



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:19 PM UTC

PDB ID : 7QOA / pdb_00007qoa
Title : Structure of CodB, a cytosine transporter in an outward-facing conformation
Authors : Hatton, C.E.; Cameron, A.D.
Deposited on : 2021-12-23
Resolution : 2.40 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

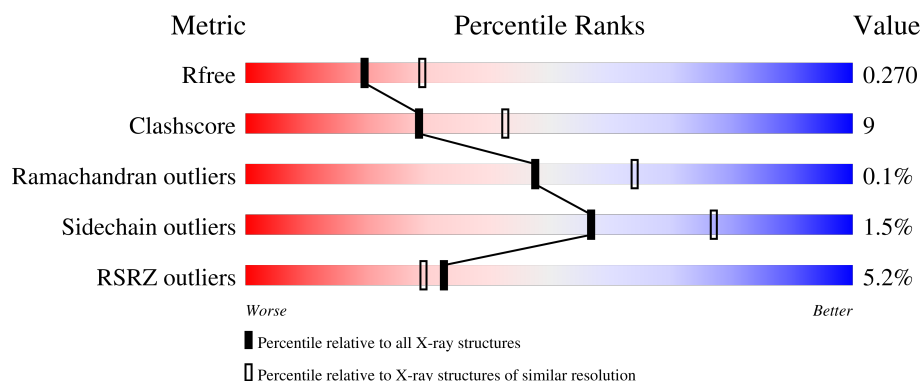
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	423	 4% 73% 21% 5%
1	B	423	 5% 77% 18% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6083 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.

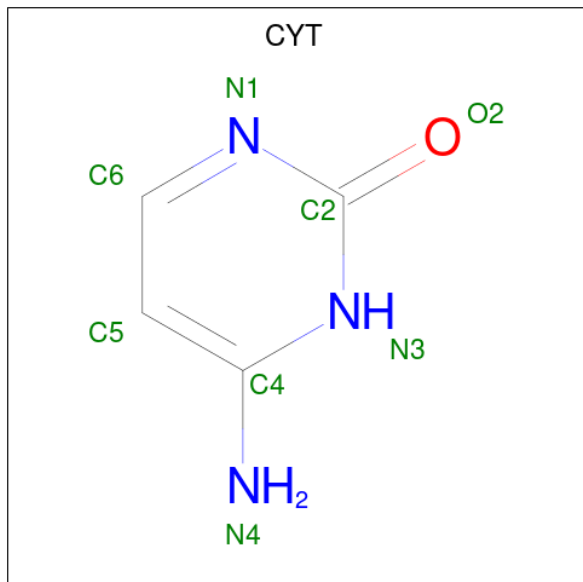
- Molecule 1 is a protein called Cytosine permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			2947	1954	470	510	13			
1	B	400	Total	C	N	O	S	0	0	0
			2936	1948	466	509	13			

There are 24 discrepancies between the modelled and reference sequences:

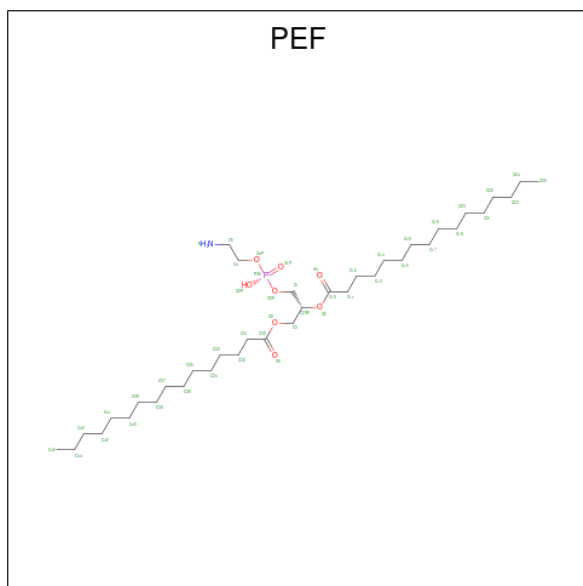
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	VAL	ILE	conflict	UNP A0A857SHB2
A	184	ASN	ALA	conflict	UNP A0A857SHB2
A	188	THR	ALA	conflict	UNP A0A857SHB2
A	309	VAL	ILE	conflict	UNP A0A857SHB2
A	312	VAL	LEU	conflict	UNP A0A857SHB2
A	417	SER	-	expression tag	UNP A0A857SHB2
A	418	LEU	-	expression tag	UNP A0A857SHB2
A	419	GLU	-	expression tag	UNP A0A857SHB2
A	420	VAL	-	expression tag	UNP A0A857SHB2
A	421	LEU	-	expression tag	UNP A0A857SHB2
A	422	PHE	-	expression tag	UNP A0A857SHB2
A	423	GLN	-	expression tag	UNP A0A857SHB2
B	152	VAL	ILE	conflict	UNP A0A857SHB2
B	184	ASN	ALA	conflict	UNP A0A857SHB2
B	188	THR	ALA	conflict	UNP A0A857SHB2
B	309	VAL	ILE	conflict	UNP A0A857SHB2
B	312	VAL	LEU	conflict	UNP A0A857SHB2
B	417	SER	-	expression tag	UNP A0A857SHB2
B	418	LEU	-	expression tag	UNP A0A857SHB2
B	419	GLU	-	expression tag	UNP A0A857SHB2
B	420	VAL	-	expression tag	UNP A0A857SHB2
B	421	LEU	-	expression tag	UNP A0A857SHB2
B	422	PHE	-	expression tag	UNP A0A857SHB2
B	423	GLN	-	expression tag	UNP A0A857SHB2

- Molecule 2 is 6-AMINOPYRIMIDIN-2(1H)-ONE (CCD ID: CYT) (formula: $C_4H_5N_3O$) (labeled as "Ligand of Interest" by depositor).



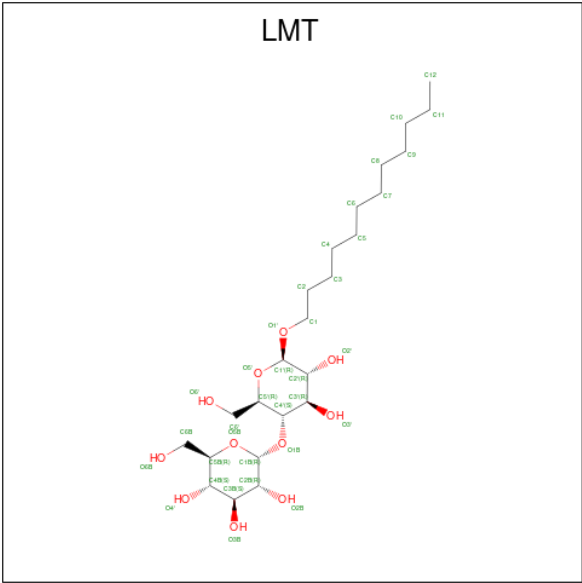
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	3	1		
2	B	1	Total	C	N	O	0	0
			8	4	3	1		

- Molecule 3 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



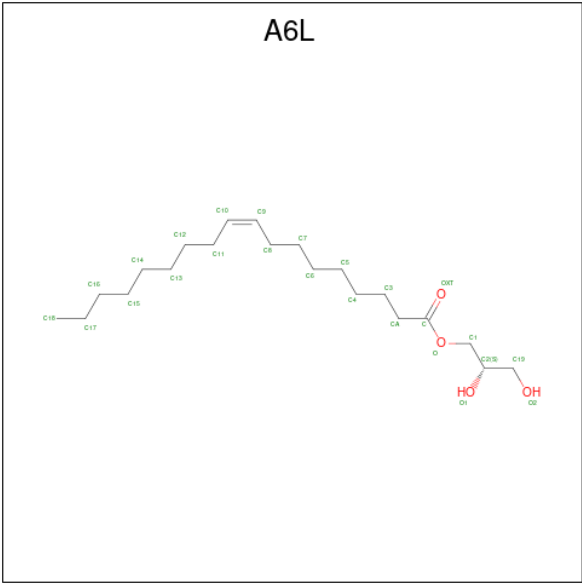
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			23	23		

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 5 is 2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: A6L) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 9 9	0	0
5	A	1	Total C 11 11	0	0
5	B	1	Total C O 8 7 1	0	0
5	B	1	Total C O 15 14 1	0	0
5	B	1	Total C 15 15	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0
6	B	1	Total Na 1 1	0	0

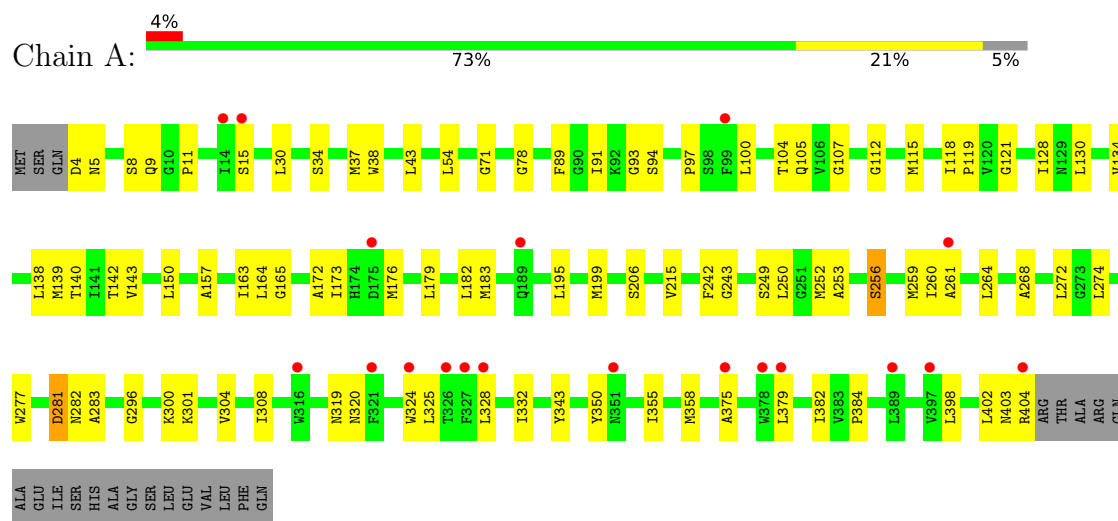
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	36	Total O 36 36	0	0
7	B	30	Total O 30 30	0	0

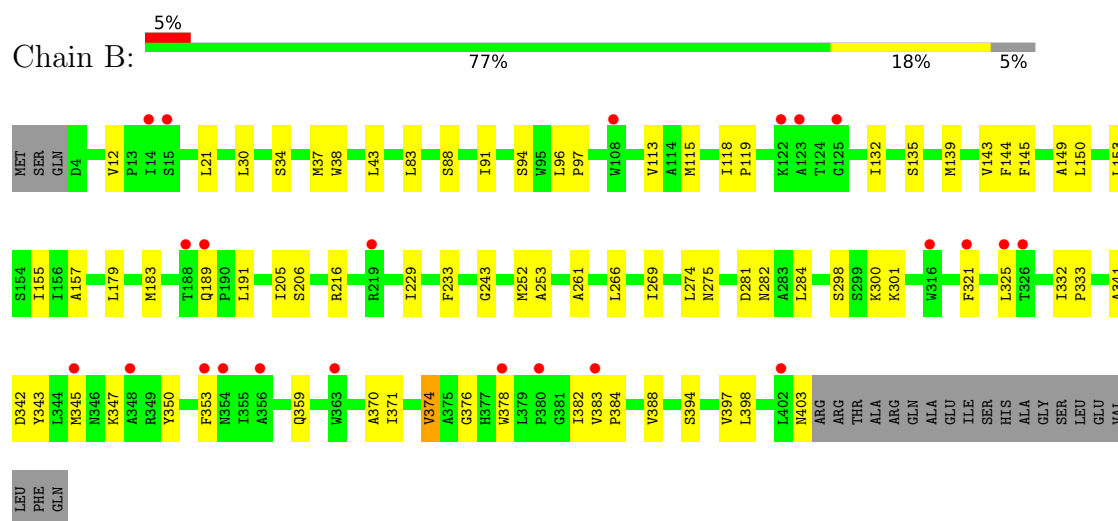
3 Residue-property plots [i](#)

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: Cytosine permease



• Molecule 1: Cytosine permease



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.25Å 209.03Å 102.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.16 – 2.40 73.16 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (73.16-2.40) 99.4 (73.16-2.40)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.218 , 0.265 (Not available) , 0.270	Depositor DCC
R_{free} test set	2210 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6083	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: LMT, PEF, CYT, NA, A6L

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	0.34	0/3015	0.52	0/4119
1	B	0.32	0/3004	0.48	0/4105
All	All	0.33	0/6019	0.50	0/8224

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2947	0	3060	63	0
1	B	2936	0	3047	43	0
2	A	8	0	4	1	0
2	B	8	0	4	0	0
3	A	23	0	38	1	0
4	A	35	0	46	12	0
5	A	20	0	0	0	0
5	B	38	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	36	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	30	0	0	2	0
All	All	6083	0	6199	107	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 9.

All (107) 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:34:SER:HA	1:A:37:MET:HE2	1.63	0.81
1:B:150:LEU:HD22	1:B:281:ASP:HB3	1.63	0.79
1:A:5:ASN:HB2	1:A:300:LYS:HE2	1.64	0.79
1:B:179:LEU:HG	1:B:183:MET:HE2	1.66	0.78
1:A:105:GLN:HE22	2:A:501:CYT:H42	1.32	0.76
1:B:143:VAL:HG21	1:B:284:LEU:HB3	1.67	0.75
1:A:355:ILE:HA	1:A:358:MET:HE2	1.68	0.75
1:A:112:GLY:HA2	1:A:115:MET:HG3	1.73	0.70
1:A:253:ALA:H	4:A:503:LMT:H6D	1.61	0.66
1:A:4:ASP:OD2	1:A:8:SER:OG	2.14	0.66
1:A:30:LEU:HB2	1:A:282:ASN:HD22	1.63	0.63
1:A:195:LEU:O	1:A:199:MET:HG3	2.00	0.62
1:B:341:ALA:O	1:B:345:MET:HG2	2.01	0.61
1:A:100:LEU:O	1:A:104:THR:HG23	2.01	0.61
1:A:382:ILE:HG22	1:A:384:PRO:HD2	1.85	0.58
1:B:34:SER:HA	1:B:37:MET:HE3	1.85	0.58
1:B:382:ILE:HG22	1:B:384:PRO:HD2	1.85	0.58
1:B:38:TRP:CH2	1:B:115:MET:HE3	2.39	0.57
1:A:118:ILE:HA	1:A:128:ILE:HD12	1.88	0.56
1:A:260:ILE:HD11	4:A:503:LMT:H91	1.87	0.56
1:B:205:ILE:HG12	1:B:333:PRO:HG3	1.87	0.56
1:B:376:GLY:O	7:B:601:HOH:O	2.18	0.56
1:A:252:MET:HE1	1:A:261:ALA:HB2	1.88	0.54
1:A:256:SER:HB3	4:A:503:LMT:H62	1.89	0.54
1:B:145:PHE:HB2	1:B:149:ALA:HB2	1.89	0.54
1:A:107:GLY:HA3	1:A:325:LEU:HD21	1.89	0.54
1:A:38:TRP:HB3	4:A:503:LMT:H1B	1.90	0.53
1:B:321:PHE:HD2	1:B:325:LEU:HG	1.74	0.52
1:A:139:MET:HG2	1:A:277:TRP:CD1	2.44	0.52
1:A:91:ILE:HG12	1:A:358:MET:HE3	1.92	0.52
1:A:398:LEU:HB3	1:A:402:LEU:HD23	1.90	0.52
1:A:301:LYS:NZ	7:A:606:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:PHE:CE1	1:B:300:LYS:HD3	2.45	0.51
1:A:11:PRO:HA	1:A:78:GLY:O	2.11	0.51
1:A:173:ILE:HA	1:A:176:MET:HE2	1.93	0.50
1:A:250:LEU:HB3	1:A:252:MET:HE2	1.93	0.50
1:B:135:SER:O	1:B:139:MET:HG3	2.13	0.49
1:A:157:ALA:HA	1:A:274:LEU:HD13	1.94	0.49
1:B:96:LEU:HB2	1:B:97:PRO:HD3	1.95	0.49
1:B:91:ILE:HG13	1:B:359:GLN:O	2.13	0.48
1:B:94:SER:O	1:B:97:PRO:HD2	2.13	0.48
1:A:15:SER:OG	7:A:601:HOH:O	2.20	0.48
1:B:189:GLN:N	1:B:189:GLN:OE1	2.47	0.48
1:A:179:LEU:O	1:A:183:MET:HG3	2.13	0.48
1:B:298:SER:HB3	1:B:301:LYS:HB2	1.96	0.47
1:A:403:ASN:O	1:A:404:ARG:HD3	2.14	0.47
1:B:397:VAL:HG12	1:B:398:LEU:HD23	1.97	0.47
1:B:229:ILE:O	1:B:233:PHE:HB3	2.14	0.47
1:A:324:TRP:O	1:A:328:LEU:HG	2.15	0.46
1:B:191:LEU:O	7:B:602:HOH:O	2.21	0.46
1:B:333:PRO:HB3	1:B:388:VAL:HG23	1.97	0.46
1:A:176:MET:HE1	1:A:182:LEU:HB2	1.98	0.46
1:A:259:MET:HB2	1:A:268:ALA:HB2	1.98	0.46
1:B:157:ALA:HB1	1:B:274:LEU:HB3	1.96	0.46
1:B:206:SER:HA	1:B:332:ILE:HG21	1.98	0.46
1:A:138:LEU:O	1:A:142:THR:HG23	2.16	0.45
1:B:88:SER:HB3	1:B:342:ASP:CB	2.45	0.45
4:A:503:LMT:H6D	7:A:611:HOH:O	2.16	0.45
1:A:38:TRP:CD1	1:A:38:TRP:N	2.82	0.45
1:A:172:ALA:HB1	1:A:249:SER:OG	2.16	0.45
1:A:89:PHE:O	1:A:93:GLY:HA3	2.16	0.45
1:A:119:PRO:HG3	4:A:503:LMT:H21	1.98	0.45
1:B:113:VAL:HG12	1:B:132:ILE:HD13	1.99	0.45
1:A:38:TRP:CZ2	4:A:503:LMT:H2'	2.52	0.44
1:B:374:VAL:O	1:B:378:TRP:HD1	2.00	0.44
1:A:150:LEU:CD2	1:A:281:ASP:HB3	2.47	0.44
1:A:150:LEU:HD22	1:A:281:ASP:HB3	1.98	0.44
1:A:172:ALA:O	1:A:176:MET:HB2	2.17	0.44
1:B:343:TYR:HA	1:B:350:TYR:CE1	2.52	0.44
1:A:243:GLY:HA2	1:A:253:ALA:O	2.17	0.44
1:B:347:LYS:HE3	1:B:347:LYS:HB2	1.63	0.44
1:A:304:VAL:O	1:A:308:ILE:HG12	2.17	0.44
1:B:266:LEU:O	1:B:269:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLN:NE2	1:A:296:GLY:HA2	2.33	0.44
1:A:343:TYR:HA	1:A:350:TYR:CE1	2.52	0.43
1:A:256:SER:OG	1:A:268:ALA:O	2.33	0.43
4:A:503:LMT:H52	4:A:503:LMT:H22	1.74	0.43
1:B:370:ALA:O	1:B:374:VAL:HG13	2.19	0.43
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.87	0.43
1:A:105:GLN:HE21	1:A:283:ALA:HA	1.84	0.43
1:B:359:GLN:NE2	1:B:403:ASN:HD21	2.17	0.43
1:A:164:LEU:HD11	1:B:155:ILE:HB	2.01	0.43
1:A:253:ALA:H	4:A:503:LMT:C6'	2.30	0.42
1:B:383:VAL:HB	1:B:384:PRO:HD3	2.01	0.42
1:A:130:LEU:O	1:A:134:VAL:HG23	2.19	0.42
1:A:253:ALA:HB3	4:A:503:LMT:H6E	2.00	0.42
3:A:502:PEF:H352	3:A:502:PEF:H122	2.00	0.42
1:A:121:GLY:HA3	1:A:128:ILE:HD13	2.02	0.42
1:B:118:ILE:HB	1:B:119:PRO:HD3	2.02	0.42
1:A:71:GLY:HA2	1:A:215:VAL:HG21	2.02	0.41
1:B:83:LEU:HD22	1:B:353:PHE:HZ	1.84	0.41
1:A:206:SER:HA	1:A:332:ILE:HG21	2.03	0.41
1:A:375:ALA:HB1	1:A:379:LEU:HD12	2.02	0.41
1:B:252:MET:HE1	1:B:261:ALA:HB2	2.03	0.41
1:B:12:VAL:HG21	1:B:216:ARG:HG3	2.03	0.41
1:A:176:MET:HE2	1:A:176:MET:HB3	1.75	0.41
1:A:272:LEU:HD22	4:A:503:LMT:C7	2.50	0.41
1:B:371:ILE:HD12	1:B:394:SER:HB2	2.03	0.41
1:A:119:PRO:HB2	4:A:503:LMT:H72	2.03	0.41
1:A:140:THR:O	1:A:143:VAL:HG12	2.20	0.41
1:A:165:GLY:HA3	1:A:242:PHE:CE2	2.55	0.41
1:B:30:LEU:HB2	1:B:282:ASN:ND2	2.36	0.41
1:A:94:SER:C	1:A:97:PRO:HD2	2.45	0.40
1:B:243:GLY:HA2	1:B:253:ALA:O	2.21	0.40
1:A:34:SER:HA	1:A:37:MET:CE	2.44	0.40
1:A:264:LEU:HD22	1:B:21:LEU:HD23	2.03	0.40
1:B:398:LEU:HD23	1:B:398:LEU:HA	1.87	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	399/423 (94%)	389 (98%)	9 (2%)	1 (0%)	36	50
1	B	398/423 (94%)	391 (98%)	7 (2%)	0	100	100
All	All	797/846 (94%)	780 (98%)	16 (2%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	ASN

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	306/324 (94%)	301 (98%)	5 (2%)	55	76
1	B	305/324 (94%)	301 (99%)	4 (1%)	61	80
All	All	611/648 (94%)	602 (98%)	9 (2%)	57	77

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

Mol	Chain	Res	Type
1	A	43	LEU
1	A	163	ILE
1	A	256	SER
1	A	281	ASP
1	A	320	ASN

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Mol	Chain	Res	Type
1	B	43	LEU
1	B	153	LEU
1	B	275	ASN
1	B	374	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	346	ASN
1	B	6	ASN
1	B	359	GLN
1	B	403	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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
5	A6L	B	503	-	13,13,24	0.29	0	12,12,25	1.07	1 (8%)
2	CYT	B	501	-	7,8,8	1.61	2 (28%)	7,10,10	3.40	3 (42%)
5	A6L	A	505	-	10,10,24	0.54	0	9,9,25	0.68	0
4	LMT	A	503	-	36,36,36	1.18	2 (5%)	47,47,47	1.41	6 (12%)
2	CYT	A	501	-	7,8,8	1.66	2 (28%)	7,10,10	3.51	3 (42%)
5	A6L	A	504	-	8,8,24	0.38	0	7,7,25	0.75	0
5	A6L	B	504	-	14,14,24	0.38	0	13,13,25	0.61	0
3	PEF	A	502	-	21,21,46	0.36	0	19,19,51	0.84	0
5	A6L	B	502	-	7,7,24	0.27	0	6,6,25	1.01	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
5	A6L	B	503	-	-	4/11/11/24	-
2	CYT	B	501	-	-	-	0/1/1/1
5	A6L	A	505	-	-	3/8/8/24	-
4	LMT	A	503	-	-	12/21/61/61	0/2/2/2
2	CYT	A	501	-	-	-	0/1/1/1
5	A6L	A	504	-	-	2/6/6/24	-
5	A6L	B	504	-	-	6/12/12/24	-
3	PEF	A	502	-	-	9/17/17/50	-
5	A6L	B	502	-	-	2/5/5/24	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	LMT	O5'-C1'	3.75	1.51	1.41
4	A	503	LMT	O5B-C1B	3.53	1.50	1.41
2	A	501	CYT	C5-C4	2.92	1.44	1.39
2	B	501	CYT	C5-C4	2.87	1.43	1.39
2	B	501	CYT	C5-C6	-2.33	1.34	1.39
2	A	501	CYT	C5-C6	-2.31	1.34	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	CYT	C5-C4-N3	6.66	121.83	118.04
2	B	501	CYT	C5-C4-N3	6.49	121.73	118.04
2	A	501	CYT	C5-C6-N1	-4.70	121.03	124.75
2	B	501	CYT	C5-C6-N1	-4.54	121.16	124.75
2	A	501	CYT	C5-C4-N4	-3.89	120.09	123.88
4	A	503	LMT	C4B-C3B-C2B	3.85	117.58	110.83
2	B	501	CYT	C5-C4-N4	-3.72	120.26	123.88
4	A	503	LMT	C1B-O1B-C4'	-3.46	109.78	117.98
4	A	503	LMT	C1B-C2B-C3B	3.31	116.98	110.01
4	A	503	LMT	O5B-C1B-C2B	2.53	115.57	110.37
4	A	503	LMT	C3B-C4B-C5B	2.28	114.36	110.23
4	A	503	LMT	O5'-C1'-C2'	2.21	114.91	110.37
5	B	503	A6L	C6-C7-C8	-2.05	104.02	113.86

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	LMT	O5'-C1'-O1'-C1
4	A	503	LMT	O5'-C5'-C6'-O6'
5	B	504	A6L	C5-C6-C7-C8
4	A	503	LMT	C4'-C5'-C6'-O6'
4	A	503	LMT	C2'-C1'-O1'-C1
4	A	503	LMT	C2-C3-C4-C5
4	A	503	LMT	C1-C2-C3-C4
5	B	502	A6L	C4-C3-CA-C
3	A	502	PEF	C15-C16-C17-C18
4	A	503	LMT	C6-C7-C8-C9
5	B	503	A6L	C3-C4-C5-C6
4	A	503	LMT	C5-C6-C7-C8
3	A	502	PEF	C34-C35-C36-C37
5	B	504	A6L	C6-C7-C8-C9
4	A	503	LMT	O1'-C1-C2-C3
5	A	505	A6L	C14-C15-C16-C17
3	A	502	PEF	C12-C13-C14-C15
5	B	504	A6L	C13-C14-C15-C16
4	A	503	LMT	C4-C5-C6-C7
3	A	502	PEF	C36-C37-C38-C39
3	A	502	PEF	C35-C36-C37-C38
5	B	503	A6L	C10-C11-C12-C13
5	A	505	A6L	C15-C16-C17-C18
5	B	504	A6L	C15-C16-C17-C18
3	A	502	PEF	C17-C18-C19-C20

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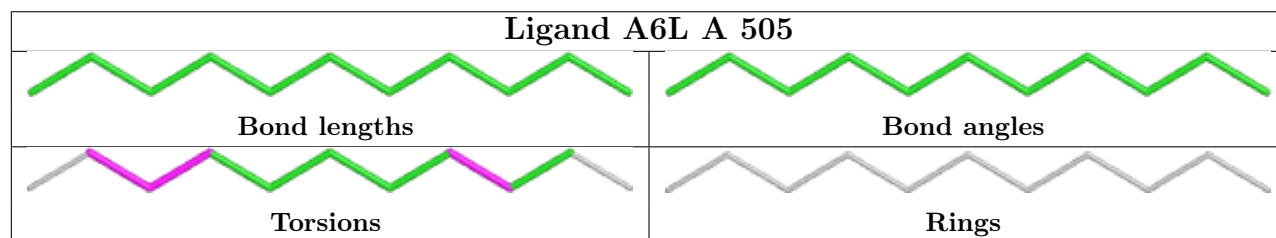
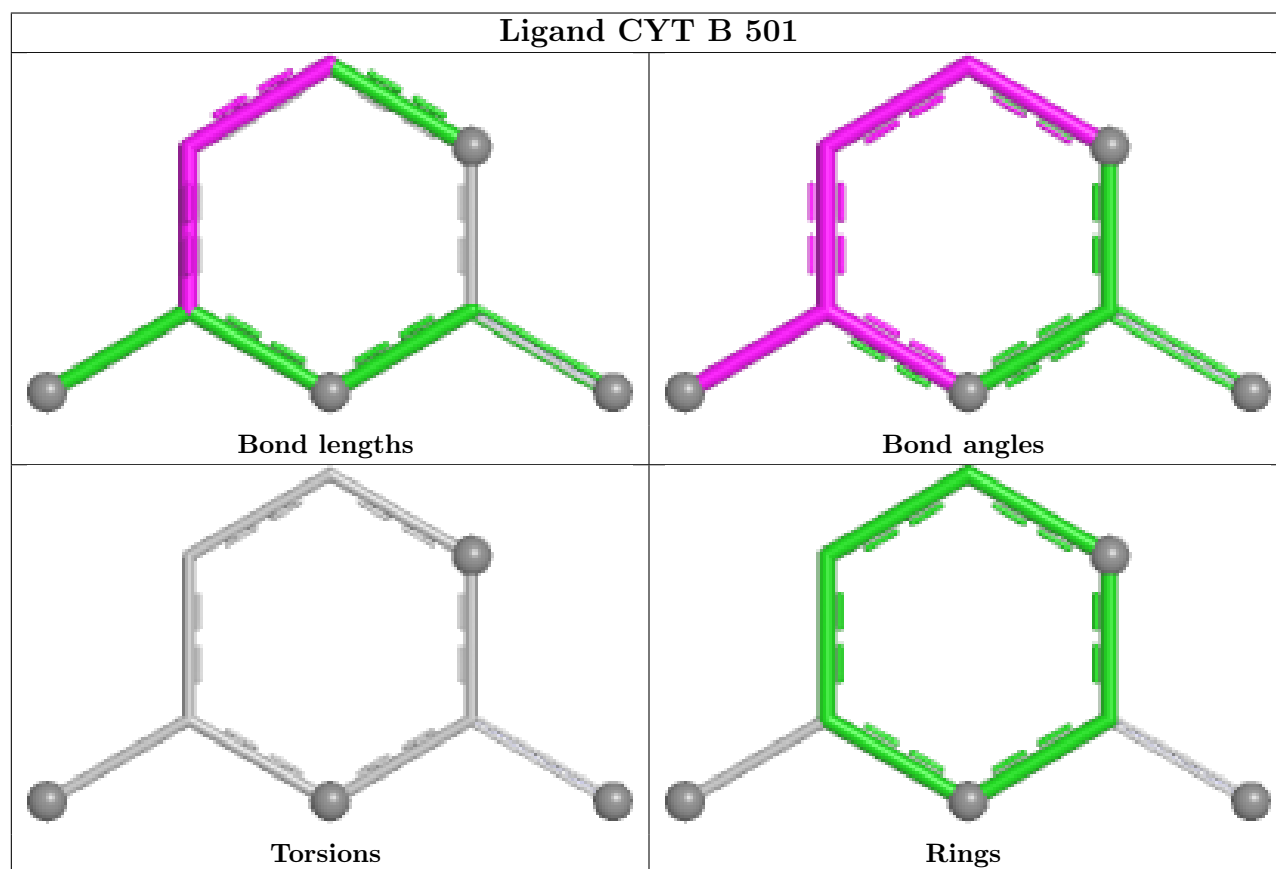
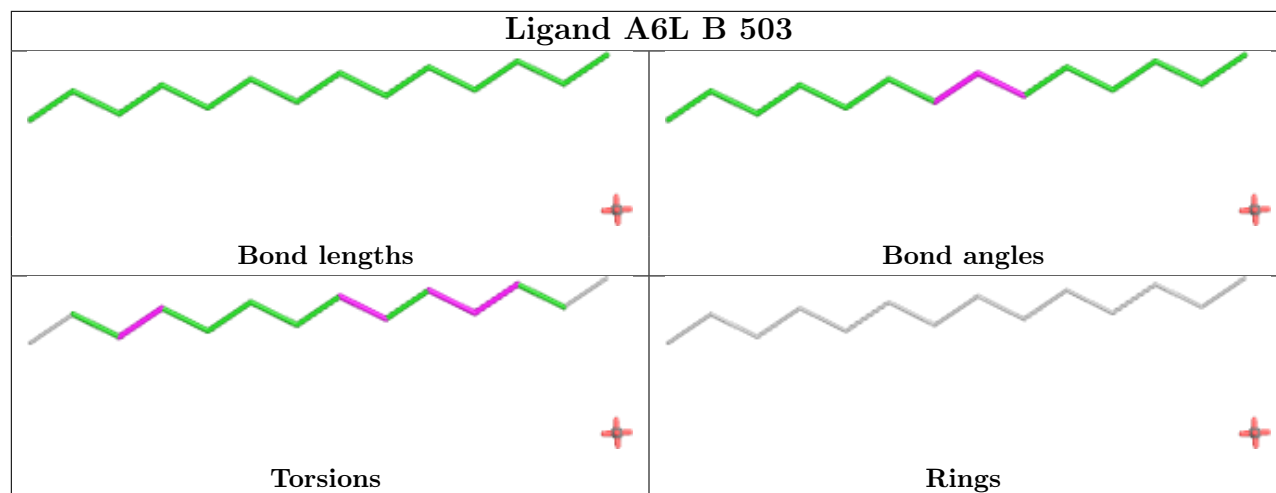
Mol	Chain	Res	Type	Atoms
3	A	502	PEF	C16-C17-C18-C19
4	A	503	LMT	C11-C10-C9-C8
5	B	503	A6L	C5-C6-C7-C8
5	A	504	A6L	C10-C11-C12-C13
5	B	502	A6L	C4-C5-C6-C7
4	A	503	LMT	C7-C8-C9-C10
5	A	504	A6L	C15-C16-C17-C18
3	A	502	PEF	C14-C15-C16-C17
5	A	505	A6L	C9-C10-C11-C12
5	B	504	A6L	C7-C8-C9-C10
5	B	503	A6L	CA-C3-C4-C5
3	A	502	PEF	C10-C11-C12-C13
5	B	504	A6L	C11-C12-C13-C14

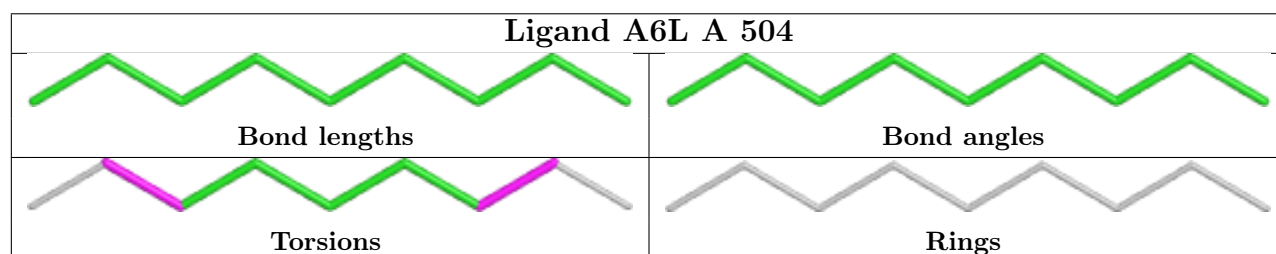
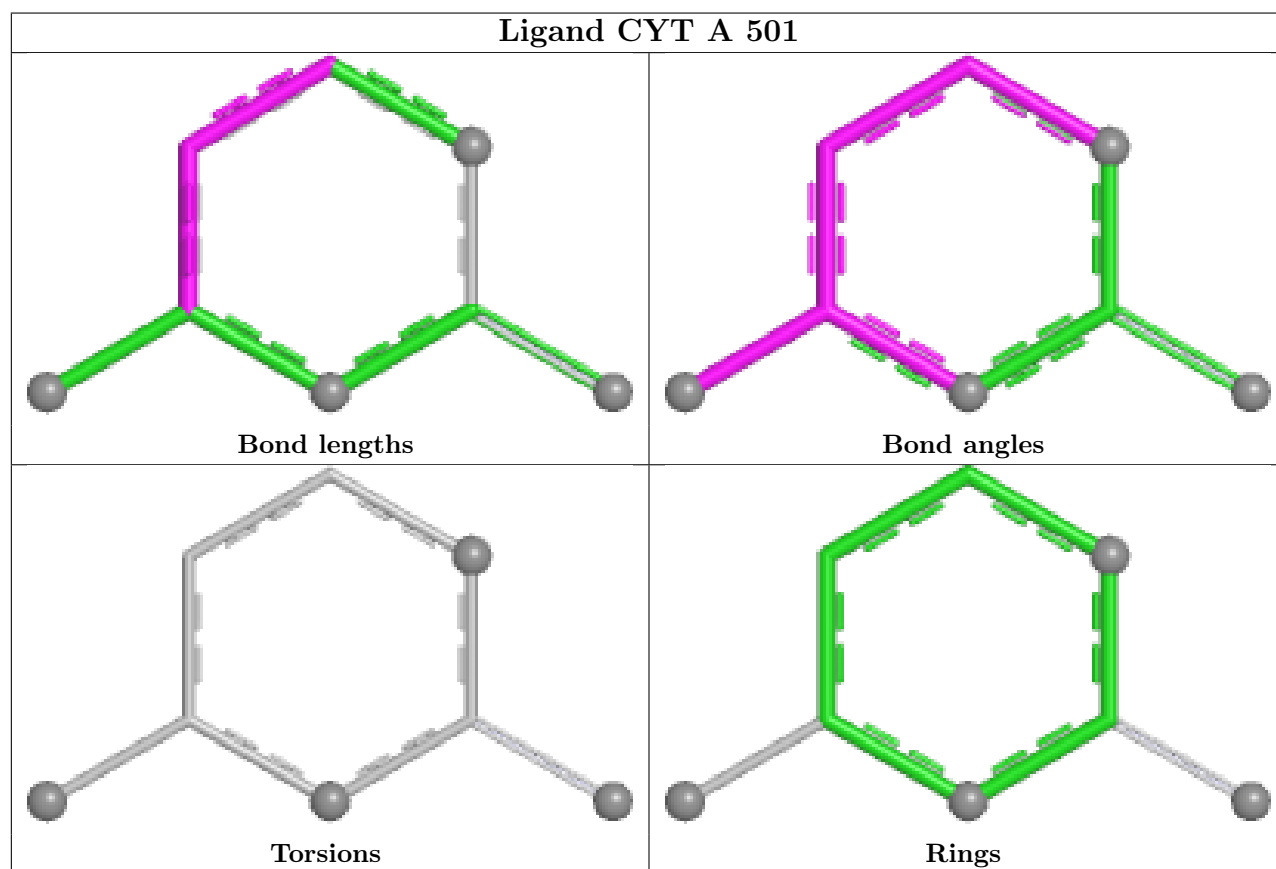
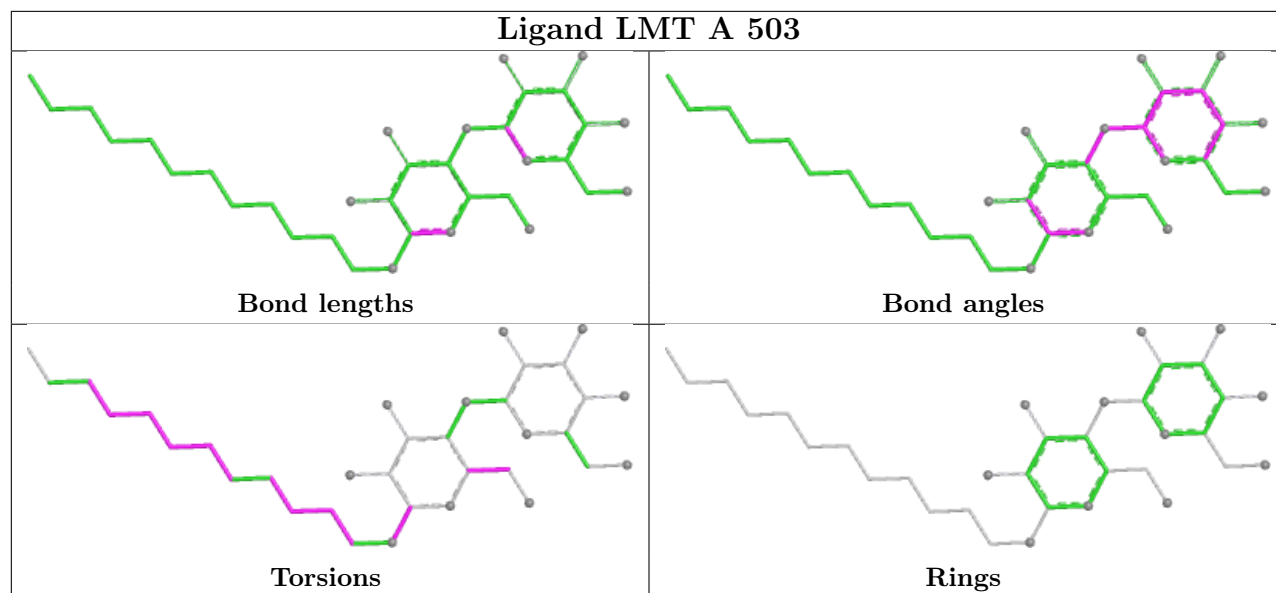
There are no ring outliers.

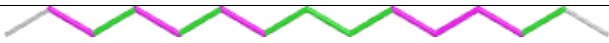
3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	LMT	12	0
2	A	501	CYT	1	0
3	A	502	PEF	1	0

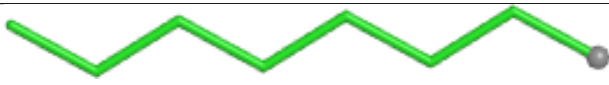
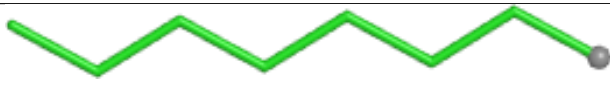
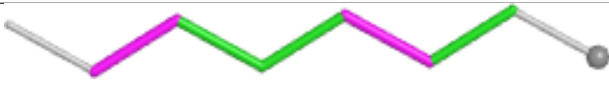
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.





Ligand A6L B 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEF A 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A6L B 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	401/423 (94%)	0.38	19 (4%) 36 32	31, 44, 64, 84	0
1	B	400/423 (94%)	0.45	23 (5%) 29 25	31, 46, 68, 81	0
All	All	801/846 (94%)	0.41	42 (5%) 33 29	31, 45, 66, 84	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	188	THR	5.4
1	A	321	PHE	5.1
1	B	356	ALA	5.0
1	B	122	LYS	4.3
1	B	123	ALA	4.2
1	B	14	ILE	4.0
1	A	326	THR	4.0
1	B	189	GLN	3.8
1	A	328	LEU	3.7
1	B	348	ALA	3.5
1	A	379	LEU	3.2
1	B	378	TRP	3.2
1	A	324	TRP	3.1
1	A	378	TRP	3.1
1	A	14	ILE	2.9
1	A	327	PHE	2.9
1	B	219	ARG	2.8
1	A	404	ARG	2.8
1	B	354	ASN	2.7
1	B	125	GLY	2.7
1	A	397	VAL	2.6
1	B	321	PHE	2.5
1	B	402	LEU	2.5
1	A	261	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	325	LEU	2.5
1	A	351	ASN	2.4
1	A	175	ASP	2.3
1	B	15	SER	2.3
1	A	15	SER	2.3
1	B	108	TRP	2.3
1	A	99	PHE	2.3
1	B	316	TRP	2.2
1	A	389	LEU	2.2
1	B	326	THR	2.2
1	B	353	PHE	2.2
1	B	380	PRO	2.1
1	B	383	VAL	2.1
1	A	316	TRP	2.1
1	A	189	GLN	2.1
1	A	375	ALA	2.1
1	B	345	MET	2.1
1	B	363	TRP	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
5	A6L	A	505	11/25	0.66	0.32	42,53,62,63	0
4	LMT	A	503	35/35	0.73	0.19	52,64,70,75	0
5	A6L	B	504	15/25	0.73	0.23	47,61,69,70	0
3	PEF	A	502	23/47	0.77	0.28	45,54,62,69	0
5	A6L	B	503	15/25	0.80	0.22	51,55,60,83	0

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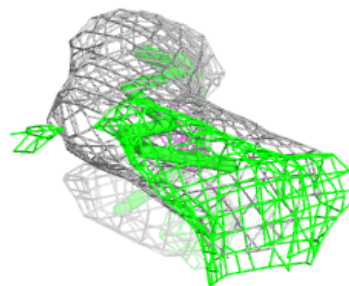
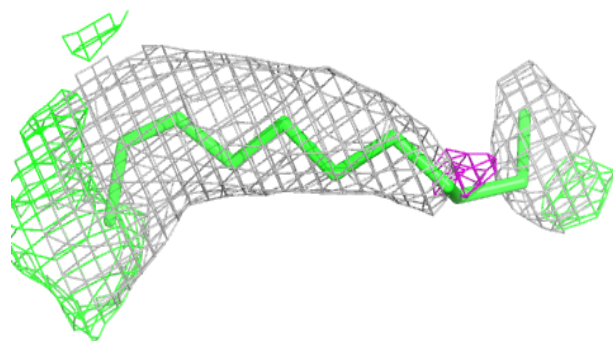
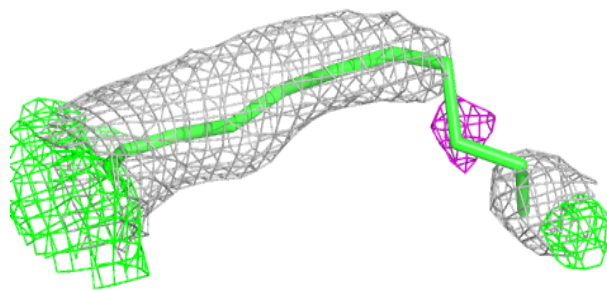
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	A6L	A	504	9/25	0.84	0.21	43,48,54,59	0
5	A6L	B	502	8/25	0.84	0.18	44,46,55,57	0
2	CYT	B	501	8/8	0.89	0.12	45,48,52,52	0
6	NA	A	506	1/1	0.93	0.09	35,35,35,35	0
2	CYT	A	501	8/8	0.96	0.07	35,39,41,41	0
6	NA	B	505	1/1	0.98	0.08	35,35,35,35	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.

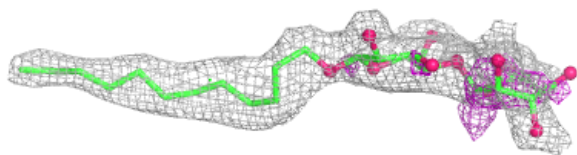
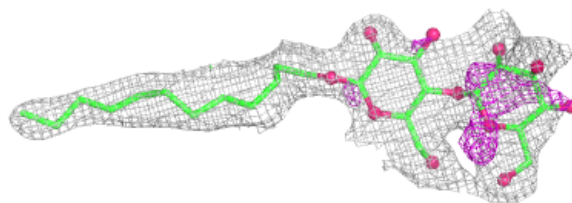
Electron density around A6L A 505:

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

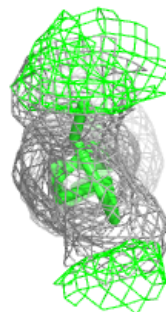
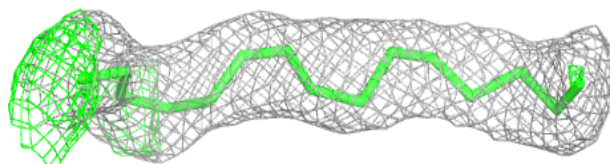
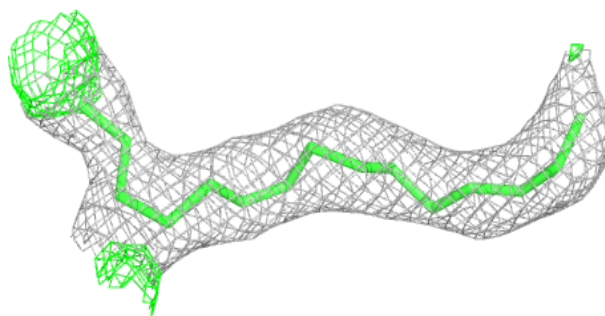


Electron density around LMT A 503:

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

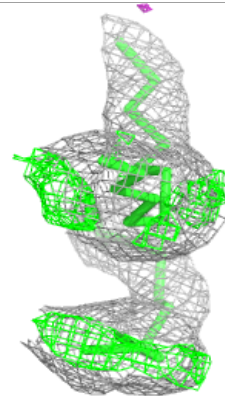
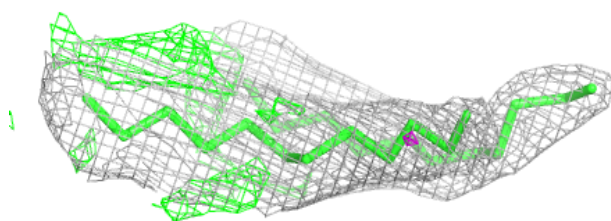
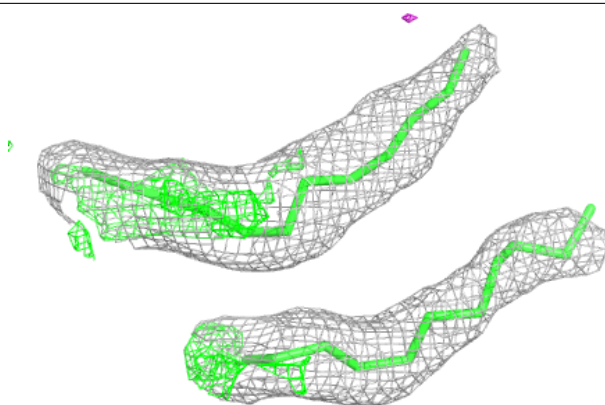
**Electron density around A6L B 504:**

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



Electron density around PEF A 502:

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

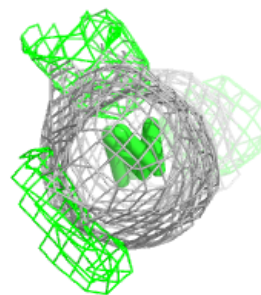
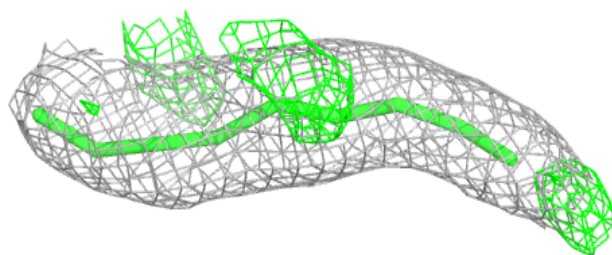
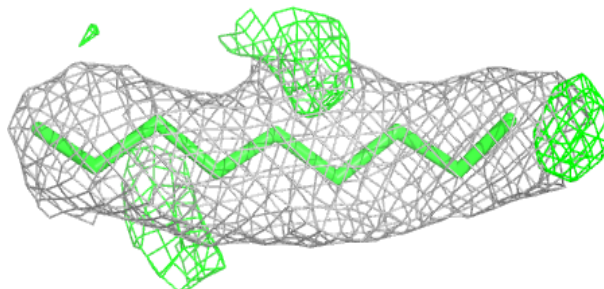
**Electron density around A6L B 503:**

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

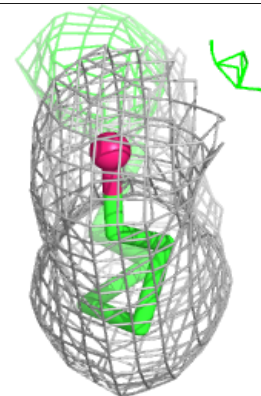
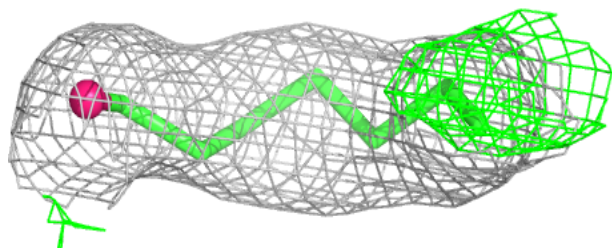
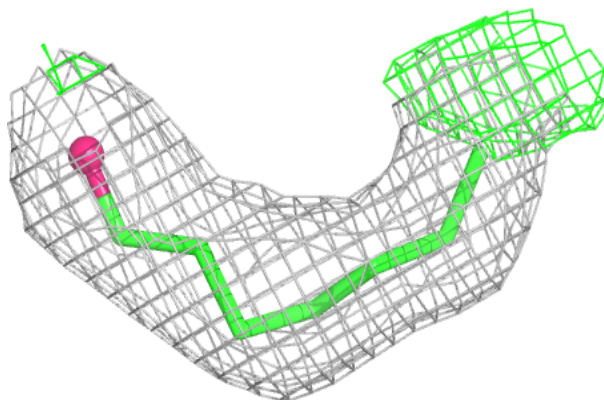


Electron density around A6L A 504:

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

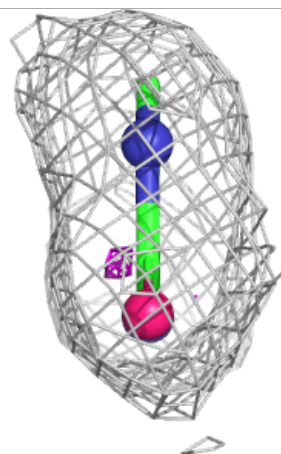
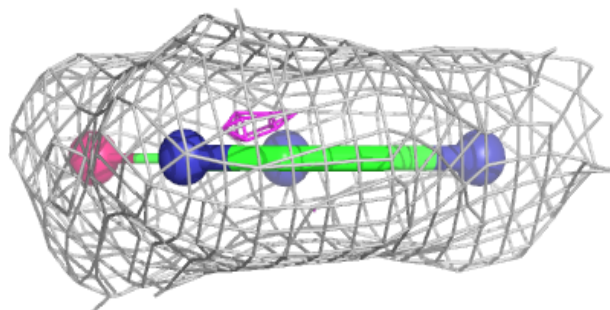
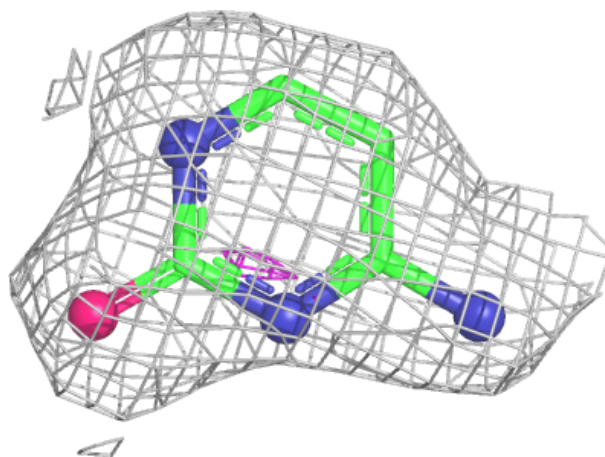
**Electron density around A6L B 502:**

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



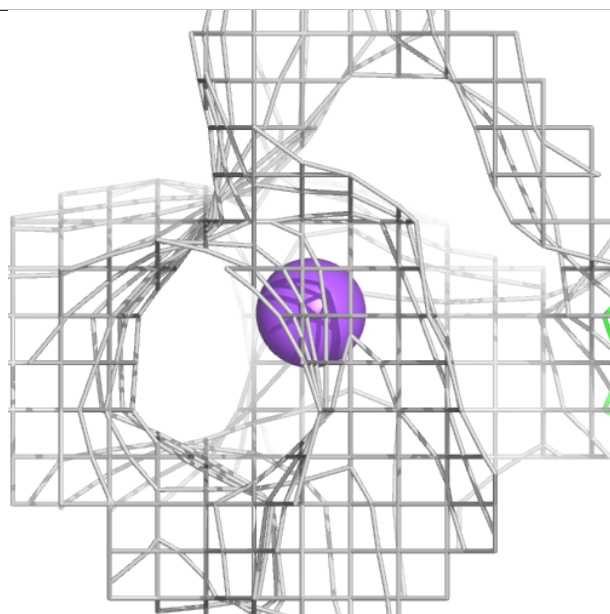
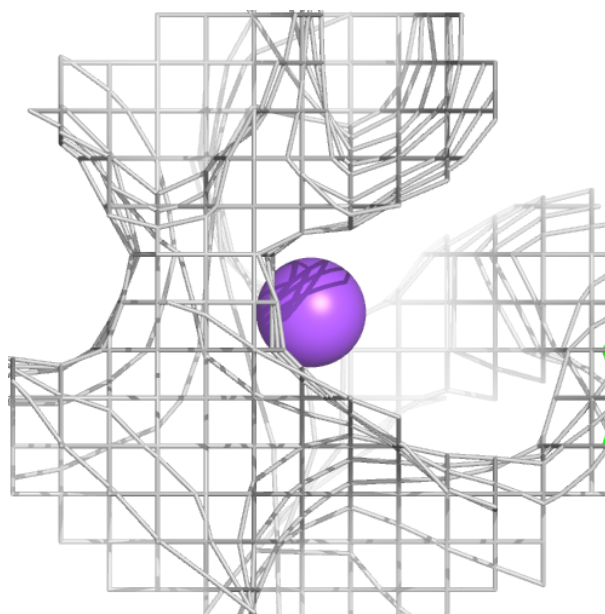
Electron density around CYT B 501:

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



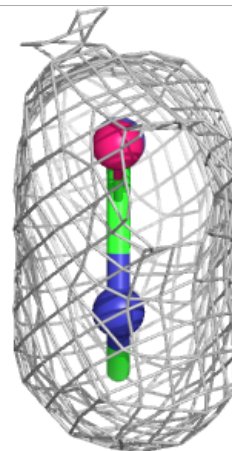
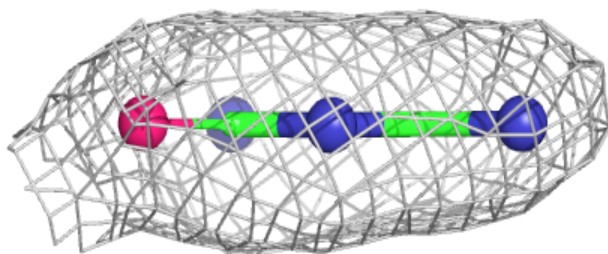
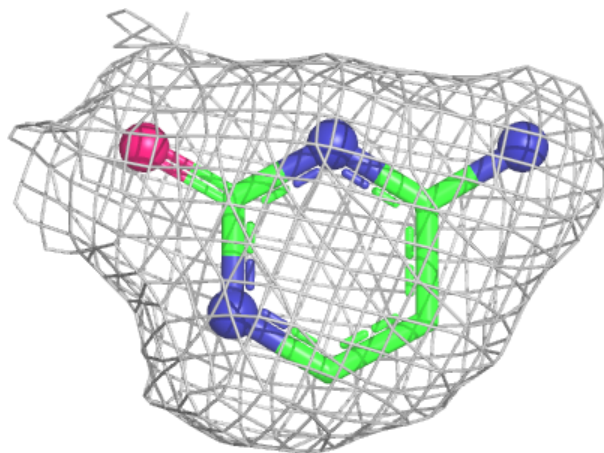
Electron density around NA A 506:

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



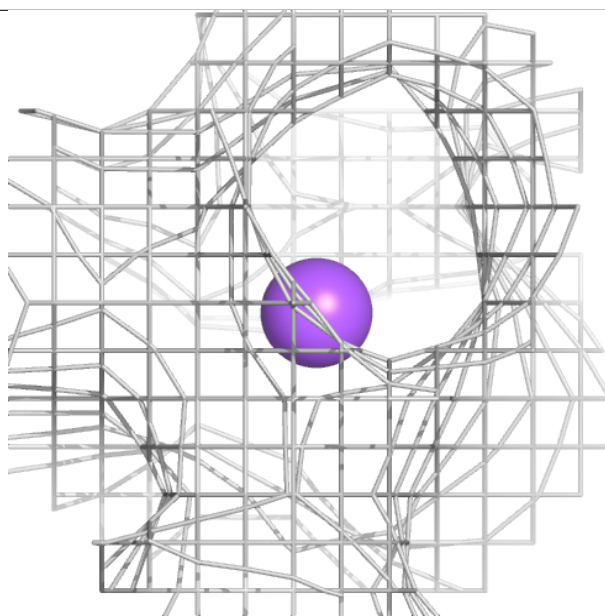
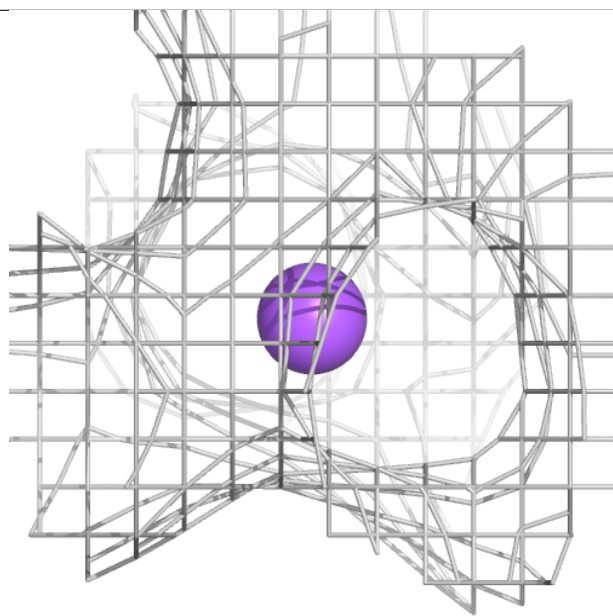
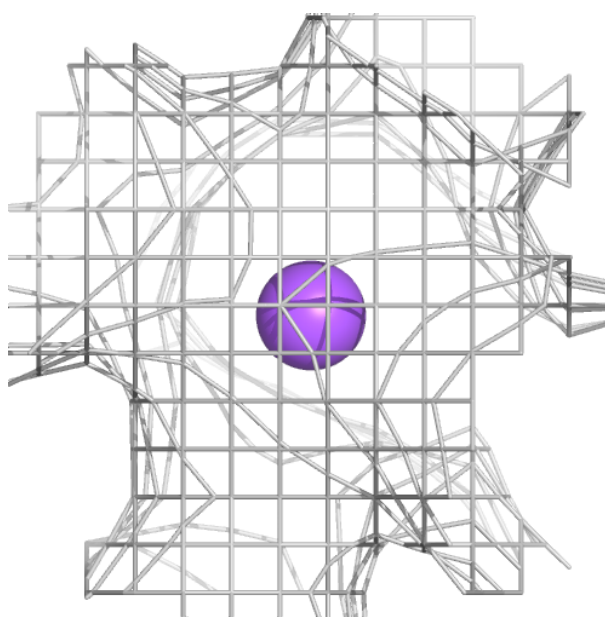
Electron density around CYT A 501:

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



Electron density around NA B 505:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.