GLN
1	B	458	ASN

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 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	3	63,65,65	1.18	7 (11%)	85,91,91	1.71	16 (18%)
5	GOL	A	1501	-	5,5,5	0.52	0	5,5,5	1.09	0
4	CIT	A	1499	-	12,12,12	1.86	2 (16%)	17,17,17	4.80	8 (47%)
5	GOL	A	1502	-	5,5,5	0.56	0	5,5,5	0.81	0
5	GOL	B	1503	-	5,5,5	0.71	0	5,5,5	1.39	1 (20%)
2	MYA	A	1497	3	63,65,65	1.30	6 (9%)	85,91,91	1.67	19 (22%)
5	GOL	B	1500	-	5,5,5	0.74	0	5,5,5	0.87	0
5	GOL	B	1501	-	5,5,5	0.94	0	5,5,5	0.70	0
5	GOL	A	1500	-	5,5,5	0.80	0	5,5,5	0.39	0
4	CIT	B	1499	-	12,12,12	1.49	2 (16%)	17,17,17	1.71	6 (35%)
5	GOL	B	1502	-	5,5,5	0.37	0	5,5,5	0.77	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	3	-	0/64/80/80	0/3/3/3
5	GOL	A	1501	-	-	2/4/4/4	-
4	CIT	A	1499	-	-	6/16/16/16	-
5	GOL	A	1502	-	-	2/4/4/4	-
5	GOL	B	1503	-	-	2/4/4/4	-
2	MYA	A	1497	3	-	1/64/80/80	0/3/3/3
5	GOL	B	1500	-	-	0/4/4/4	-
5	GOL	B	1501	-	-	4/4/4/4	-
5	GOL	A	1500	-	-	0/4/4/4	-
4	CIT	B	1499	-	-	2/16/16/16	-
5	GOL	B	1502	-	-	2/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1499	CIT	C3-C6	4.93	1.58	1.53
2	A	1497	MYA	P1A-O3A	4.46	1.64	1.59
2	A	1497	MYA	O10-C10	3.37	1.48	1.42
2	B	1497	MYA	P1A-O3A	3.22	1.63	1.59
2	A	1497	MYA	C4A-N9A	-3.19	1.31	1.37
2	B	1497	MYA	C8A-N7A	2.72	1.36	1.31
2	A	1497	MYA	C8A-N7A	2.58	1.36	1.31
2	A	1497	MYA	P3X-O7A	-2.41	1.45	1.54
4	B	1499	CIT	C2-C3	-2.40	1.51	1.54
2	B	1497	MYA	C2A-N3A	2.38	1.38	1.33
2	B	1497	MYA	O10-C10	2.19	1.46	1.42
4	A	1499	CIT	O5-C6	2.17	1.28	1.22
2	A	1497	MYA	C2A-N1A	2.14	1.37	1.33
2	B	1497	MYA	O5-C5	2.09	1.27	1.23
4	B	1499	CIT	O5-C6	2.06	1.28	1.22
2	B	1497	MYA	O2M-C2M	2.04	1.24	1.21
2	B	1497	MYA	C1X-N9A	2.01	1.51	1.46

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1499	CIT	O7-C3-C6	-11.23	93.03	108.96
4	A	1499	CIT	C4-C3-C6	-10.53	86.73	110.03
2	B	1497	MYA	C3M-C2M-S1	6.79	121.49	113.40
4	A	1499	CIT	C2-C3-C6	-6.23	96.26	110.03
2	B	1497	MYA	N3A-C2A-N1A	-5.89	119.66	128.58
4	A	1499	CIT	O7-C3-C4	5.67	122.31	109.38
4	A	1499	CIT	O6-C6-C3	5.61	123.89	113.14
2	A	1497	MYA	C4A-C5A-N7A	-4.88	105.00	110.58
4	A	1499	CIT	C4-C3-C2	4.81	121.66	109.31
2	A	1497	MYA	C3M-C2M-S1	4.66	118.96	113.40
2	A	1497	MYA	O2M-C2M-S1	-4.51	116.94	122.68
2	B	1497	MYA	O2M-C2M-C3M	-4.38	118.92	123.98
2	A	1497	MYA	N9A-C8A-N7A	-3.85	108.48	113.94
2	B	1497	MYA	C5A-C4A-N3A	-3.70	121.63	126.72
2	A	1497	MYA	N3A-C2A-N1A	-3.58	123.16	128.58
2	A	1497	MYA	O6A-C12-C11	-3.50	104.92	110.55
2	A	1497	MYA	C5A-C4A-N9A	3.46	109.58	105.81
2	A	1497	MYA	C5A-C4A-N3A	-3.28	122.20	126.72
4	B	1499	CIT	O7-C3-C6	3.26	113.58	108.96
2	B	1497	MYA	C2A-N3A-C4A	3.23	119.72	111.83
4	B	1499	CIT	C2-C3-C6	-3.01	103.37	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1497	MYA	C5A-N7A-C8A	2.86	107.95	103.45
2	A	1497	MYA	C4A-N9A-C8A	2.84	108.72	105.74
4	A	1499	CIT	O7-C3-C2	2.77	115.70	109.38
4	A	1499	CIT	O6-C6-O5	-2.71	115.19	123.86
4	B	1499	CIT	O1-C1-C2	-2.64	115.47	122.95
2	B	1497	MYA	C4M-C3M-C2M	-2.59	106.55	112.27
2	A	1497	MYA	O5A-P2A-O3A	-2.56	100.37	107.27
4	B	1499	CIT	O2-C1-O1	2.55	129.89	123.33
2	B	1497	MYA	C4A-C5A-N7A	-2.54	107.67	110.58
2	B	1497	MYA	O2M-C2M-S1	-2.47	119.54	122.68
2	A	1497	MYA	C6A-C5A-C4A	2.47	120.55	117.18
2	B	1497	MYA	O8A-P3X-O7A	2.43	116.91	107.80
2	B	1497	MYA	P3X-O3X-C3X	-2.43	116.94	123.43
2	B	1497	MYA	C2A-N1A-C6A	2.42	122.71	118.73
2	B	1497	MYA	C13-C11-C10	2.42	112.89	108.77
2	B	1497	MYA	C5A-C4A-N9A	2.41	108.44	105.81
4	B	1499	CIT	O4-C5-C4	2.38	121.90	114.35
4	B	1499	CIT	O3-C5-C4	-2.30	116.42	122.95
2	A	1497	MYA	C4M-C3M-C2M	-2.28	107.23	112.27
2	A	1497	MYA	C2A-N1A-C6A	2.26	122.44	118.73
2	B	1497	MYA	N9A-C8A-N7A	-2.24	110.76	113.94
2	A	1497	MYA	O5A-P2A-O4A	2.17	122.53	112.44
2	A	1497	MYA	C10-C9-N8	2.11	120.50	116.48
2	A	1497	MYA	O1A-P1A-O2A	2.07	122.09	112.44
2	A	1497	MYA	C7-C6-C5	2.04	115.80	112.39
5	B	1503	GOL	O3-C3-C2	2.04	119.57	110.38
2	B	1497	MYA	C6-C7-N8	-2.01	107.71	112.00
2	A	1497	MYA	CAM-C9M-C8M	-2.01	104.20	114.37
2	B	1497	MYA	C6-C5-N4	-2.01	112.68	116.34

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1499	CIT	O7-C3-C4-C5
5	A	1502	GOL	O1-C1-C2-C3
5	B	1501	GOL	O1-C1-C2-C3
5	B	1502	GOL	C1-C2-C3-O3
5	B	1501	GOL	O1-C1-C2-O2
5	B	1502	GOL	O2-C2-C3-O3
4	A	1499	CIT	C1-C2-C3-O7
5	B	1501	GOL	C1-C2-C3-O3

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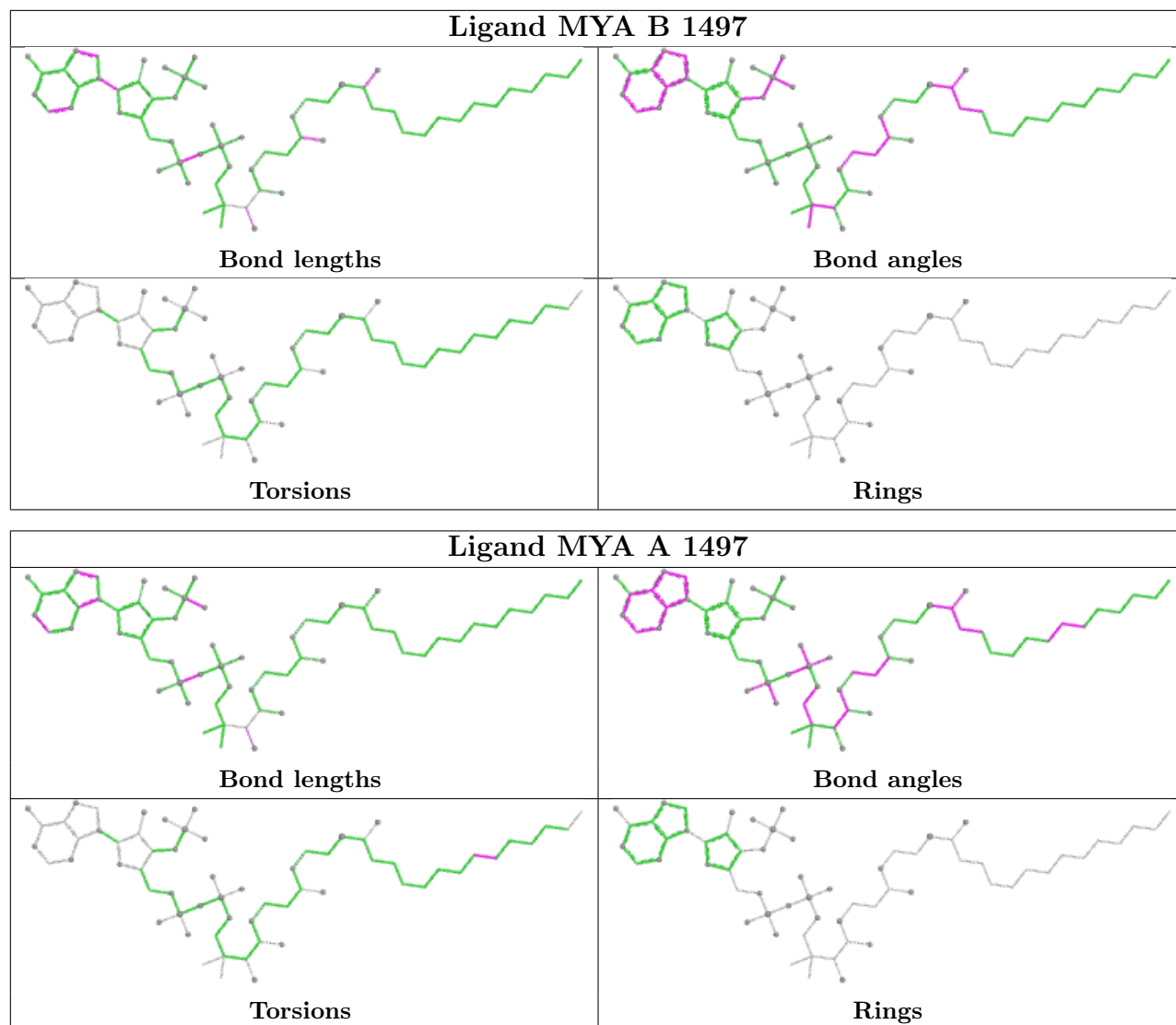
Mol	Chain	Res	Type	Atoms
5	B	1503	GOL	O1-C1-C2-C3
5	B	1501	GOL	O2-C2-C3-O3
5	B	1503	GOL	O1-C1-C2-O2
4	A	1499	CIT	C6-C3-C4-C5
5	A	1502	GOL	O1-C1-C2-O2
5	A	1501	GOL	O1-C1-C2-O2
5	A	1501	GOL	O1-C1-C2-C3
4	A	1499	CIT	O2-C1-C2-C3
4	A	1499	CIT	C1-C2-C3-C4
2	A	1497	MYA	C8M-C9M-CAM-CBM
4	A	1499	CIT	O1-C1-C2-C3
4	B	1499	CIT	C3-C4-C5-O3
4	B	1499	CIT	C3-C4-C5-O4

There are no ring outliers.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1503	GOL	5	0
5	B	1500	GOL	14	0
5	B	1501	GOL	3	0
4	B	1499	CIT	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 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 [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, 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	382/410 (93%)	-0.15	12 (3%)	51	56	8, 18, 41, 84	27 (7%)
1	B	382/410 (93%)	-0.21	12 (3%)	51	56	7, 16, 42, 70	25 (6%)
All	All	764/820 (93%)	-0.18	24 (3%)	51	56	7, 17, 42, 84	52 (6%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	VAL	3.6
1	A	316	ARG	3.4
1	B	317	ASN	3.3
1	A	314	LEU	3.1
1	B	411	PRO	3.1
1	A	317	ASN	3.1
1	A	315	SER	2.7
1	A	409	ASN	2.7
1	B	412	THR	2.6
1	B	416	LEU	2.6
1	A	319	THR	2.5
1	B	188	PHE	2.5
1	A	115	ARG	2.5
1	A	313	HIS	2.4
1	B	185	ASP	2.4
1	A	307	ILE	2.3
1	B	133	ASN	2.2
1	B	414	LYS	2.2
1	A	410	HIS	2.2
1	B	184	ASP	2.1
1	B	128	LEU	2.1
1	A	412	THR	2.1
1	A	408	MET	2.0
1	B	192	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

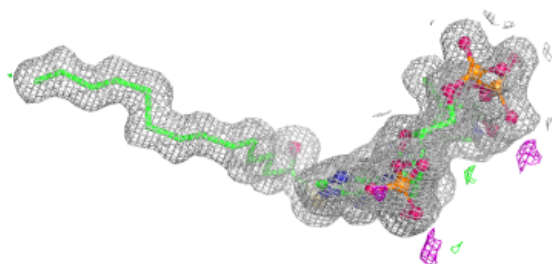
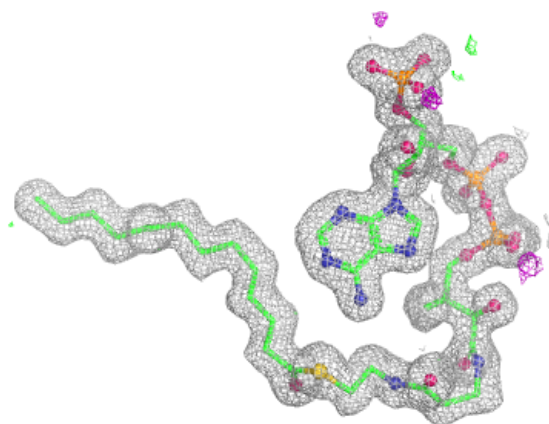
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	GOL	B	1501	6/6	0.73	0.14	29,33,38,38	0
5	GOL	A	1502	6/6	0.77	0.15	42,47,48,49	0
5	GOL	B	1503	6/6	0.78	0.14	31,33,34,40	0
4	CIT	A	1499	13/13	0.81	0.13	35,43,45,45	0
5	GOL	B	1502	6/6	0.82	0.15	32,41,43,45	0
4	CIT	B	1499	13/13	0.85	0.11	27,33,40,41	0
5	GOL	A	1501	6/6	0.88	0.15	27,36,41,55	0
5	GOL	B	1500	6/6	0.92	0.09	19,23,26,32	0
5	GOL	A	1500	6/6	0.96	0.07	21,23,26,30	0
2	MYA	B	1497	63/63	0.98	0.04	9,14,18,20	0
3	MG	A	1498	1/1	0.98	0.10	28,28,28,28	0
3	MG	B	1498	1/1	0.98	0.05	25,25,25,25	0
2	MYA	A	1497	63/63	0.98	0.05	9,16,21,23	0

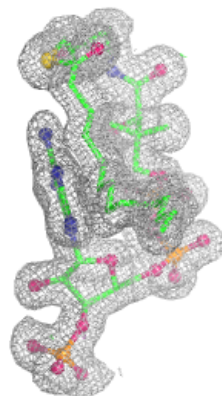
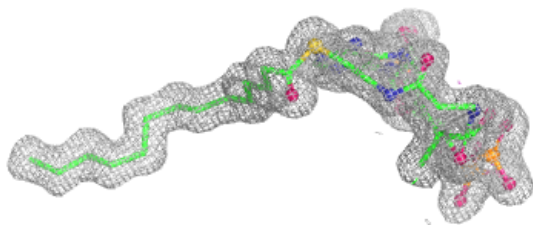
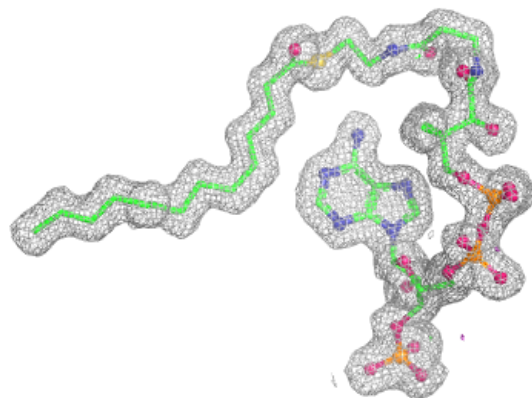
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MYA 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 [i](#)

There are no such residues in this entry.