



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 10:33 PM EDT

PDB ID : 6PAV
Title : Structure of Human NMT1 with products CoA and myristoyl-lysine peptide with acetylated N-terminus
Authors : Price, I.R.; Lin, H.
Deposited on : 2019-06-12
Resolution : 2.52 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

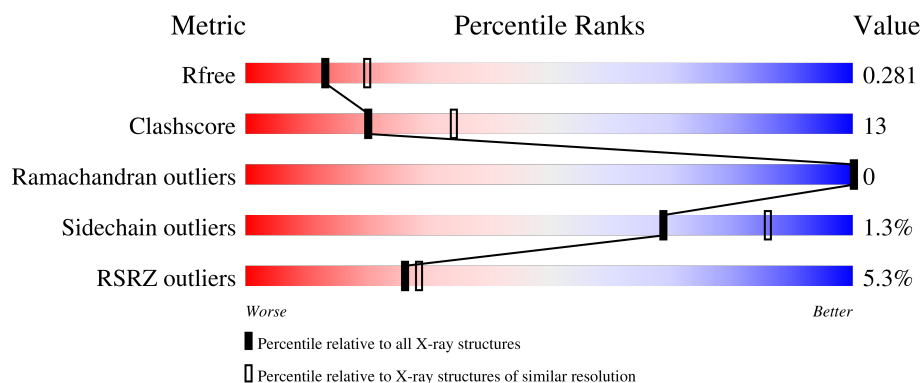
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	388	<div> <div>5%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
1	B	388	<div> <div>5%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
2	D	8	<div> <div>12%</div> <div>50%</div> <div>38%</div> <div>12%</div> </div>
3	C	8	<div> <div>25%</div> <div>50%</div> <div>38%</div> <div>12%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12926 atoms, of which 6407 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	B	379	Total	C	H	N	O	S	0	0	0
			6196	2013	3092	523	552	16			
1	A	377	Total	C	H	N	O	S	0	0	0
			6108	1990	3044	512	546	16			

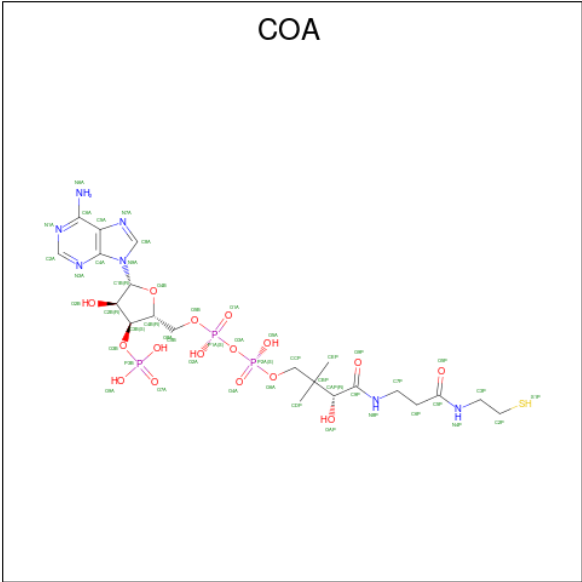
- Molecule 2 is a protein called acetyl-Arf6 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	8	Total	C	H	N	O	0	0	0
			132	43	71	9	9			

- Molecule 3 is a protein called ARF6 peptide.

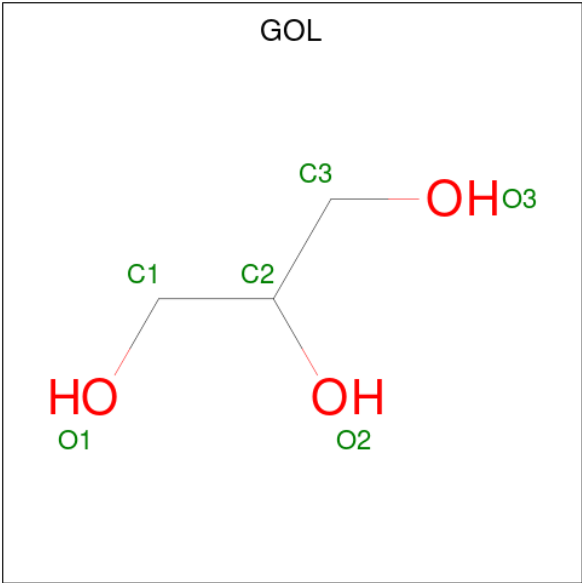
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	8	Total	C	H	N	O	0	0	0
			130	43	69	9	9			

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	P	0	0
			72	19	27	7	16	3		
4	A	1	Total	C	H	N	O	P	0	0
			80	21	32	7	16	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



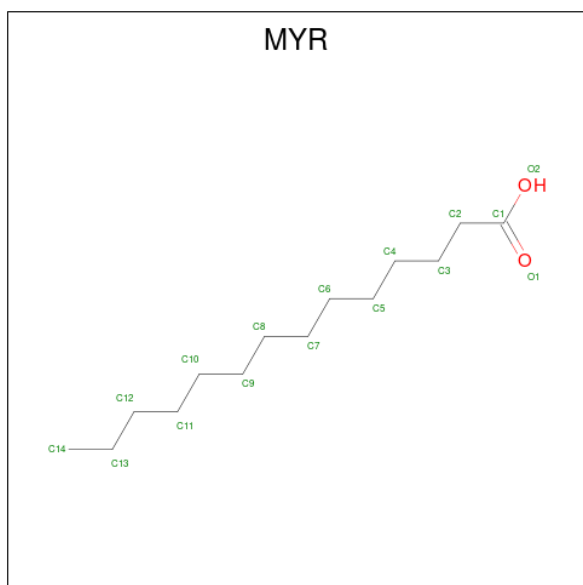
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			10	3	4	3		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			11	3	5	3		
5	A	1	Total	C	H	O	0	0
			10	3	4	3		

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			42	14	27	1		
6	C	1	Total	C	H	O	0	0
			42	14	27	1		

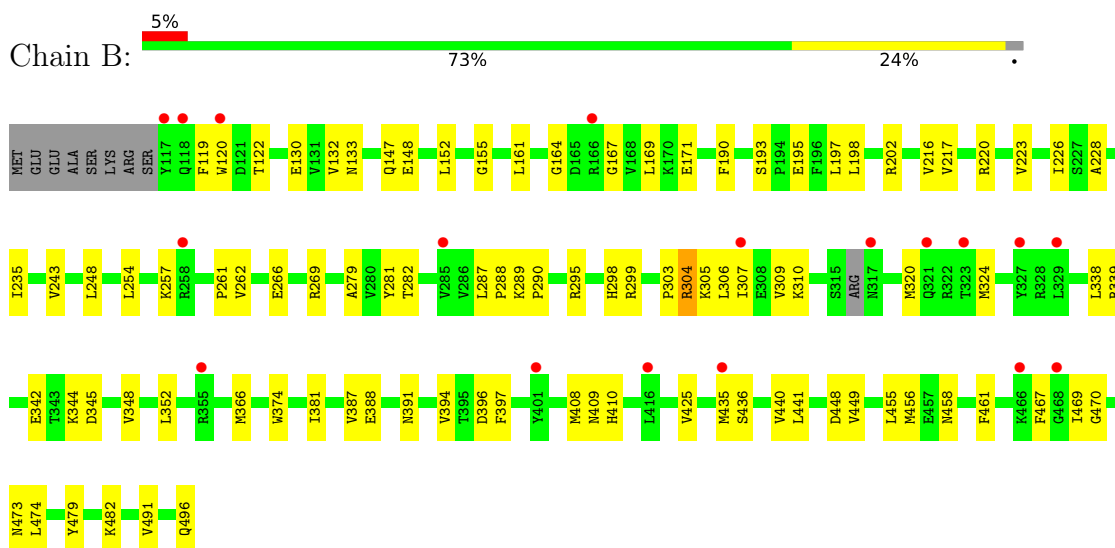
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	35	Total	O	0	0
			35	35		
7	D	1	Total	O	0	0
			1	1		
7	A	45	Total	O	0	0
			45	45		
7	C	1	Total	O	0	0
			1	1		

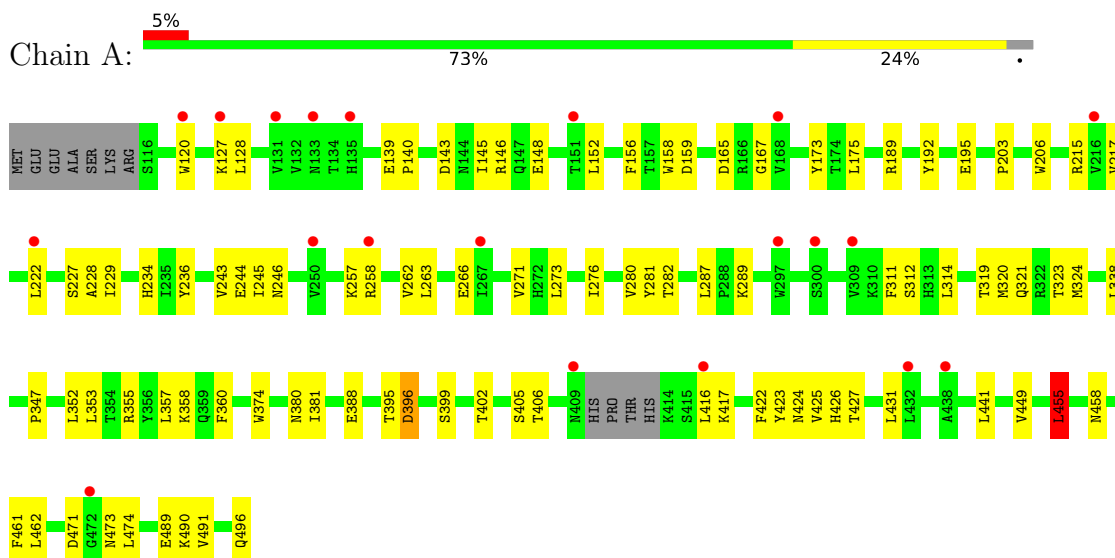
3 Residue-property plots

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

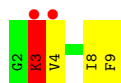


- Molecule 2: acetyl-Arf6 peptide





● Molecule 3: ARF6 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.36Å 58.22Å 154.03Å 90.00° 90.66° 90.00°	Depositor
Resolution (Å)	77.01 – 2.52 77.01 – 2.52	Depositor EDS
% Data completeness (in resolution range)	98.5 (77.01-2.52) 98.5 (77.01-2.52)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.265 , 0.280 0.266 , 0.281	Depositor DCC
R_{free} test set	1467 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12926	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.22% 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: GOL, ACE, MYR, COA

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	0.57	0/3149	0.77	1/4280 (0.0%)
1	B	0.60	3/3192 (0.1%)	0.77	0/4338
2	D	1.42	1/59 (1.7%)	1.07	0/77
3	C	0.99	0/61	1.61	1/79 (1.3%)
All	All	0.60	4/6461 (0.1%)	0.79	2/8774 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	LYS	CE-NZ	9.65	1.73	1.49
1	B	266	GLU	CD-OE1	-5.38	1.19	1.25
1	B	410	HIS	N-CA	-5.05	1.36	1.46
1	B	269	ARG	CZ-NH1	-5.01	1.26	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	LYS	CD-CE-NZ	8.04	130.20	111.70
1	A	455	LEU	CB-CG-CD1	5.01	119.52	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	3064	3044	3044	80	2
1	B	3104	3092	3090	70	1
2	D	61	71	74	5	0
3	C	61	69	69	5	0
4	A	48	32	32	8	0
4	B	45	27	26	3	0
5	A	12	9	16	0	0
5	B	12	9	16	2	0
6	B	15	27	27	1	0
6	C	15	27	27	3	0
7	A	45	0	0	12	0
7	B	35	0	0	6	0
7	C	1	0	0	1	0
7	D	1	0	0	0	0
All	All	6519	6407	6421	161	3

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 13.

All (161) 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)
2:D:3:LYS:CE	2:D:3:LYS:NZ	1.73	1.52
1:A:228:ALA:HB1	1:A:243:VAL:HG21	1.31	1.09
1:A:422:PHE:O	7:A:601:HOH:O	1.85	0.92
1:A:395:THR:O	7:A:602:HOH:O	1.86	0.91
1:B:228:ALA:HB1	1:B:243:VAL:HG21	1.53	0.88
1:A:424:ASN:OD1	7:A:603:HOH:O	1.92	0.87
1:B:228:ALA:HB1	1:B:243:VAL:CG2	2.06	0.85
1:A:405:SER:OG	7:A:604:HOH:O	1.95	0.85
3:C:3:LYS:O	7:C:201:HOH:O	1.97	0.81
1:A:120:TRP:NE1	4:A:501:COA:O2B	2.16	0.79
1:B:409:ASN:N	7:B:603:HOH:O	2.14	0.79
1:A:399:SER:OG	1:A:423:TYR:O	2.00	0.78
1:A:120:TRP:CD1	4:A:501:COA:O2B	2.36	0.77
1:A:396:ASP:HA	7:A:602:HOH:O	1.84	0.76
1:A:228:ALA:HB1	1:A:243:VAL:CG2	2.13	0.76
1:A:338:LEU:HD21	1:A:441:LEU:HD11	1.68	0.75
1:B:338:LEU:HD21	1:B:441:LEU:HD11	1.67	0.75
1:B:190:PHE:O	7:B:601:HOH:O	2.04	0.75
1:B:303:PRO:O	1:B:307:ILE:HD12	1.87	0.73
1:A:282:THR:HB	1:A:474:LEU:HD11	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ARG:HB2	1:B:467:PHE:CD2	2.26	0.70
1:A:319:THR:HG22	1:A:320:MET:N	2.07	0.70
1:B:304:ARG:HD3	1:B:324:MET:HE3	1.73	0.69
1:A:496:GLN:OXT	7:A:605:HOH:O	2.12	0.67
1:A:229:ILE:O	1:A:243:VAL:HG23	1.93	0.67
1:A:312:SER:OG	3:C:8:ILE:HG13	1.94	0.67
1:B:147:GLN:OE1	7:B:602:HOH:O	2.12	0.67
1:B:295:ARG:HG2	1:B:469:ILE:HD11	1.78	0.66
1:A:143:ASP:OD2	7:A:606:HOH:O	2.14	0.65
1:B:397:PHE:CD1	1:B:425:VAL:HG22	2.32	0.64
1:A:175:LEU:HD22	1:A:222:LEU:HG	1.80	0.63
1:B:226:ILE:HD12	1:B:248:LEU:HD13	1.80	0.62
1:A:458:ASN:HA	1:A:461:PHE:CE2	2.34	0.62
2:D:3:LYS:NZ	2:D:3:LYS:CD	2.60	0.62
1:B:133:ASN:O	7:B:604:HOH:O	2.15	0.61
1:B:195:GLU:HB3	1:B:381:ILE:HD11	1.83	0.60
1:B:119:PHE:CE1	1:B:261:PRO:HB3	2.36	0.60
1:B:304:ARG:HD3	1:B:324:MET:CE	2.32	0.60
1:B:470:GLY:HA2	2:D:7:LYS:O	2.02	0.59
1:A:380:ASN:O	1:A:402:THR:HB	2.02	0.59
1:A:416:LEU:HD21	1:A:449:VAL:HG12	1.83	0.59
1:B:391:ASN:N	1:B:391:ASN:OD1	2.36	0.58
1:A:234:HIS:CE1	1:A:236:TYR:O	2.57	0.58
1:B:261:PRO:HD3	4:B:501:COA:O1A	2.05	0.57
1:A:143:ASP:HB3	7:A:606:HOH:O	2.05	0.56
1:B:299:ARG:HB2	1:B:467:PHE:CE2	2.41	0.56
1:B:147:GLN:NE2	1:A:347:PRO:HD3	2.20	0.56
1:A:319:THR:CG2	1:A:320:MET:N	2.68	0.56
1:B:281:TYR:CD2	6:B:504:MYR:H41	2.41	0.55
1:B:436:SER:O	1:B:440:VAL:HG23	2.06	0.55
1:A:320:MET:O	1:A:324:MET:HG3	2.05	0.55
1:B:132:VAL:HG11	1:B:482:LYS:HG2	1.88	0.55
1:B:133:ASN:HB3	7:B:604:HOH:O	2.06	0.55
1:A:399:SER:OG	1:A:423:TYR:N	2.36	0.55
1:A:203:PRO:O	1:A:206:TRP:HD1	1.89	0.55
1:A:128:LEU:HD21	1:A:287:LEU:O	2.06	0.55
1:A:319:THR:O	1:A:323:THR:OG1	2.20	0.55
1:B:408:MET:C	7:B:603:HOH:O	2.41	0.55
1:B:152:LEU:HD23	1:B:262:VAL:HG11	1.89	0.54
1:B:235:ILE:O	1:B:235:ILE:HG23	2.08	0.54
1:B:223:VAL:HB	1:B:254:LEU:HD12	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:HG2	1:A:280:VAL:CG1	2.38	0.53
1:A:352:LEU:HB3	1:A:425:VAL:HG11	1.91	0.52
1:B:305:LYS:O	1:B:309:VAL:HG22	2.10	0.52
1:A:353:LEU:HD11	1:A:357:LEU:HD11	1.91	0.52
1:A:427:THR:N	7:A:602:HOH:O	2.42	0.52
1:A:228:ALA:HB2	1:A:245:ILE:CD1	2.40	0.51
1:B:458:ASN:HA	1:B:461:PHE:CE2	2.46	0.51
1:A:228:ALA:HB2	1:A:245:ILE:HD13	1.92	0.51
1:A:120:TRP:HE1	4:A:501:COA:HO2A	1.57	0.50
1:B:282:THR:HB	1:B:474:LEU:HD11	1.93	0.50
4:A:501:COA:O5P	4:A:501:COA:C2P	2.59	0.50
1:B:455:LEU:HD12	1:B:455:LEU:C	2.32	0.50
1:A:311:PHE:CD2	1:A:416:LEU:CD1	2.94	0.50
1:B:257:LYS:O	1:B:257:LYS:HG2	2.11	0.49
1:A:143:ASP:CG	7:A:606:HOH:O	2.49	0.49
1:A:244:GLU:HG2	1:A:280:VAL:HG13	1.93	0.49
1:B:228:ALA:HB1	1:B:243:VAL:HG22	1.93	0.49
1:A:229:ILE:C	1:A:243:VAL:HG23	2.32	0.49
1:B:456:MET:HG3	1:B:491:VAL:O	2.13	0.48
1:A:158:TRP:HZ3	1:A:263:LEU:HD23	1.78	0.48
1:A:458:ASN:O	1:A:462:LEU:HG	2.14	0.48
1:A:152:LEU:HD21	1:A:158:TRP:CZ2	2.48	0.48
1:B:119:PHE:CD1	1:B:261:PRO:HB3	2.49	0.48
1:A:360:PHE:HB3	1:A:490:LYS:O	2.15	0.47
1:B:287:LEU:O	1:B:290:PRO:HD3	2.15	0.47
4:A:501:COA:N6A	4:A:501:COA:H32	2.30	0.47
1:B:339:ARG:NE	1:B:388:GLU:OE1	2.48	0.46
1:A:319:THR:HG22	1:A:321:GLN:H	1.79	0.46
1:A:227:SER:OG	1:A:246:ASN:O	2.28	0.46
1:B:169:LEU:HD22	1:B:198:LEU:HD11	1.98	0.46
1:B:298:HIS:CD2	1:B:298:HIS:N	2.84	0.46
3:C:9:PHE:C	3:C:9:PHE:CD2	2.89	0.46
1:B:155:GLY:O	1:B:217:VAL:HG23	2.16	0.46
4:A:501:COA:O5P	4:A:501:COA:N8P	2.44	0.45
1:B:345:ASP:O	1:B:348:VAL:HG12	2.17	0.45
1:B:435:MET:HG3	1:B:461:PHE:CZ	2.52	0.45
4:A:501:COA:N6A	4:A:501:COA:C3P	2.79	0.45
1:B:132:VAL:CG1	1:B:482:LYS:HG2	2.47	0.45
1:B:167:GLY:O	1:B:171:GLU:HG3	2.17	0.45
1:A:266:GLU:HA	1:A:266:GLU:OE1	2.17	0.44
1:B:193:SER:O	1:B:197:LEU:HG	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ARG:O	1:B:449:VAL:HG23	2.18	0.44
1:A:257:LYS:O	1:A:258:ARG:HB2	2.18	0.44
1:A:281:TYR:CE2	6:C:101:MYR:H62	2.53	0.44
1:A:426:HIS:CD2	1:A:431:LEU:HB2	2.53	0.44
1:A:473:ASN:O	3:C:4:VAL:HG21	2.18	0.44
1:B:279:ALA:HB3	1:B:479:TYR:HB3	2.00	0.43
1:B:342:GLU:OE2	1:B:344:LYS:HE2	2.17	0.43
1:B:216:VAL:O	1:B:220:ARG:N	2.50	0.43
1:B:366:MET:HE2	1:B:374:TRP:CD1	2.53	0.43
4:B:501:COA:N8P	4:B:501:COA:H131	2.32	0.43
1:A:257:LYS:HB3	1:A:257:LYS:HE2	1.69	0.43
1:A:258:ARG:O	1:A:262:VAL:HG23	2.18	0.43
1:A:455:LEU:HD22	1:A:491:VAL:HG12	2.01	0.43
1:B:309:VAL:O	1:B:310:LYS:HB2	2.18	0.43
4:B:501:COA:H121	4:B:501:COA:C8A	2.49	0.43
1:A:195:GLU:HB3	1:A:381:ILE:HD11	2.00	0.43
1:B:289:LYS:O	5:B:502:GOL:H32	2.19	0.43
1:A:245:ILE:HG22	6:C:101:MYR:H21	2.01	0.43
1:A:355:ARG:HA	1:A:358:LYS:HE2	2.01	0.43
1:A:471:ASP:OD2	1:A:471:ASP:N	2.52	0.43
1:B:120:TRP:HB3	1:B:288:PRO:HG2	2.00	0.43
1:B:352:LEU:HB3	1:B:425:VAL:HG21	2.00	0.43
1:B:306:LEU:HD11	1:B:449:VAL:HB	2.00	0.42
1:A:165:ASP:OD1	1:A:167:GLY:N	2.49	0.42
1:A:203:PRO:HB3	1:A:374:TRP:CZ2	2.54	0.42
1:A:396:ASP:CA	7:A:602:HOH:O	2.57	0.42
1:B:120:TRP:CB	1:B:288:PRO:HG2	2.49	0.42
1:A:139:GLU:HB2	1:A:140:PRO:HD2	2.00	0.42
1:A:159:ASP:OD2	1:A:215:ARG:NE	2.43	0.42
1:A:189:ARG:O	1:A:405:SER:HA	2.20	0.42
1:A:355:ARG:HA	1:A:358:LYS:CE	2.49	0.42
1:B:161:LEU:N	1:B:161:LEU:HD23	2.34	0.42
1:B:164:GLY:H	1:B:202:ARG:NH2	2.17	0.42
1:B:164:GLY:N	1:B:202:ARG:NH2	2.68	0.42
1:A:127:LYS:O	1:A:289:LYS:HD2	2.19	0.42
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.67	0.42
1:A:173:TYR:CE1	1:A:192:TYR:O	2.72	0.42
1:A:489:GLU:H	1:A:489:GLU:CD	2.23	0.42
4:A:501:COA:N6A	4:A:501:COA:S1P	2.94	0.41
1:B:305:LYS:HE2	1:B:448:ASP:OD2	2.20	0.41
1:A:189:ARG:O	1:A:406:THR:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:O	1:B:130:GLU:CG	2.68	0.41
1:A:152:LEU:HD21	1:A:158:TRP:CH2	2.55	0.41
1:A:416:LEU:HD23	1:A:417:LYS:N	2.35	0.41
1:A:245:ILE:HG21	6:C:101:MYR:H51	2.02	0.41
1:A:145:ILE:HB	1:A:273:LEU:HD23	2.01	0.41
1:B:130:GLU:O	1:B:130:GLU:HG3	2.21	0.41
1:A:143:ASP:CB	7:A:606:HOH:O	2.66	0.41
1:A:156:PHE:CA	1:A:217:VAL:HG23	2.51	0.41
1:B:374:TRP:CE2	5:B:503:GOL:H31	2.55	0.41
1:B:387:VAL:O	1:B:394:VAL:HA	2.20	0.41
1:B:397:PHE:CD1	1:B:425:VAL:CG2	3.04	0.41
1:A:311:PHE:CD2	1:A:416:LEU:HD13	2.56	0.41
1:B:304:ARG:CD	1:B:324:MET:CE	2.99	0.40
2:D:8:ILE:HD13	2:D:8:ILE:HA	1.77	0.40
1:A:271:VAL:HG13	1:A:276:ILE:HB	2.03	0.40
1:A:474:LEU:HD13	3:C:4:VAL:HG23	2.03	0.40
1:B:119:PHE:O	1:B:122:THR:OG1	2.33	0.40
1:B:473:ASN:O	2:D:4:VAL:HG11	2.21	0.40

All (3) 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:B:148:GLU:OE2	1:B:388:GLU:OE2[1_565]	1.96	0.24
1:A:148:GLU:OE1	1:A:388:GLU:OE1[1_545]	1.99	0.21
1:A:146:ARG:NH1	1:A:388:GLU:O[1_545]	2.18	0.02

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	373/388 (96%)	360 (96%)	13 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	375/388 (97%)	362 (96%)	13 (4%)	0	100	100
2	D	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
3	C	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
All	All	760/792 (96%)	732 (96%)	28 (4%)	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	337/353 (96%)	334 (99%)	3 (1%)	78	91
1	B	344/353 (98%)	340 (99%)	4 (1%)	71	87
2	D	7/7 (100%)	6 (86%)	1 (14%)	3	5
3	C	7/7 (100%)	6 (86%)	1 (14%)	3	5
All	All	695/720 (96%)	686 (99%)	9 (1%)	69	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	304	ARG
1	B	320	MET
1	B	396	ASP
1	B	496	GLN
2	D	3	LYS
1	A	314	LEU
1	A	396	ASP
1	A	455	LEU
3	C	3	LYS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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
4	COA	A	501	-	41,50,50	0.86	1 (2%)	52,75,75	1.68	12 (23%)
5	GOL	B	502	-	5,5,5	0.84	0	5,5,5	1.04	0
4	COA	B	501	-	39,47,50	0.73	0	49,72,75	1.63	11 (22%)
5	GOL	B	503	-	5,5,5	0.65	0	5,5,5	0.73	0
5	GOL	A	502	-	5,5,5	0.97	0	5,5,5	0.86	0
6	MYR	B	504	-	14,14,15	0.64	0	13,13,15	0.77	0
5	GOL	A	503	-	5,5,5	1.02	0	5,5,5	1.12	0
6	MYR	C	101	3	14,14,15	0.79	1 (7%)	13,13,15	1.83	2 (15%)

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
4	COA	A	501	-	-	12/44/64/64	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	502	-	-	0/4/4/4	-
4	COA	B	501	-	-	14/40/60/64	0/3/3/3
5	GOL	B	503	-	-	2/4/4/4	-
5	GOL	A	502	-	-	0/4/4/4	-
6	MYR	B	504	-	-	1/11/12/13	-
5	GOL	A	503	-	-	0/4/4/4	-
6	MYR	C	101	3	-	5/11/12/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	101	MYR	C2-C1	2.41	1.69	1.46
4	A	501	COA	C2B-C1B	-2.15	1.50	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	101	MYR	O1-C1-C2	-5.72	89.31	126.89
4	B	501	COA	C1B-N9A-C4A	-4.58	118.59	126.64
4	A	501	COA	N3A-C2A-N1A	-3.73	122.84	128.68
4	A	501	COA	CDP-CBP-CCP	3.68	114.24	108.23
4	B	501	COA	C7P-N8P-C9P	-3.51	116.33	122.59
4	A	501	COA	P2A-O3A-P1A	-3.27	121.62	132.83
4	A	501	COA	C7P-C6P-C5P	-3.25	106.95	112.36
4	B	501	COA	C4A-C5A-N7A	-3.23	106.03	109.40
4	B	501	COA	N3A-C2A-N1A	-3.21	123.67	128.68
4	B	501	COA	P2A-O3A-P1A	-3.03	122.44	132.83
4	A	501	COA	C6P-C7P-N8P	-2.92	105.99	111.90
4	A	501	COA	C4A-C5A-N7A	-2.92	106.35	109.40
4	B	501	COA	C6P-C7P-N8P	2.79	117.53	111.90
4	A	501	COA	C6P-C5P-N4P	-2.75	111.78	116.42
4	A	501	COA	C2B-C3B-C4B	2.55	107.75	103.22
4	A	501	COA	O2B-C2B-C1B	-2.55	101.44	110.85
4	B	501	COA	O2B-C2B-C3B	2.48	118.20	111.17
4	A	501	COA	C1B-N9A-C4A	-2.45	122.33	126.64
4	B	501	COA	O4B-C1B-C2B	2.33	110.34	106.93
4	B	501	COA	O9A-P3B-O8A	2.28	116.35	107.64
6	C	101	MYR	C10-C9-C8	-2.27	102.90	114.42
4	A	501	COA	O2A-P1A-O1A	2.18	123.04	112.24
4	B	501	COA	O5A-P2A-O4A	2.03	122.27	112.24
4	A	501	COA	O5P-C5P-N4P	2.01	126.81	123.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	COA	O2B-C2B-C1B	-2.01	103.45	110.85

There are no chirality outliers.

All (34) torsion outliers are listed below:

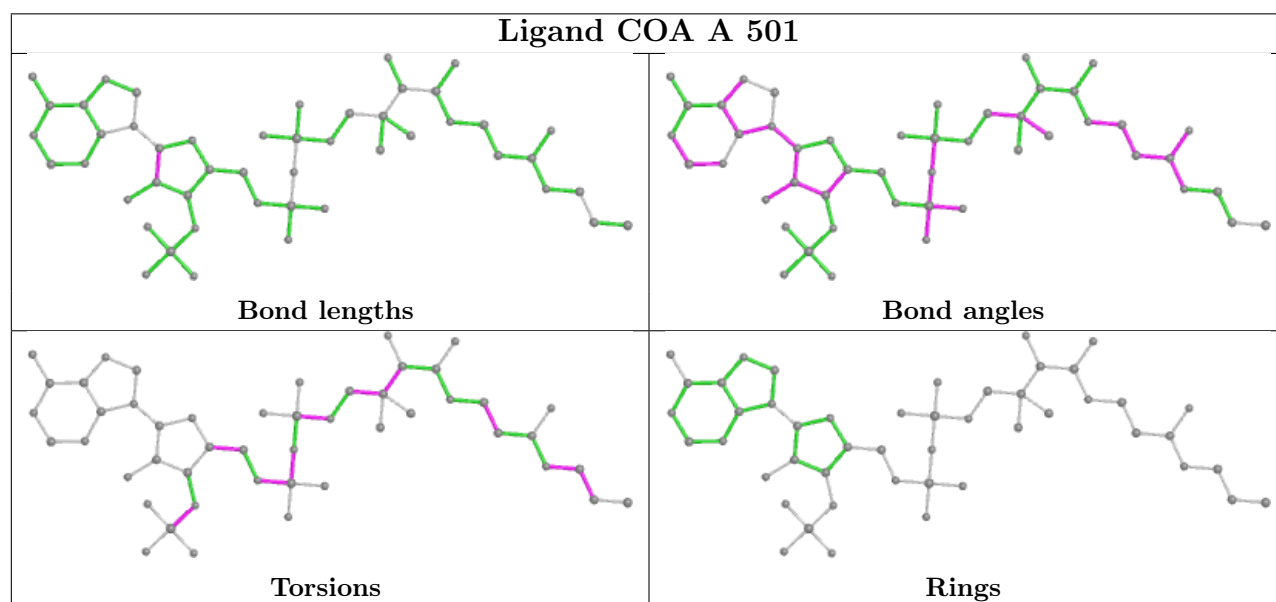
Mol	Chain	Res	Type	Atoms
4	B	501	COA	O4B-C4B-C5B-O5B
4	B	501	COA	C5B-O5B-P1A-O2A
4	B	501	COA	C5B-O5B-P1A-O3A
4	B	501	COA	CAP-CBP-CCP-O6A
4	A	501	COA	C3B-O3B-P3B-O7A
4	A	501	COA	C2P-C3P-N4P-C5P
5	B	503	GOL	O1-C1-C2-C3
6	C	101	MYR	C1-C2-C3-C4
4	B	501	COA	C3B-C4B-C5B-O5B
4	B	501	COA	CDP-CBP-CCP-O6A
6	C	101	MYR	C4-C5-C6-C7
6	C	101	MYR	C2-C3-C4-C5
5	B	503	GOL	O1-C1-C2-O2
4	A	501	COA	C5P-C6P-C7P-N8P
6	C	101	MYR	C3-C4-C5-C6
4	B	501	COA	O9P-C9P-CAP-OAP
4	B	501	COA	CEP-CBP-CCP-O6A
4	A	501	COA	CDP-CBP-CCP-O6A
4	A	501	COA	CEP-CBP-CCP-O6A
4	A	501	COA	OAP-CAP-CBP-CDP
6	C	101	MYR	C9-C10-C11-C12
4	A	501	COA	S1P-C2P-C3P-N4P
4	B	501	COA	O9P-C9P-N8P-C7P
4	A	501	COA	P2A-O3A-P1A-O1A
4	B	501	COA	C4B-C5B-O5B-P1A
4	A	501	COA	CCP-O6A-P2A-O4A
6	B	504	MYR	C4-C5-C6-C7
4	A	501	COA	C3B-C4B-C5B-O5B
4	B	501	COA	P1A-O3A-P2A-O5A
4	B	501	COA	CAP-C9P-N8P-C7P
4	A	501	COA	O4B-C4B-C5B-O5B
4	B	501	COA	N8P-C9P-CAP-OAP
4	A	501	COA	C5B-O5B-P1A-O3A
4	B	501	COA	C5B-O5B-P1A-O1A

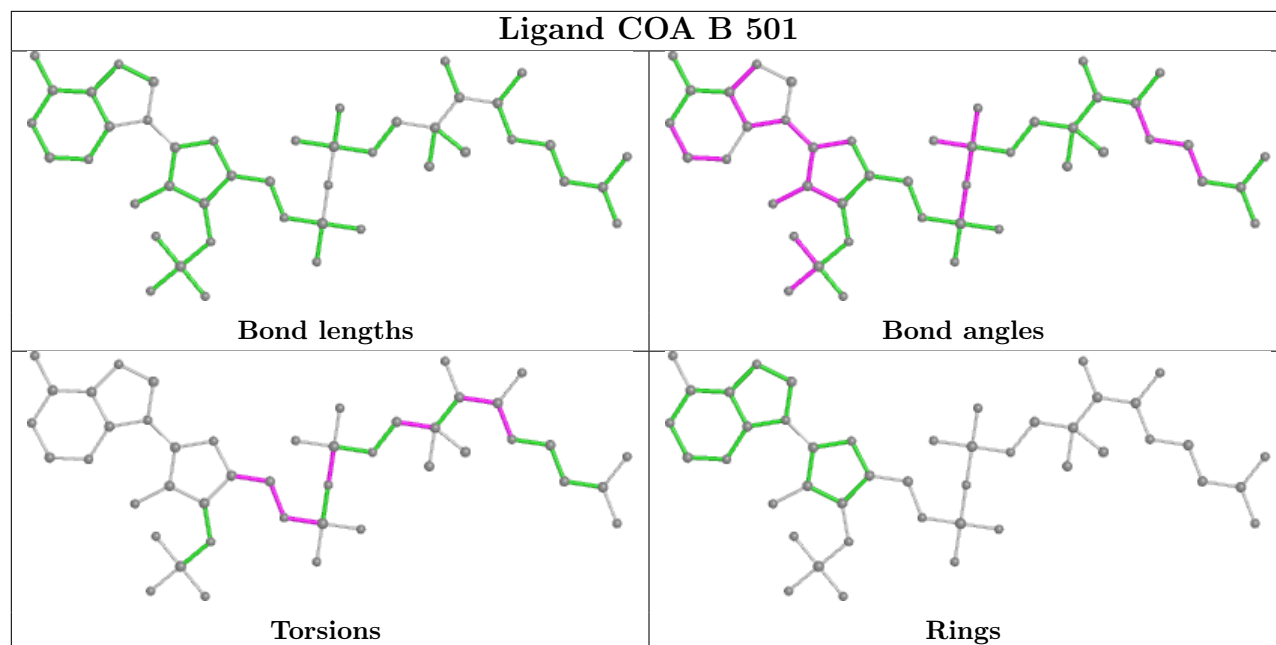
There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	COA	8	0
5	B	502	GOL	1	0
4	B	501	COA	3	0
5	B	503	GOL	1	0
6	B	504	MYR	1	0
6	C	101	MYR	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 [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	377/388 (97%)	0.63	20 (5%) 26 28	43, 55, 74, 118	0
1	B	379/388 (97%)	0.68	18 (4%) 31 34	43, 56, 82, 112	0
2	D	7/8 (87%)	1.18	1 (14%) 2 2	62, 70, 82, 93	0
3	C	8/8 (100%)	1.43	2 (25%) 0 0	59, 64, 71, 139	0
All	All	771/792 (97%)	0.67	41 (5%) 26 28	43, 56, 78, 139	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	ARG	5.5
1	B	166	ARG	4.0
1	A	250	VAL	3.6
1	A	258	ARG	3.5
2	D	9	PHE	3.4
1	A	222	LEU	3.3
1	B	118	GLN	3.3
1	B	327	TYR	3.2
1	A	416	LEU	3.2
1	B	321	GLN	2.9
1	A	133	ASN	2.9
1	A	135	HIS	2.8
1	B	468	GLY	2.8
1	B	323	THR	2.8
1	A	309	VAL	2.7
1	B	317	ASN	2.7
1	A	409	ASN	2.7
1	A	267	ILE	2.7
1	B	285	VAL	2.7
1	A	168	VAL	2.5
1	B	466	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	432	LEU	2.5
1	B	401	TYR	2.4
1	A	472	GLY	2.4
1	B	416	LEU	2.4
1	A	151	THR	2.4
3	C	4	VAL	2.3
1	A	300	SER	2.3
1	A	120	TRP	2.3
3	C	3	LYS	2.2
1	B	329	LEU	2.2
1	B	117	TYR	2.2
1	A	216	VAL	2.2
1	A	297	TRP	2.2
1	A	127	LYS	2.2
1	B	355	ARG	2.2
1	B	307	ILE	2.2
1	B	120	TRP	2.1
1	B	435	MET	2.0
1	A	131	VAL	2.0
1	A	438	ALA	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 monosaccharides 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.

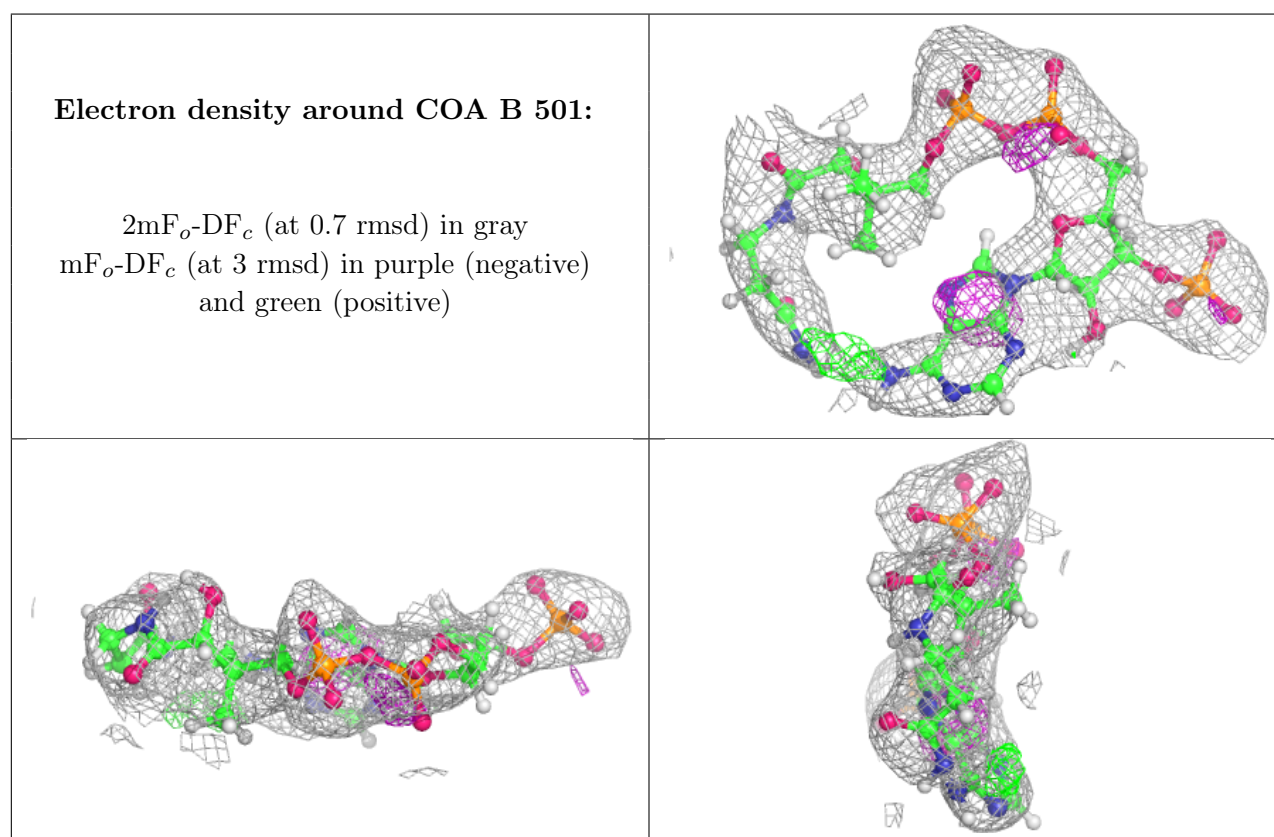
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MYR	B	504	15/16	0.71	0.34	21,62,121,129	0
6	MYR	C	101	15/16	0.80	0.35	30,30,30,30	0
4	COA	B	501	45/48	0.81	0.24	48,79,95,101	0

Continued on next page...

Continued from previous page...

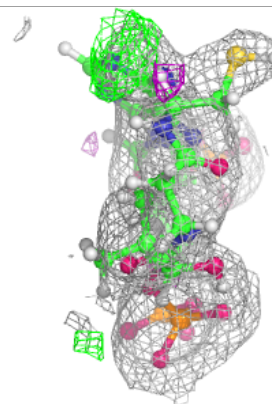
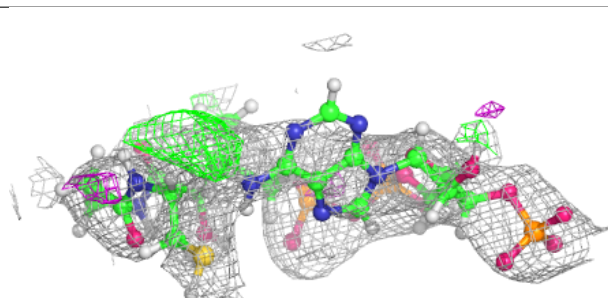
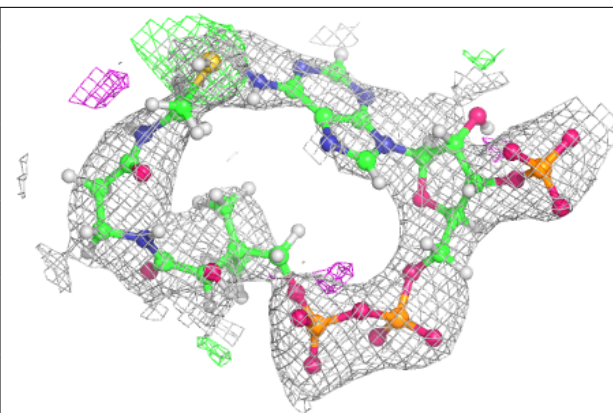
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	COA	A	501	48/48	0.81	0.24	52,78,196,245	0
5	GOL	B	503	6/6	0.87	0.23	49,61,73,76	0
5	GOL	A	502	6/6	0.87	0.27	53,56,68,70	0
5	GOL	B	502	6/6	0.89	0.24	53,60,72,75	0
5	GOL	A	503	6/6	0.89	0.44	51,58,66,69	0

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 A 501:

$2mF_o-DF_c$ (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.