Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2024 – 11:21 AM EDT

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PDB ID	:	8FBT
Title	:	Crystal structure of Cryptosporidium parvum N-myristoyltransferase with bound myristoyl-CoA
Authors	:	Staker, B.L.; Fenwick, M.K.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2022-11-30
Resolution	:	2.20 Å(reported)

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 2.20 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		3.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
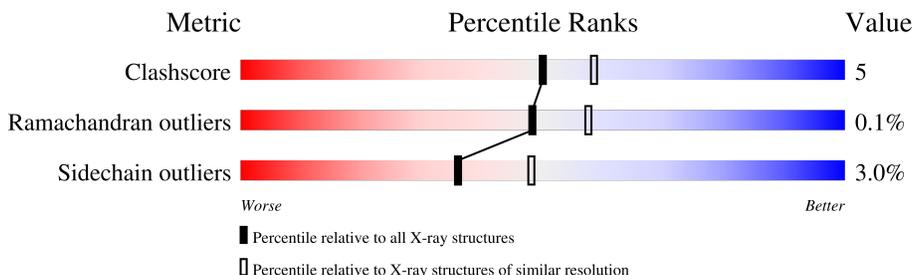
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	432	82% 14% •
1	B	432	82% 12% • 5%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 14061 atoms, of which 6781 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	B	411	Total 6711	C 2186	H 3328	N 567	O 609	S 21	0	8	0
1	A	418	Total 6721	C 2201	H 3307	N 573	O 618	S 22	0	11	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	35	GLY	-	expression tag	UNP Q5CV46
B	36	PRO	-	expression tag	UNP Q5CV46
B	37	GLY	-	expression tag	UNP Q5CV46
B	38	SER	-	expression tag	UNP Q5CV46
B	310	ALA	LYS	engineered mutation	UNP Q5CV46
B	311	ALA	GLU	engineered mutation	UNP Q5CV46
A	35	GLY	-	expression tag	UNP Q5CV46
A	36	PRO	-	expression tag	UNP Q5CV46
A	37	GLY	-	expression tag	UNP Q5CV46
A	38	SER	-	expression tag	UNP Q5CV46
A	310	ALA	LYS	engineered mutation	UNP Q5CV46
A	311	ALA	GLU	engineered mutation	UNP Q5CV46

- Molecule 2 is TETRADECANOYL-COA (three-letter code: MYA) (formula: $C_{35}H_{62}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).
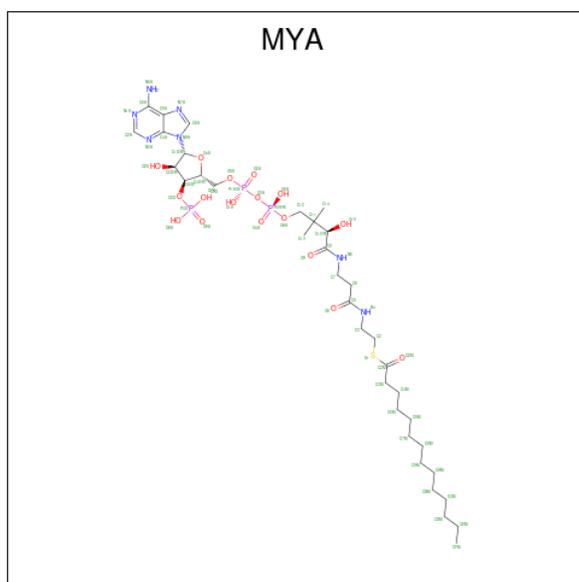
MYA

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	S	0	0
			121	35	58	7	17	3	1		
2	A	1	Total	C	H	N	O	P	S	0	0
			121	35	58	7	17	3	1		

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
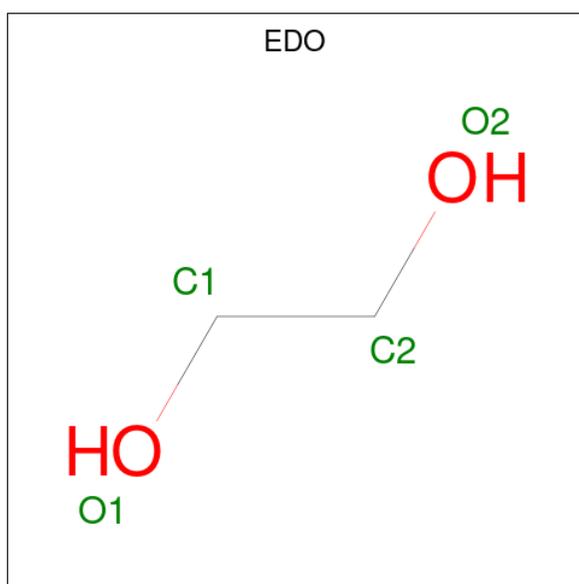
EDO

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
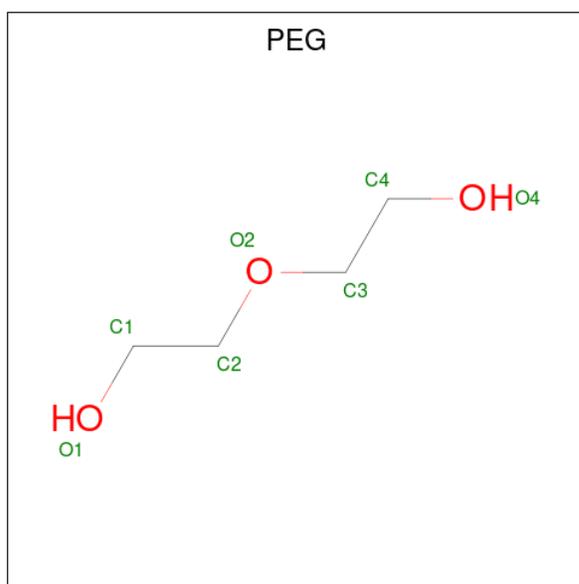
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	B	1	17	4	10	3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
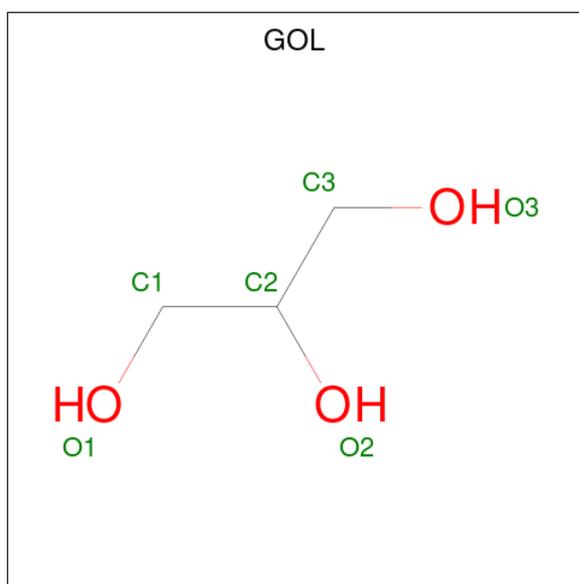
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	14	3	8	3	0	1

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	185	Total 185	O 185	0	13
6	A	151	Total 151	O 151	0	19

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain B:
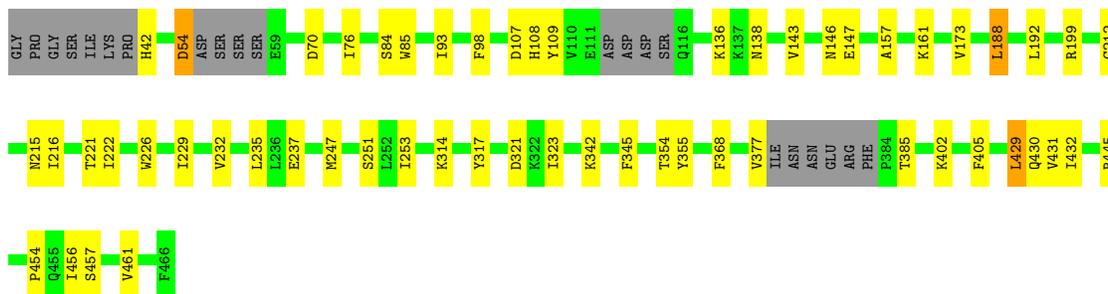
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain A:
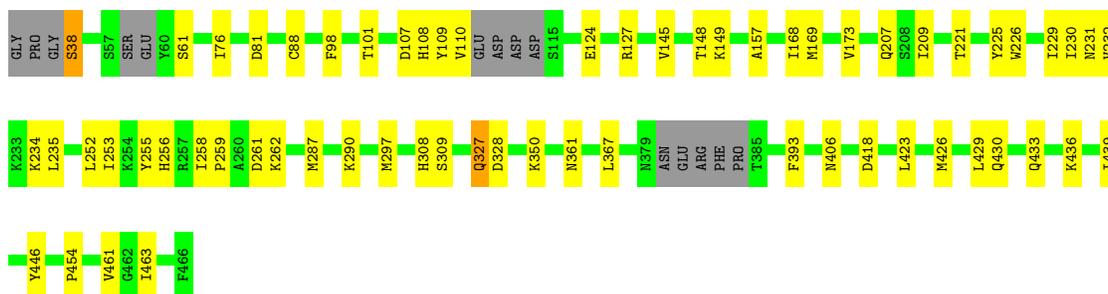
4 Data and refinement statistics ⓘ

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.43Å　　105.34Å　　71.12Å 90.00°　　112.48°　　90.00°	Depositor
Resolution (Å)	49.83　–　2.20	Depositor
% Data completeness (in resolution range)	99.0 (49.83-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.98 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.164　,　0.217	Depositor
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.150	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14061	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MYA, EDO, PEG, 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	0.61	0/3491	0.68	0/4731
1	B	0.68	0/3462	0.75	1/4686 (0.0%)
All	All	0.65	0/6953	0.72	1/9417 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	429	LEU	CB-CG-CD2	-5.19	102.17	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3414	3307	3296	39	0
1	B	3383	3328	3321	31	0
2	A	63	58	56	0	0
2	B	63	58	57	3	0
3	A	4	6	6	0	0
3	B	4	6	6	0	0
4	B	7	10	10	0	0
5	A	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	151	0	0	8	0
6	B	185	0	0	2	0
All	All	7280	6781	6760	71	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 5.

All (71) 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:54:ASP:N	1:B:54:ASP:OD1	2.15	0.80
1:A:109:TYR:O	1:A:110:VAL:HG23	1.87	0.72
1:B:188:LEU:HD23	1:B:192[B]:LEU:HD13	1.75	0.68
1:A:226:TRP:CZ2	1:A:439:ILE:HD12	2.30	0.66
1:B:221:THR:HG21	1:B:461:VAL:HG21	1.81	0.63
1:A:221:THR:HG21	1:A:461:VAL:HG21	1.85	0.59
2:B:501:MYA:H8A	6:B:757:HOH:O	2.03	0.57
1:A:430:GLN:NE2	6:A:602:HOH:O	2.23	0.57
1:B:377:VAL:HG23	1:B:377:VAL:O	2.08	0.54
1:A:234:LYS:HD3	1:A:418:ASP:OD1	2.09	0.53
1:B:232:VAL:HG21	1:B:253:ILE:HA	1.91	0.53
1:A:327:GLN:NE2	1:A:328:ASP:OD1	2.42	0.52
1:B:229:ILE:HG23	1:B:235:LEU:HD12	1.92	0.51
1:A:88[A]:CYS:HG	1:A:101:THR:HG1	1.56	0.51
1:A:230:ILE:O	6:A:601[B]:HOH:O	2.19	0.50
1:A:308:HIS:ND1	6:A:607:HOH:O	2.34	0.50
1:A:256:HIS:CD2	6:A:656:HOH:O	2.65	0.50
1:A:127:ARG:HH11	1:A:127:ARG:HG2	1.76	0.50
1:A:38:SER:N	6:A:611:HOH:O	2.45	0.50
1:A:287:MET:HG2	6:A:640:HOH:O	2.11	0.50
1:B:222:ILE:CD1	1:B:445:ARG:HG3	2.42	0.49
1:B:345:PHE:HB3	1:B:354:THR:HG21	1.95	0.49
1:B:42:HIS:ND1	2:B:501:MYA:O7A	2.46	0.48
1:A:169[A]:MET:HE1	1:A:207:GLN:HB2	1.94	0.48
1:A:393:PHE:HE2	1:A:426:MET:HE3	1.78	0.48
1:A:258:ILE:HG23	1:A:259:PRO:HD2	1.95	0.48
1:B:76:ILE:HD11	1:B:85:TRP:CD1	2.49	0.47
1:A:61:SER:O	1:A:454:PRO:HD3	2.13	0.47
1:B:314:LYS:HG2	1:B:317:TYR:HE2	1.79	0.46
1:B:109:TYR:CD1	2:B:501:MYA:H6A	2.50	0.46
1:A:262:LYS:O	1:A:406:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LYS:NZ	6:A:609[A]:HOH:O	2.42	0.45
1:A:255:TYR:O	1:A:436:LYS:HE3	2.16	0.45
1:A:393:PHE:CE2	1:A:426:MET:HE3	2.52	0.45
1:B:157:ALA:HA	1:B:173:VAL:O	2.18	0.44
1:B:385:THR:HG23	1:B:385:THR:O	2.18	0.44
1:B:84:SER:HB3	1:B:146:ASN:HD21	1.83	0.44
1:B:143:VAL:HG21	1:B:192[B]:LEU:HD11	2.00	0.44
1:A:231[B]:ASN:O	1:A:235:LEU:HG	2.17	0.44
1:A:232:VAL:HB	1:A:253:ILE:HG12	1.99	0.44
1:B:138:ASN:O	1:B:199:ARG:HD3	2.18	0.43
1:A:124:GLU:H	1:A:124:GLU:CD	2.22	0.43
1:A:209:ILE:HD13	1:A:463[B]:ILE:HD13	2.01	0.43
1:A:221:THR:HG22	1:A:446:TYR:HB2	1.99	0.43
1:B:402:LYS:HE2	1:B:430:GLN:O	2.19	0.43
1:B:226:TRP:CD1	1:B:432:ILE:HD12	2.54	0.43
1:B:107:ASP:HB2	1:B:108:HIS:CD2	2.53	0.42
1:A:225:TYR:CE1	1:A:423:LEU:HG	2.54	0.42
1:A:367:LEU:C	1:A:367:LEU:HD23	2.40	0.42
1:B:212[B]:CYS:SG	1:B:216:ILE:HD11	2.59	0.42
1:A:231[A]:ASN:O	1:A:235:LEU:HG	2.18	0.42
1:A:290:LYS:HD2	1:A:297:MET:HG2	2.01	0.42
1:A:157:ALA:HA	1:A:173:VAL:O	2.19	0.42
1:A:290:LYS:HD2	1:A:297:MET:CG	2.50	0.42
1:B:377:VAL:O	1:B:377:VAL:CG2	2.67	0.42
1:A:107:ASP:HB2	1:A:108:HIS:CD2	2.55	0.42
1:B:429:LEU:HA	1:B:432:ILE:HG12	2.01	0.42
1:B:222:ILE:CD1	1:B:445:ARG:CG	2.98	0.42
1:B:454:PRO:O	1:B:456:ILE:HG23	2.20	0.41
1:B:247:MET:HB2	1:B:251:SER:OG	2.20	0.41
1:B:355:TYR:HB2	1:B:368:PHE:CZ	2.55	0.41
1:A:148:THR:O	1:A:149:LYS:HB2	2.20	0.41
1:B:323:ILE:H	1:B:323:ILE:HG13	1.72	0.41
1:A:145:VAL:O	1:A:149:LYS:N	2.49	0.41
1:A:231[B]:ASN:ND2	6:A:620:HOH:O	2.53	0.41
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.97	0.41
1:A:229:ILE:HG23	1:A:235:LEU:HD12	2.02	0.41
1:B:405:PHE:CD1	1:B:431:VAL:HG21	2.55	0.41
1:B:429:LEU:HD12	1:B:432:ILE:CG1	2.51	0.41
1:A:226:TRP:CH2	1:A:439:ILE:HD12	2.56	0.40
1:B:161:LYS:NZ	6:B:618:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/432 (97%)	400 (96%)	18 (4%)	1 (0%)	44	52
1	B	410/432 (95%)	387 (94%)	23 (6%)	0	100	100
All	All	829/864 (96%)	787 (95%)	41 (5%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/403 (92%)	360 (97%)	10 (3%)	40	53
1	B	373/403 (93%)	361 (97%)	12 (3%)	34	45
All	All	743/806 (92%)	721 (97%)	22 (3%)	36	48

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	ASP
1	B	70	ASP
1	B	93	ILE
1	B	98	PHE
1	B	136	LYS

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Mol	Chain	Res	Type
1	B	147	GLU
1	B	188	LEU
1	B	215	ASN
1	B	237	GLU
1	B	321	ASP
1	B	342	LYS
1	B	457	SER
1	A	38	SER
1	A	81	ASP
1	A	98	PHE
1	A	168	ILE
1	A	252	LEU
1	A	261	ASP
1	A	309	SER
1	A	327	GLN
1	A	361	ASN
1	A	433	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

6 ligands are modelled in this entry.

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	A	501	-	59,65,65	3.06	15 (25%)	72,91,91	1.50	15 (20%)
5	GOL	A	503[A]	-	5,5,5	1.03	0	5,5,5	1.16	0
2	MYA	B	501	-	59,65,65	3.30	15 (25%)	72,91,91	1.46	10 (13%)
3	EDO	A	502	-	3,3,3	0.52	0	2,2,2	0.29	0
3	EDO	B	502	-	3,3,3	0.48	0	2,2,2	0.35	0
4	PEG	B	503	-	6,6,6	0.35	0	5,5,5	0.29	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	A	501	-	-	7/60/80/80	0/3/3/3
5	GOL	A	503[A]	-	-	4/4/4/4	-
2	MYA	B	501	-	-	10/60/80/80	0/3/3/3
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
4	PEG	B	503	-	-	2/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MYA	O4X-C1X	12.87	1.57	1.40
2	A	501	MYA	C2X-C3X	-12.09	1.26	1.53
2	B	501	MYA	C2X-C3X	-11.78	1.27	1.53
2	A	501	MYA	O4X-C1X	10.14	1.54	1.40
2	B	501	MYA	C1X-N9A	-7.28	1.31	1.49
2	A	501	MYA	C1X-N9A	-7.04	1.32	1.49
2	A	501	MYA	C3X-C4X	6.89	1.70	1.52
2	B	501	MYA	C3X-C4X	6.38	1.69	1.52
2	B	501	MYA	O4X-C4X	-6.22	1.31	1.45
2	A	501	MYA	O4X-C4X	-6.11	1.31	1.45
2	B	501	MYA	P1A-O3A	6.09	1.66	1.59
2	A	501	MYA	P1A-O3A	6.06	1.66	1.59
2	B	501	MYA	C5-N4	5.83	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MYA	P2A-O3A	5.45	1.65	1.59
2	B	501	MYA	C9-N8	5.15	1.45	1.33
2	A	501	MYA	C5-N4	4.52	1.44	1.33
2	A	501	MYA	P2A-O3A	4.15	1.64	1.59
2	A	501	MYA	C9-N8	4.14	1.43	1.33
2	A	501	MYA	P3X-O3X	3.64	1.65	1.59
2	B	501	MYA	C3M-C2M	3.30	1.54	1.50
2	B	501	MYA	C6A-N6A	3.27	1.45	1.34
2	A	501	MYA	C6A-N6A	2.92	1.44	1.34
2	B	501	MYA	O2X-C2X	2.91	1.50	1.43
2	B	501	MYA	P3X-O3X	2.81	1.64	1.59
2	A	501	MYA	O2X-C2X	2.80	1.49	1.43
2	A	501	MYA	C3M-C2M	2.74	1.53	1.50
2	A	501	MYA	O9-C9	-2.52	1.18	1.23
2	A	501	MYA	C2M-S1	2.44	1.82	1.76
2	B	501	MYA	O9-C9	-2.40	1.18	1.23
2	B	501	MYA	O5-C5	-2.15	1.19	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	MYA	C3M-C2M-S1	5.69	120.19	113.40
2	A	501	MYA	N3A-C2A-N1A	-4.75	122.22	128.67
2	B	501	MYA	N3A-C2A-N1A	-4.57	122.47	128.67
2	B	501	MYA	O2M-C2M-C3M	-3.77	119.63	123.98
2	A	501	MYA	C7-C6-C5	3.70	118.56	112.39
2	B	501	MYA	C2-S1-C2M	3.64	112.59	101.84
2	B	501	MYA	C2-C3-N4	-2.87	106.42	112.41
2	A	501	MYA	O4X-C1X-N9A	2.84	112.51	108.75
2	A	501	MYA	C4X-O4X-C1X	-2.83	107.34	109.92
2	A	501	MYA	O5-C5-N4	-2.71	117.72	123.03
2	A	501	MYA	O3X-C3X-C2X	2.69	121.32	111.68
2	B	501	MYA	C4A-C5A-N7A	-2.64	106.55	109.34
2	A	501	MYA	C3X-C2X-C1X	2.59	105.59	99.89
2	A	501	MYA	O3A-P1A-O2A	2.59	118.48	110.70
2	B	501	MYA	C2X-C3X-C4X	2.55	107.70	103.24
2	A	501	MYA	O5-C5-C6	2.47	126.49	122.02
2	A	501	MYA	C6-C7-N8	-2.37	106.95	112.00
2	A	501	MYA	O2M-C2M-C3M	-2.36	121.26	123.98
2	A	501	MYA	O3X-C3X-C4X	-2.33	101.80	110.03
2	A	501	MYA	C4A-C5A-N7A	-2.29	106.92	109.34
2	A	501	MYA	C1X-N9A-C4A	-2.25	122.68	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MYA	C2-C3-N4	-2.12	107.99	112.41
2	B	501	MYA	C6-C7-N8	-2.09	107.55	112.00
2	B	501	MYA	C3X-C2X-C1X	2.05	104.39	99.89
2	B	501	MYA	C14-C11-C12	2.04	111.60	108.22

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	MYA	C3M-C2M-S1-C2
2	B	501	MYA	S1-C2-C3-N4
2	A	501	MYA	C5X-O5X-P1A-O3A
5	A	503[A]	GOL	C1-C2-C3-O3
4	B	503	PEG	O2-C3-C4-O4
5	A	503[A]	GOL	O1-C1-C2-C3
5	A	503[A]	GOL	O2-C2-C3-O3
2	B	501	MYA	CAM-CBM-CCM-CDM
3	B	502	EDO	O1-C1-C2-O2
5	A	503[A]	GOL	O1-C1-C2-O2
2	B	501	MYA	C5M-C6M-C7M-C8M
2	B	501	MYA	O2M-C2M-S1-C2
2	A	501	MYA	C8M-C9M-CAM-CBM
2	A	501	MYA	C3M-C2M-S1-C2
2	B	501	MYA	C8M-C9M-CAM-CBM
2	B	501	MYA	C3M-C4M-C5M-C6M
2	B	501	MYA	C12-O6A-P2A-O3A
2	B	501	MYA	C12-O6A-P2A-O4A
2	A	501	MYA	C3X-O3X-P3X-O8A
4	B	503	PEG	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2
2	B	501	MYA	P2A-O3A-P1A-O2A
2	A	501	MYA	C3X-O3X-P3X-O7A
2	A	501	MYA	C3X-O3X-P3X-O9A
2	A	501	MYA	C3M-C4M-C5M-C6M

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand MYA A 501

Bond lengths — Bond angles — Torsions — Rings

Ligand MYA B 501

Bond lengths — Bond angles — Torsions — Rings
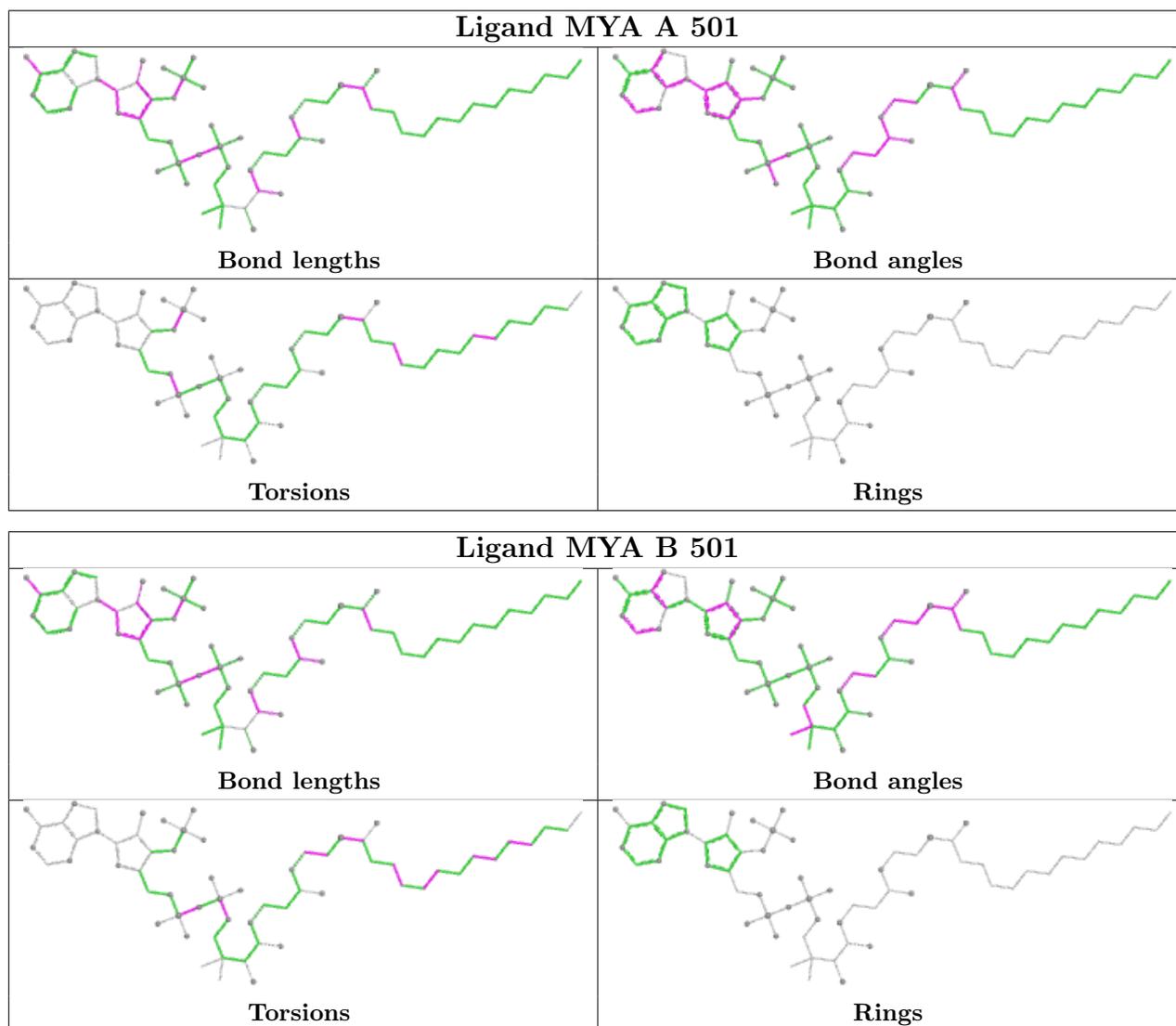
5.7 Other polymers ⓘ

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 ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.