



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:40 PM UTC

PDB ID : 4C7H / pdb_00004c7h
Title : Leishmania major N-myristoyltransferase in complex with a peptidomimetic (-NH₂) molecule
Authors : Olaleye, T.O.; Brannigan, J.A.; Goncalves, V.; Roberts, S.M.; Leatherbarrow, R.J.; Wilkinson, A.J.; Tate, E.W.
Deposited on : 2013-09-20
Resolution : 1.40 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

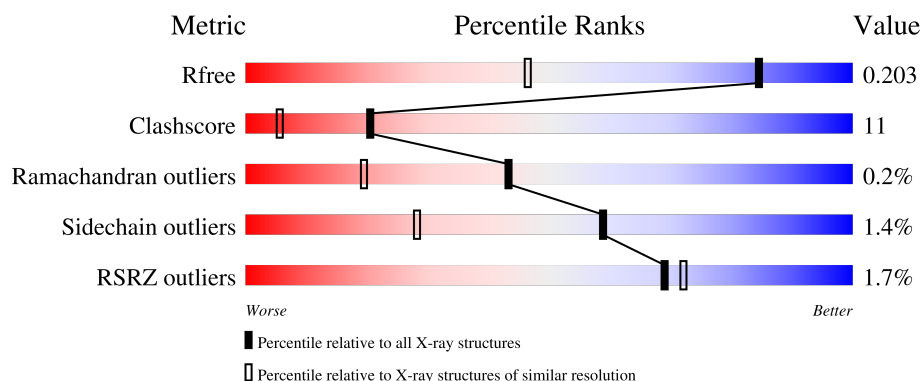
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	411	2% 73% 23% .

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
7	DMS	A	1428	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4223 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.

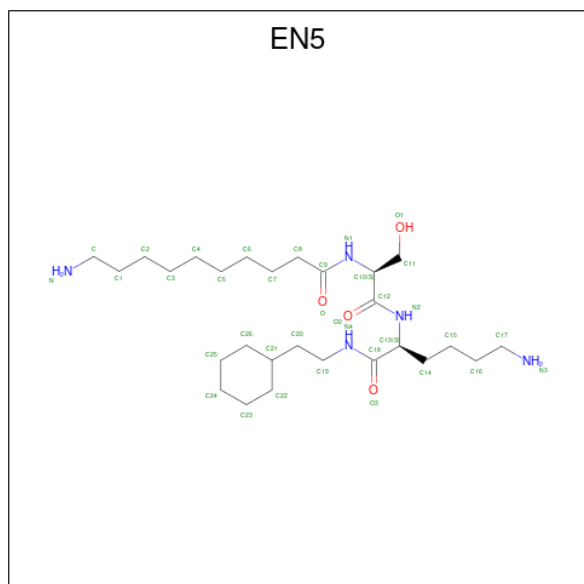
- Molecule 1 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	23	0
			3476	2253	582	623	18			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

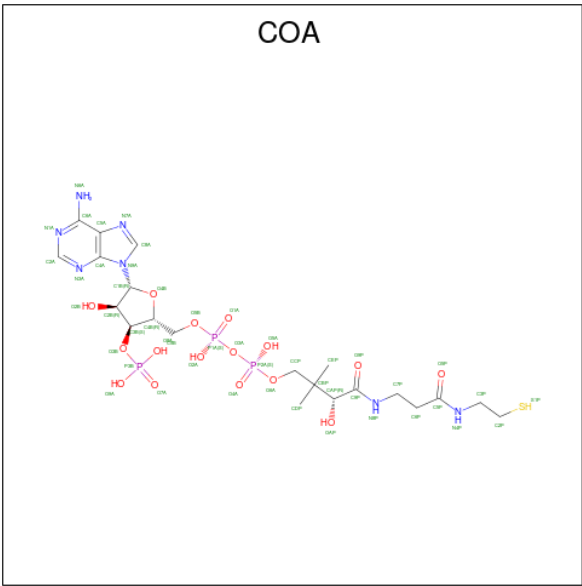
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is N-(10-aminodecanoyl)-L-seryl-N-(2-cyclohexylethyl)-L-lysineamide (CCD ID: EN5) (formula: C₂₇H₅₃N₅O₄).



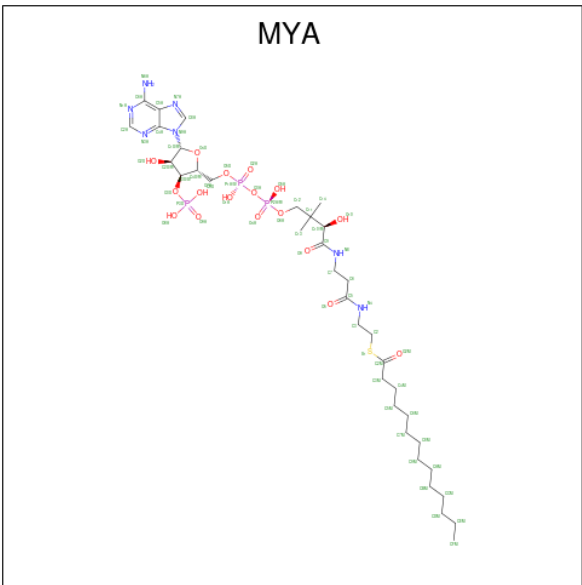
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			36	27	5	4		

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



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

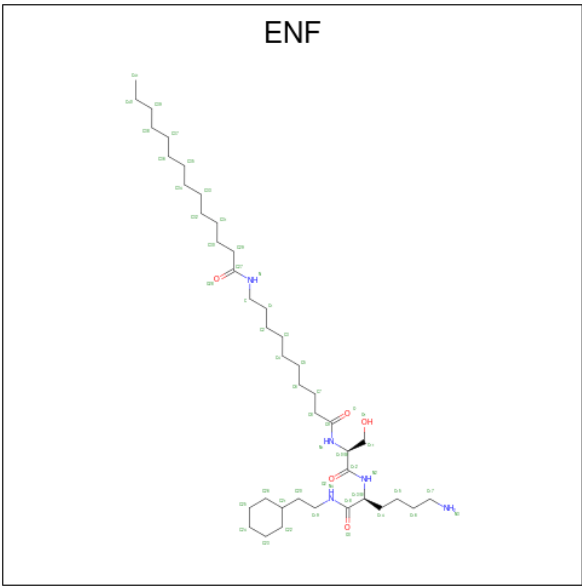
- Molecule 5 is TETRADECANOYL-COA (CCD ID: MYA) (formula: C₃₅H₆₂N₇O₁₇P₃S).



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

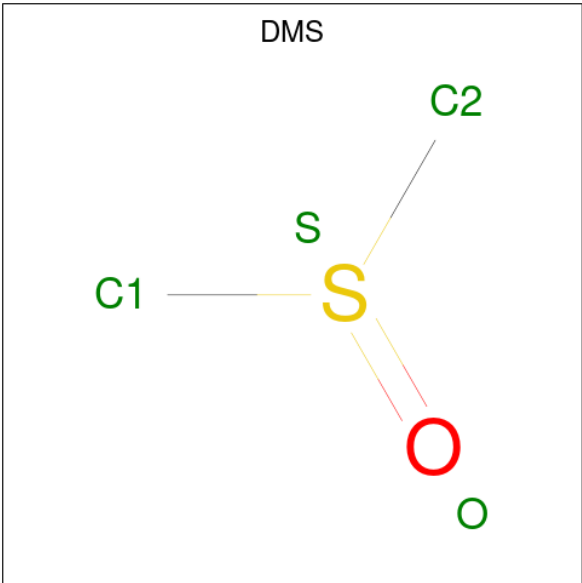
- Molecule 6 is N-{(5E)-10-[(9E)-tetradec-9-enoylamino]dec-5-enoyl}-L-seryl-N-(2-cyclohexyle

thyl)-L-lysynamide (CCD ID: ENF) (formula: C₄₁H₇₉N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	1
			51	41	5	5		

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		

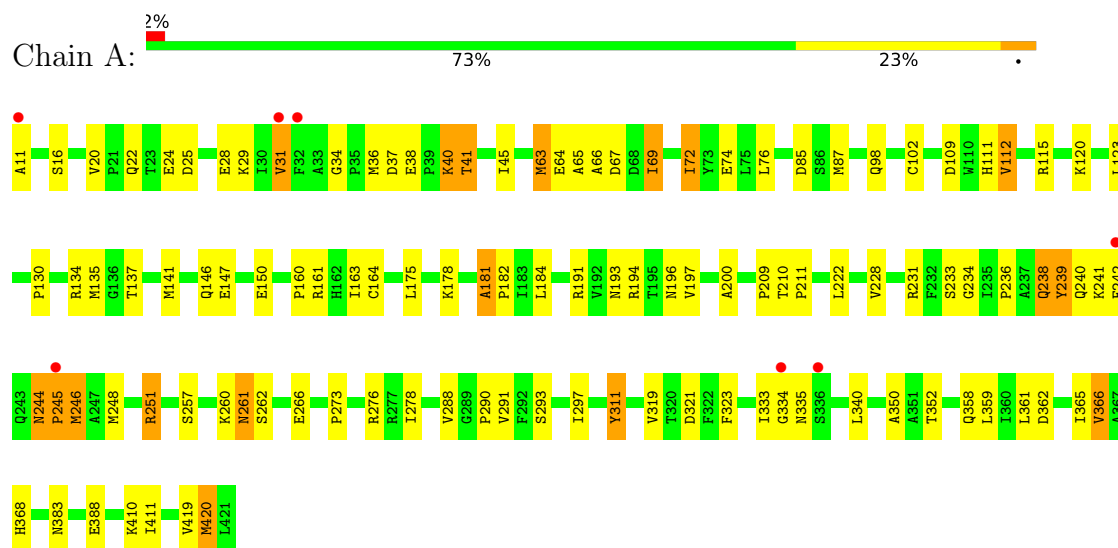
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	540	Total	O	0	0
			540	540		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.66Å 91.13Å 53.78Å 90.00° 113.85° 90.00°	Depositor
Resolution (Å)	22.26 – 1.40 22.26 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (22.26-1.40) 98.7 (22.26-1.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.173 , 0.205 0.171 , 0.203	Depositor DCC
R_{free} test set	4168 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4223	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EN5, MG, MYA, COA, ENF, DMS

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	1.84	55/3641 (1.5%)	1.59	37/4945 (0.7%)

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	ALA	CA-C	9.00	1.63	1.52
1	A	160	PRO	N-CA	8.10	1.56	1.47
1	A	359	LEU	N-CA	8.06	1.55	1.46
1	A	197	VAL	C-O	7.76	1.31	1.24
1	A	40	LYS	CA-C	-6.97	1.44	1.52
1	A	209	PRO	CA-C	6.92	1.59	1.52
1	A	350	ALA	N-CA	6.88	1.54	1.46
1	A	319	VAL	N-CA	6.54	1.53	1.46
1	A	362	ASP	C-O	-6.48	1.16	1.24
1	A	184	LEU	C-O	6.46	1.31	1.24
1	A	361	LEU	C-O	-6.44	1.16	1.24
1	A	20	VAL	C-O	6.37	1.28	1.24
1	A	45	ILE	CA-C	-6.36	1.46	1.52
1	A	38	GLU	C-N	6.33	1.41	1.33
1	A	112	VAL	N-CA	6.18	1.53	1.46
1	A	181	ALA	N-CA	6.17	1.52	1.46
1	A	321	ASP	N-CA	6.09	1.53	1.46
1	A	234	GLY	CA-C	-6.07	1.46	1.52
1	A	333	ILE	N-CA	5.97	1.53	1.46
1	A	366	VAL	N-CA	5.92	1.53	1.46
1	A	161	ARG	C-O	5.89	1.31	1.24
1	A	288	VAL	CA-C	5.88	1.60	1.52
1	A	257	SER	CA-CB	5.85	1.63	1.53
1	A	290	PRO	CA-CB	5.84	1.60	1.53
1	A	130	PRO	C-O	5.66	1.30	1.23
1	A	196	ASN	N-CA	-5.65	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	VAL	N-CA	5.62	1.53	1.46
1	A	411	ILE	C-O	5.59	1.30	1.23
1	A	236	PRO	C-O	5.58	1.29	1.23
1	A	134	ARG	CZ-NH2	-5.57	1.26	1.33
1	A	63[A]	MET	C-O	-5.57	1.15	1.24
1	A	63[B]	MET	C-O	-5.57	1.15	1.24
1	A	200	ALA	N-CA	5.54	1.53	1.45
1	A	323	PHE	N-CA	5.53	1.53	1.45
1	A	311	TYR	CA-C	-5.47	1.45	1.52
1	A	163	ILE	N-CA	5.46	1.53	1.46
1	A	150	GLU	N-CA	5.45	1.52	1.46
1	A	164	CYS	N-CA	5.44	1.52	1.46
1	A	266	GLU	CA-C	-5.42	1.45	1.52
1	A	257	SER	C-O	5.36	1.31	1.24
1	A	37	ASP	N-CA	5.34	1.52	1.45
1	A	273	PRO	CA-CB	5.31	1.61	1.53
1	A	365	ILE	N-CA	5.31	1.52	1.46
1	A	66	ALA	CA-C	-5.29	1.45	1.52
1	A	67	ASP	CA-C	-5.25	1.46	1.52
1	A	261	ASN	CG-OD1	5.25	1.33	1.23
1	A	228	VAL	C-O	5.23	1.30	1.24
1	A	352	THR	N-CA	5.21	1.53	1.46
1	A	350	ALA	CA-C	-5.18	1.46	1.52
1	A	211	PRO	N-CA	5.17	1.53	1.47
1	A	34	GLY	N-CA	-5.13	1.37	1.44
1	A	293	SER	N-CA	5.12	1.52	1.45
1	A	193	ASN	CG-OD1	5.12	1.33	1.23
1	A	335	ASN	CA-C	5.12	1.58	1.52
1	A	87	MET	N-CA	-5.01	1.39	1.45

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	GLY	N-CA-C	11.73	140.98	113.18
1	A	41	THR	N-CA-CB	7.65	123.59	111.20
1	A	233	SER	CA-C-N	-7.63	115.38	122.17
1	A	233	SER	C-N-CA	-7.63	115.38	122.17
1	A	388	GLU	CA-C-O	-7.38	112.60	120.42
1	A	365	ILE	O-C-N	6.96	128.73	121.91
1	A	38	GLU	CA-C-N	-6.84	112.61	119.93
1	A	38	GLU	C-N-CA	-6.84	112.61	119.93
1	A	246	MET	N-CA-C	6.35	118.28	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	THR	CB-CA-C	-6.33	97.38	109.66
1	A	244	ASN	CA-C-N	-6.12	112.26	119.05
1	A	244	ASN	C-N-CA	-6.12	112.26	119.05
1	A	419	VAL	CA-C-N	-6.07	114.13	122.93
1	A	419	VAL	C-N-CA	-6.07	114.13	122.93
1	A	137	THR	O-C-N	6.03	126.33	121.38
1	A	76	LEU	CA-C-O	-6.01	114.05	120.42
1	A	278	ILE	N-CA-CB	5.93	119.47	110.58
1	A	228	VAL	O-C-N	5.89	127.90	121.83
1	A	245	PRO	N-CA-C	5.78	121.57	113.53
1	A	333	ILE	CB-CA-C	5.75	120.71	111.29
1	A	239	TYR	N-CA-C	-5.65	106.43	113.15
1	A	383	ASN	N-CA-C	5.62	118.17	111.71
1	A	31	VAL	N-CA-C	-5.51	108.13	113.53
1	A	368	HIS	O-C-N	5.38	127.82	122.12
1	A	74	GLU	CB-CG-CD	-5.29	103.60	112.60
1	A	193	ASN	CB-CG-ND2	5.26	124.29	116.40
1	A	72	ILE	N-CA-C	-5.25	105.42	110.72
1	A	222	LEU	N-CA-C	-5.19	107.01	113.55
1	A	85	ASP	CA-C-O	5.15	125.59	119.56
1	A	210	THR	CA-C-N	-5.11	114.69	119.85
1	A	210	THR	C-N-CA	-5.11	114.69	119.85
1	A	420	MET	CA-C-O	5.11	126.13	120.71
1	A	45	ILE	O-C-N	-5.07	115.32	121.10
1	A	135	MET	CA-C-N	-5.04	114.46	121.67
1	A	135	MET	C-N-CA	-5.04	114.46	121.67
1	A	69[A]	ILE	O-C-N	-5.02	117.00	121.87
1	A	69[B]	ILE	O-C-N	-5.02	117.00	121.87

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	3476	0	3477	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	36	0	53	4	0
4	A	48	0	32	11	0
5	A	63	0	58	0	0
6	A	51	0	79	11	0
7	A	8	0	12	5	0
8	A	540	0	0	15	0
All	All	4223	0	3711	83	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 11.

All (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63[B]:MET:HE1	1:A:72:ILE:CD1	1.36	1.54
1:A:63[B]:MET:CE	1:A:72:ILE:HD12	1.58	1.31
1:A:63[B]:MET:CE	1:A:72:ILE:CD1	2.11	1.28
4:A:1424[A]:COA:S1P	6:A:1426[A]:ENF:H	1.73	1.26
4:A:1424[A]:COA:S1P	6:A:1426[A]:ENF:C27	2.30	1.19
4:A:1424[A]:COA:S1P	6:A:1426[A]:ENF:C	2.29	1.19
1:A:194[B]:ARG:HH11	1:A:194[B]:ARG:CG	1.57	1.14
1:A:63[B]:MET:HG3	1:A:69[B]:ILE:HD11	1.33	1.11
1:A:231[B]:ARG:NH1	8:A:2361:HOH:O	1.83	1.11
1:A:63[B]:MET:HE1	1:A:72:ILE:HD11	1.27	1.08
1:A:63[B]:MET:HE1	1:A:72:ILE:HD12	1.15	1.07
1:A:194[B]:ARG:HG3	1:A:194[B]:ARG:NH1	1.62	1.07
4:A:1424[A]:COA:S1P	6:A:1426[A]:ENF:N	2.32	1.01
1:A:231[B]:ARG:CZ	8:A:2361:HOH:O	2.08	1.00
1:A:194[B]:ARG:HH11	1:A:194[B]:ARG:HG3	0.78	0.93
4:A:1424[A]:COA:HS1	6:A:1426[A]:ENF:H	1.46	0.79
1:A:231[B]:ARG:NH2	8:A:2361:HOH:O	2.15	0.78
1:A:260:LYS:HD3	8:A:2390:HOH:O	1.85	0.76
1:A:63[B]:MET:HG3	1:A:69[B]:ILE:CD1	2.14	0.76
1:A:41:THR:HB	8:A:2078:HOH:O	1.86	0.76
1:A:11:ALA:HB3	8:A:2009:HOH:O	1.85	0.75
1:A:24[A]:GLU:OE2	1:A:28[A]:GLU:OE2	2.05	0.74
1:A:31:VAL:HA	1:A:141:MET:HE2	1.74	0.69
1:A:240:GLN:HA	1:A:240:GLN:OE1	1.95	0.67
1:A:63[B]:MET:HE2	1:A:72:ILE:CD1	2.18	0.66
1:A:147:GLU:HG3	8:A:2264:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63[B]:MET:CE	1:A:72:ILE:HD13	2.23	0.64
4:A:1424[A]:COA:C2P	6:A:1426[A]:ENF:C	2.76	0.63
1:A:63[B]:MET:HE3	1:A:69[B]:ILE:HD13	1.81	0.62
1:A:63[B]:MET:CE	1:A:69[B]:ILE:HD13	2.28	0.62
1:A:261:ASN:HD21	1:A:358:GLN:HE21	1.48	0.62
4:A:1424[A]:COA:S1P	6:A:1426[A]:ENF:C29	2.89	0.60
4:A:1424[A]:COA:C2P	6:A:1426[A]:ENF:H	2.32	0.59
1:A:261:ASN:ND2	1:A:358:GLN:HE21	1.99	0.58
1:A:16:SER:HA	1:A:22:GLN:HE22	1.69	0.58
1:A:146:GLN:HG2	8:A:2262:HOH:O	2.05	0.57
1:A:63[B]:MET:HE2	1:A:72:ILE:HD12	1.73	0.56
1:A:231[B]:ARG:NH1	8:A:2357:HOH:O	2.29	0.55
3:A:1423[B]:EN5:HN1	7:A:1428:DMS:H13	1.72	0.55
1:A:41:THR:HG22	8:A:2079:HOH:O	2.07	0.54
1:A:63[A]:MET:HB3	1:A:102:CYS:SG	2.47	0.54
1:A:194[B]:ARG:CG	1:A:194[B]:ARG:NH1	2.32	0.54
1:A:251[A]:ARG:HH11	1:A:251[A]:ARG:CG	2.21	0.53
1:A:242:PHE:CD2	1:A:248[B]:MET:HG2	2.44	0.52
4:A:1424[A]:COA:H22	6:A:1426[A]:ENF:HA	1.92	0.52
1:A:16:SER:HA	1:A:22:GLN:NE2	2.26	0.51
1:A:239:TYR:O	1:A:245:PRO:HG3	2.10	0.51
4:A:1424[A]:COA:C2P	6:A:1426[A]:ENF:HA	2.40	0.50
1:A:248[A]:MET:HA	1:A:248[A]:MET:HE2	1.95	0.49
3:A:1423[B]:EN5:HN1	7:A:1428:DMS:C1	2.27	0.48
1:A:251[A]:ARG:HH11	1:A:251[A]:ARG:HG2	1.78	0.48
1:A:63[B]:MET:HB3	1:A:102:CYS:SG	2.52	0.48
1:A:24[A]:GLU:OE2	1:A:410:LYS:HE2	2.15	0.47
3:A:1423[B]:EN5:H8A	7:A:1428:DMS:C1	2.44	0.47
1:A:109:ASP:O	1:A:191[A]:ARG:HD3	2.16	0.46
1:A:178:LYS:HE2	8:A:2305:HOH:O	2.17	0.45
1:A:238:GLN:C	1:A:240:GLN:H	2.25	0.45
1:A:420:MET:HB3	1:A:420:MET:HE2	1.56	0.45
1:A:246:MET:HB2	1:A:246:MET:HE2	1.58	0.45
7:A:1428:DMS:H11	8:A:2473:HOH:O	2.17	0.43
1:A:31:VAL:CA	1:A:141:MET:HE2	2.45	0.43
1:A:36[B]:MET:HE2	1:A:36[B]:MET:HB3	1.91	0.43
1:A:112:VAL:HG22	1:A:191[B]:ARG:HD2	2.00	0.43
1:A:248[B]:MET:HE3	1:A:251[B]:ARG:NH1	2.34	0.43
3:A:1423[B]:EN5:H8A	7:A:1428:DMS:H12	2.01	0.43
1:A:22:GLN:NE2	8:A:2013:HOH:O	2.52	0.43
1:A:25:ASP:O	1:A:29:LYS:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251[A]:ARG:NH1	8:A:2373:HOH:O	2.52	0.42
4:A:1424[A]:COA:S1P	6:A:1426[A]:ENF:H29	2.58	0.42
1:A:276[A]:ARG:HB2	1:A:297:ILE:HG13	2.01	0.42
1:A:276[A]:ARG:HH11	1:A:276[A]:ARG:HD2	1.69	0.42
1:A:123:LEU:HD22	1:A:175[A]:LEU:CD1	2.50	0.42
1:A:63[A]:MET:HE3	1:A:111:HIS:ND1	2.34	0.42
1:A:240:GLN:C	1:A:242:PHE:H	2.27	0.42
1:A:311:TYR:CE1	1:A:366:VAL:HG11	2.56	0.41
1:A:112:VAL:HG22	1:A:191[A]:ARG:HD2	2.03	0.41
1:A:181:ALA:HB3	1:A:182:PRO:HD3	2.01	0.41
1:A:115:ARG:CZ	1:A:120:LYS:HD2	2.51	0.41
1:A:63[B]:MET:HE2	1:A:72:ILE:HD13	1.95	0.41
1:A:40:LYS:HE2	8:A:2071:HOH:O	2.19	0.41
1:A:244:ASN:OD1	1:A:244:ASN:C	2.63	0.41

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	432/411 (105%)	420 (97%)	11 (2%)	1 (0%)	43 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	LYS

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	385/362 (106%)	378 (98%)	7 (2%)	51 20

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	GLU
1	A	238	GLN
1	A	251[A]	ARG
1	A	251[B]	ARG
1	A	262[A]	SER
1	A	262[B]	SER
1	A	340	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	22	GLN
1	A	146	GLN
1	A	243	GLN
1	A	252	ASN
1	A	254	GLN
1	A	261	ASN
1	A	339	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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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
7	DMS	A	1428	-	3,3,3	1.66	1 (33%)	3,3,3	1.54	1 (33%)
5	MYA	A	1425[B]	2	63,65,65	1.36	8 (12%)	85,91,91	1.60	16 (18%)
4	COA	A	1424[A]	2	47,50,50	1.67	13 (27%)	69,75,75	1.50	10 (14%)
3	EN5	A	1423[B]	-	36,36,36	0.92	2 (5%)	41,42,42	1.60	9 (21%)
7	DMS	A	1427	-	3,3,3	0.57	0	3,3,3	0.75	0
6	ENF	A	1426[A]	-	51,51,51	1.23	3 (5%)	57,58,58	1.25	4 (7%)

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	EN5	A	1423[B]	-	-	5/39/47/47	0/1/1/1
5	MYA	A	1425[B]	2	-	1/64/80/80	0/3/3/3
6	ENF	A	1426[A]	-	-	7/55/63/63	0/1/1/1
4	COA	A	1424[A]	2	-	1/48/64/64	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1426[A]	ENF	O28-C27	-5.11	1.13	1.23
6	A	1426[A]	ENF	O3-C18	-4.17	1.15	1.23
4	A	1424[A]	COA	C4A-N9A	-3.96	1.29	1.37
4	A	1424[A]	COA	C5A-N7A	-3.77	1.32	1.39
5	A	1425[B]	MYA	C2A-N1A	3.67	1.40	1.33
6	A	1426[A]	ENF	O2-C12	-3.50	1.16	1.23
4	A	1424[A]	COA	P2A-O4A	-3.14	1.39	1.50
5	A	1425[B]	MYA	C13-C11	3.11	1.60	1.53
4	A	1424[A]	COA	O9P-C9P	-3.02	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1425[B]	MYA	C3M-C2M	2.92	1.53	1.50
4	A	1424[A]	COA	C8A-N9A	-2.90	1.32	1.37
5	A	1425[B]	MYA	C4A-N9A	-2.80	1.31	1.37
4	A	1424[A]	COA	O5P-C5P	-2.77	1.17	1.23
4	A	1424[A]	COA	P3B-O8A	-2.77	1.44	1.54
4	A	1424[A]	COA	C5A-C4A	2.76	1.44	1.39
5	A	1425[B]	MYA	P1A-O3A	2.49	1.62	1.59
4	A	1424[A]	COA	P2A-O5A	-2.42	1.44	1.55
4	A	1424[A]	COA	C5A-C6A	2.37	1.47	1.41
5	A	1425[B]	MYA	P3X-O3X	2.34	1.63	1.59
5	A	1425[B]	MYA	O10-C10	2.27	1.46	1.42
5	A	1425[B]	MYA	P2A-O4A	-2.27	1.43	1.50
7	A	1428	DMS	O-S	2.25	1.65	1.50
4	A	1424[A]	COA	P1A-O2A	-2.19	1.45	1.55
3	A	1423[B]	EN5	C20-C19	2.17	1.59	1.52
3	A	1423[B]	EN5	O-C9	2.14	1.27	1.23
4	A	1424[A]	COA	C4A-N3A	-2.01	1.30	1.34
4	A	1424[A]	COA	C5P-N4P	-2.01	1.28	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1424[A]	COA	C5A-C4A-N3A	-5.92	118.57	126.72
5	A	1425[B]	MYA	O6A-C12-C11	-5.35	101.94	110.55
5	A	1425[B]	MYA	C5A-C4A-N3A	-4.95	119.91	126.72
3	A	1423[B]	EN5	C7-C8-C9	-4.89	99.63	113.19
6	A	1426[A]	ENF	C29-C27-N	-4.64	107.88	116.34
4	A	1424[A]	COA	N3A-C4A-N9A	4.39	134.63	127.17
6	A	1426[A]	ENF	O28-C27-C29	3.98	129.23	122.02
4	A	1424[A]	COA	C2A-N3A-C4A	3.71	120.90	111.83
4	A	1424[A]	COA	C4A-C5A-N7A	-3.61	106.46	110.58
5	A	1425[B]	MYA	N9A-C8A-N7A	-3.42	109.08	113.94
5	A	1425[B]	MYA	C4A-C5A-N7A	-3.35	106.75	110.58
3	A	1423[B]	EN5	O-C9-N1	-3.23	117.48	122.95
5	A	1425[B]	MYA	C4A-N9A-C8A	3.21	109.11	105.74
4	A	1424[A]	COA	C6P-C5P-N4P	-3.20	110.51	116.34
5	A	1425[B]	MYA	N3A-C4A-N9A	3.09	132.41	127.17
5	A	1425[B]	MYA	C4M-C3M-C2M	-2.99	105.66	112.27
3	A	1423[B]	EN5	C3-C2-C1	-2.88	99.80	114.37
3	A	1423[B]	EN5	C8-C9-N1	2.76	120.73	115.86
3	A	1423[B]	EN5	O3-C18-C13	2.71	126.14	120.48
5	A	1425[B]	MYA	C6A-C5A-C4A	2.70	120.87	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1428	DMS	C2-S-C1	2.66	112.03	98.42
6	A	1426[A]	ENF	C7-C8-C9	-2.63	105.89	113.19
6	A	1426[A]	ENF	C6-C7-C8	2.62	122.75	113.13
4	A	1424[A]	COA	C4A-N9A-C8A	2.51	108.37	105.74
5	A	1425[B]	MYA	C3M-C2M-S1	2.48	116.36	113.40
3	A	1423[B]	EN5	C25-C26-C21	-2.48	106.86	112.08
5	A	1425[B]	MYA	C5A-N7A-C8A	2.38	107.20	103.45
4	A	1424[A]	COA	C5A-N7A-C8A	2.37	107.17	103.45
3	A	1423[B]	EN5	C18-C13-N2	-2.36	104.72	111.11
5	A	1425[B]	MYA	C2-C3-N4	-2.28	107.66	112.41
5	A	1425[B]	MYA	C13-C11-C10	2.23	112.56	108.77
4	A	1424[A]	COA	O4B-C1B-C2B	-2.23	101.85	106.62
4	A	1424[A]	COA	C6A-C5A-N7A	2.17	136.28	132.09
5	A	1425[B]	MYA	C13-C11-C12	-2.16	104.67	108.22
3	A	1423[B]	EN5	C6-C7-C8	2.12	120.92	113.13
3	A	1423[B]	EN5	C20-C21-C26	-2.10	106.77	112.05
4	A	1424[A]	COA	O5A-P2A-O4A	2.06	122.04	112.44
5	A	1425[B]	MYA	O2M-C2M-S1	-2.06	120.06	122.68
5	A	1425[B]	MYA	O4X-C1X-C2X	-2.03	102.27	106.62
5	A	1425[B]	MYA	C7-N8-C9	2.01	126.16	122.55

There are no chirality outliers.

All (14) torsion outliers are listed below:

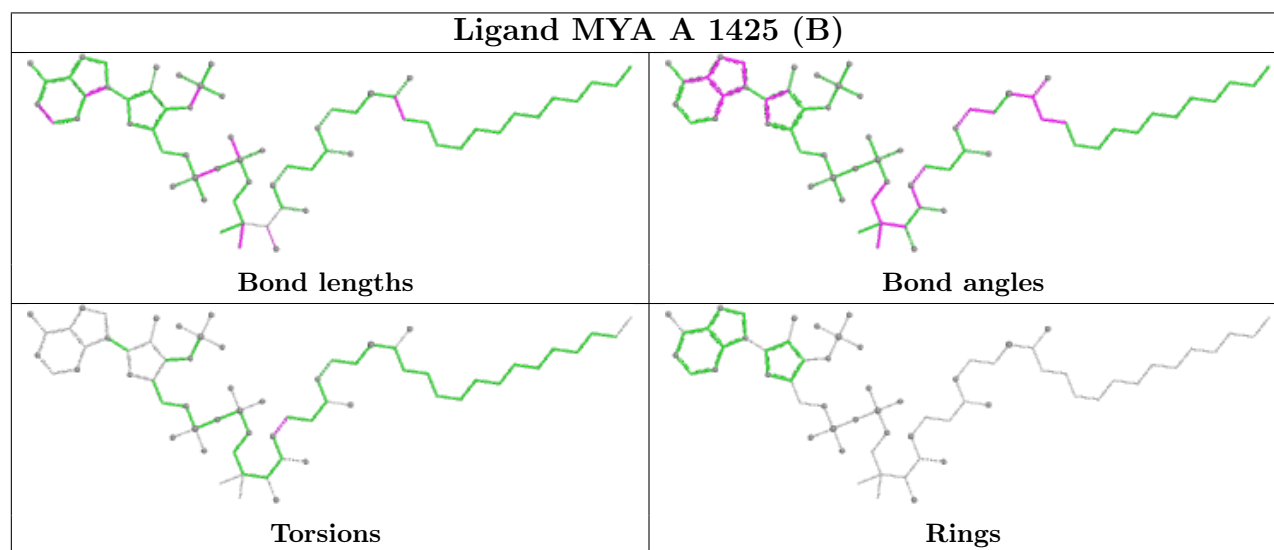
Mol	Chain	Res	Type	Atoms
6	A	1426[A]	ENF	O28-C27-N-C
6	A	1426[A]	ENF	C6-C7-C8-C9
6	A	1426[A]	ENF	N-C-C1-C2
6	A	1426[A]	ENF	C29-C27-N-C
6	A	1426[A]	ENF	C5-C6-C7-C8
3	A	1423[B]	EN5	C5-C6-C7-C8
3	A	1423[B]	EN5	C6-C7-C8-C9
4	A	1424[A]	COA	C6P-C7P-N8P-C9P
5	A	1425[B]	MYA	C6-C7-N8-C9
3	A	1423[B]	EN5	N-C-C1-C2
3	A	1423[B]	EN5	N2-C13-C18-O3
6	A	1426[A]	ENF	N2-C13-C18-O3
3	A	1423[B]	EN5	N2-C13-C18-N4
6	A	1426[A]	ENF	N2-C13-C18-N4

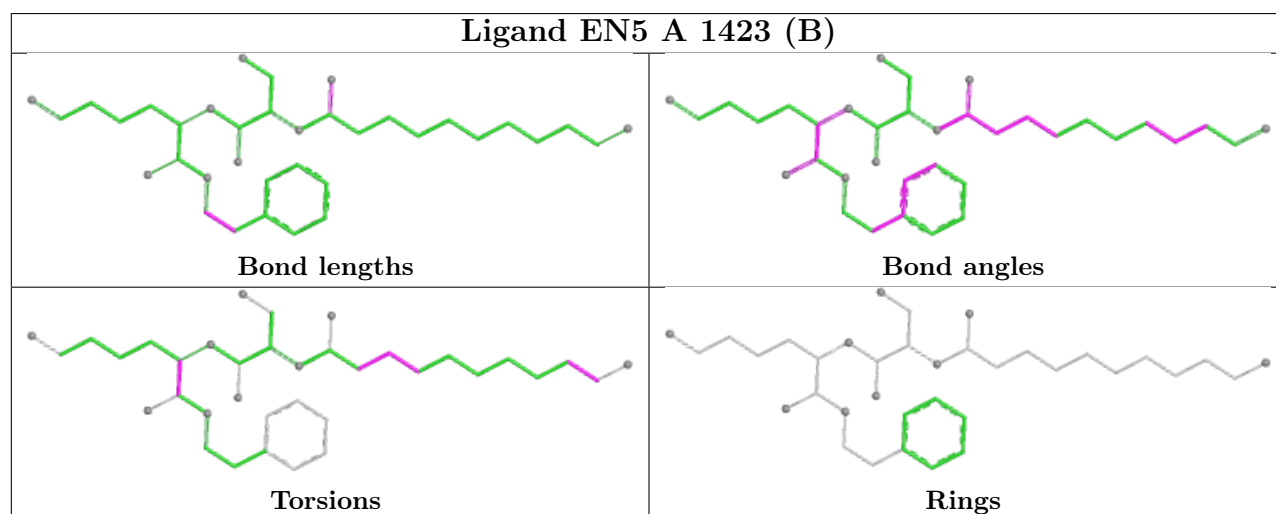
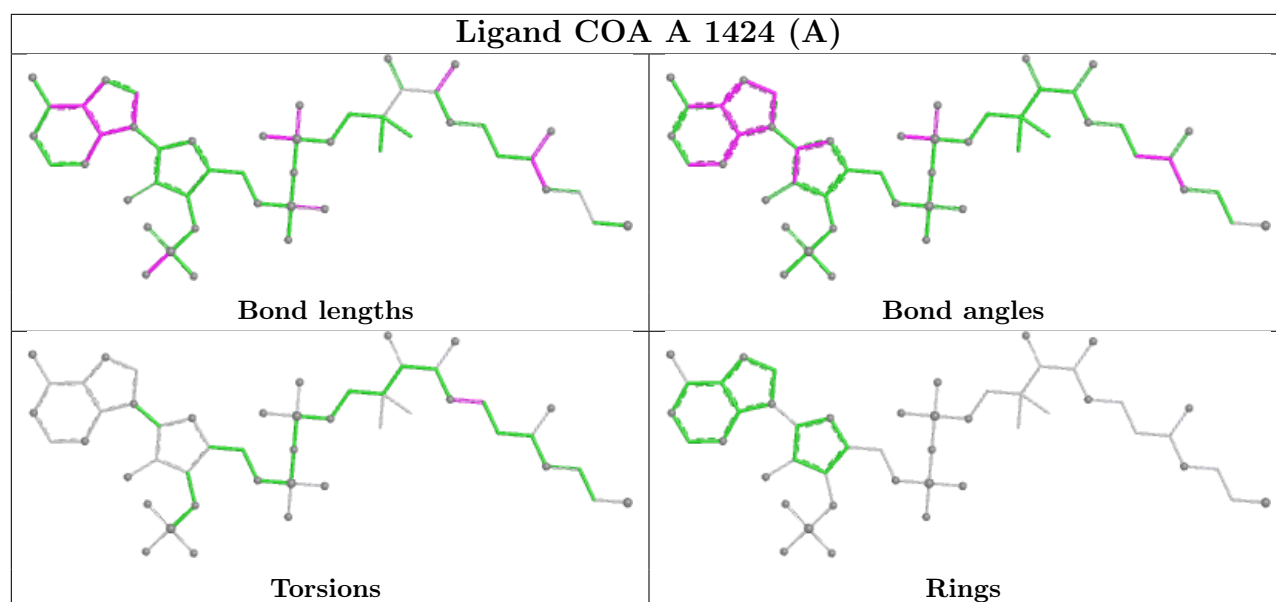
There are no ring outliers.

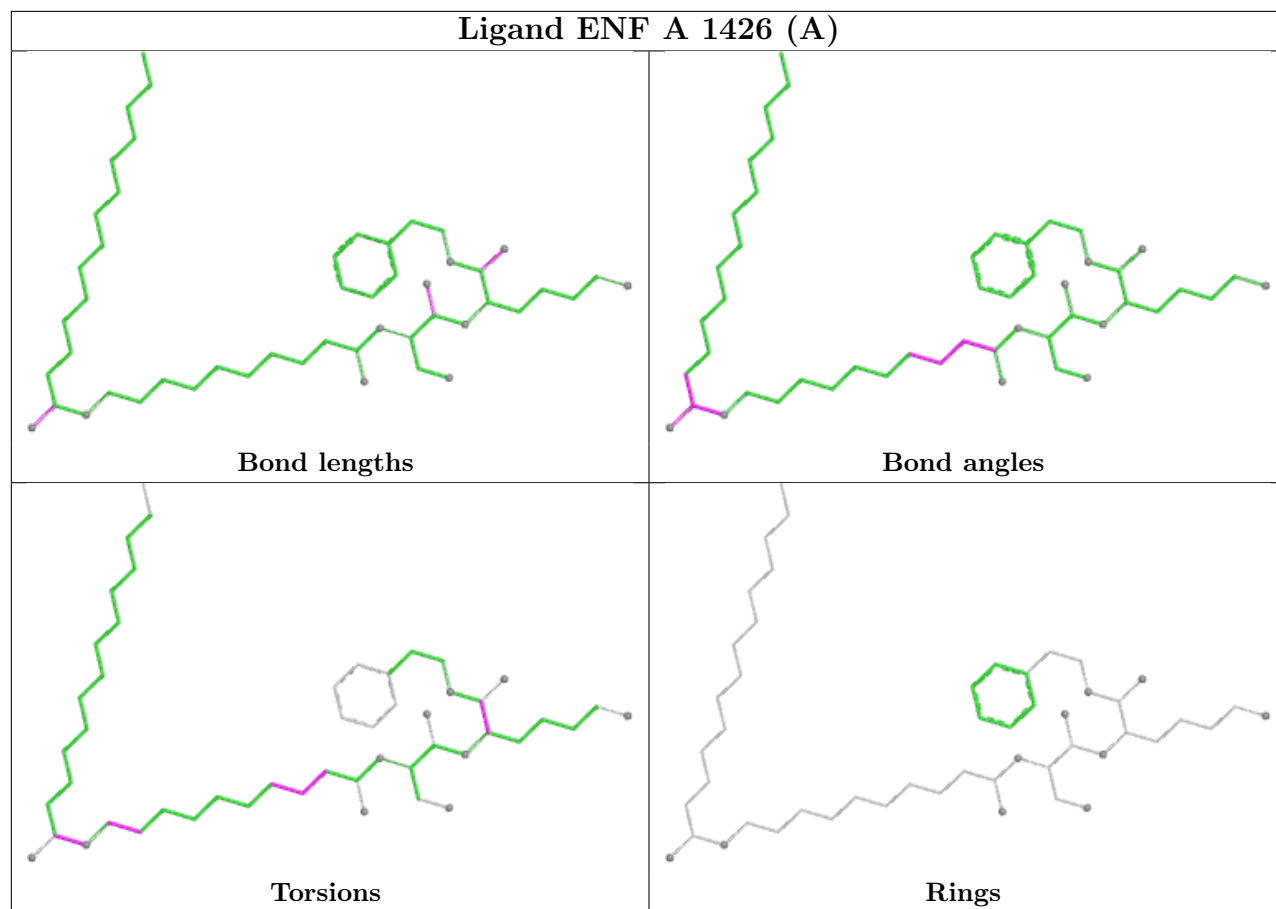
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1428	DMS	5	0
4	A	1424[A]	COA	11	0
3	A	1423[B]	EN5	4	0
6	A	1426[A]	ENF	11	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 [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	411/411 (100%)	-0.20	7 (1%) 69 72	7, 15, 34, 58	23 (5%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	GLY	3.7
1	A	242	PHE	3.1
1	A	245	PRO	2.3
1	A	336	SER	2.3
1	A	31	VAL	2.1
1	A	11	ALA	2.0
1	A	32	PHE	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(Å ²)	Q<0.9
4	COA	A	1424[A]	48/48	0.80	0.13	19,34,39,42	48

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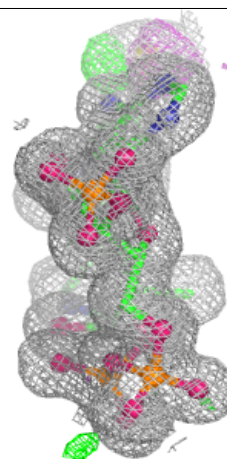
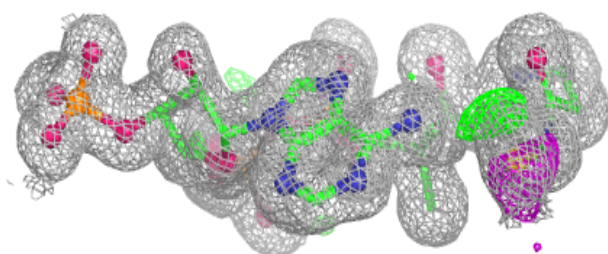
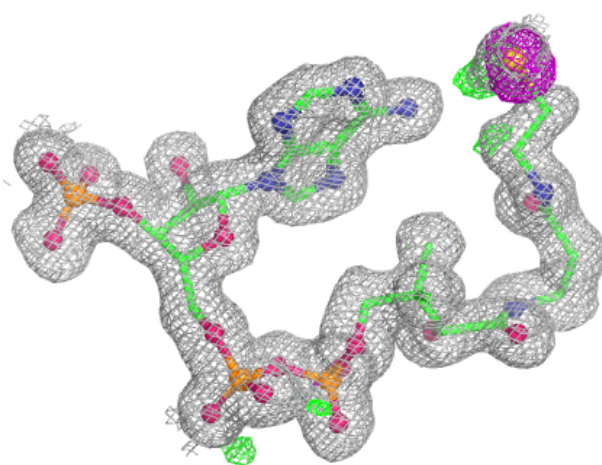
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ENF	A	1426[A]	51/51	0.80	0.09	10,16,21,21	51
7	DMS	A	1427	4/4	0.92	0.16	13,14,15,17	4
7	DMS	A	1428	4/4	0.94	0.11	12,18,18,20	4
3	EN5	A	1423[B]	36/36	0.97	0.06	9,12,27,31	36
2	MG	A	1422	1/1	0.97	0.08	26,26,26,26	0
5	MYA	A	1425[B]	63/63	0.97	0.05	10,13,16,18	63

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.

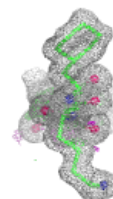
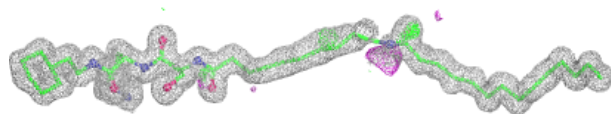
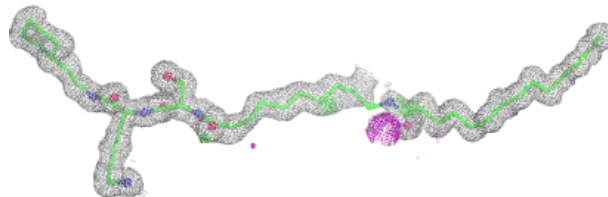
Electron density around COA A 1424 (A):

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

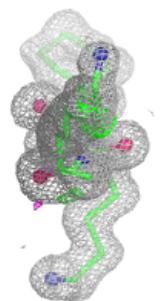
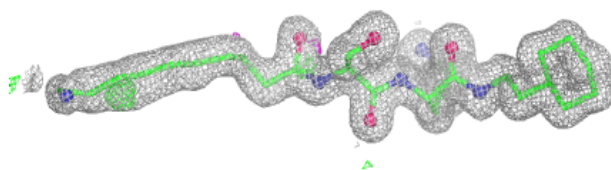
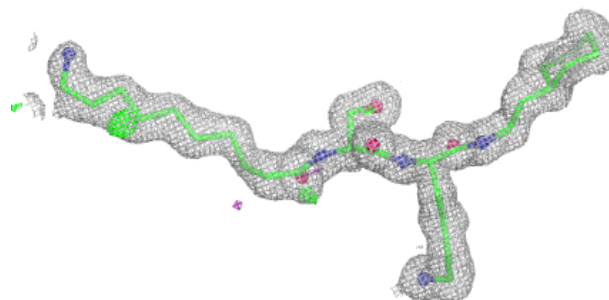


Electron density around ENF A 1426 (A):

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

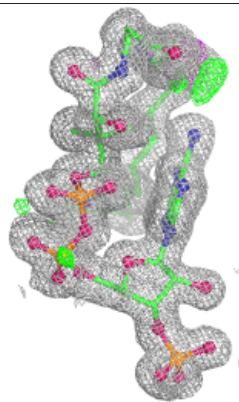
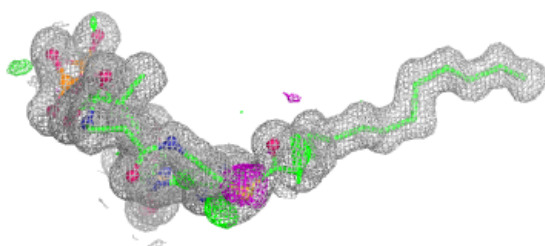
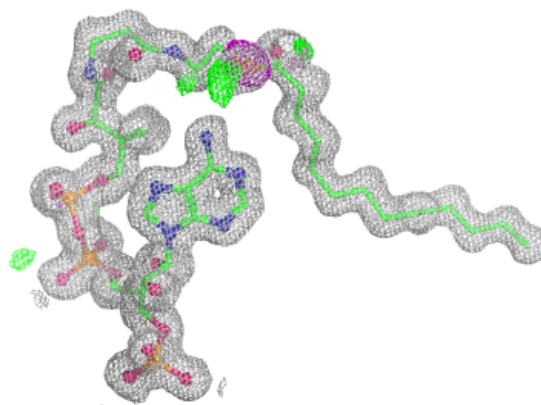
**Electron density around EN5 A 1423 (B):**

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



Electron density around MYA A 1425 (B):

$2mF_o-DF_c$ (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.