



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2024 – 06:57 PM JST

PDB ID : 8I40
Title : Crystal structure of ASCT from Trypanosoma brucei in complex with CoA.
Authors : Mochizuki, K.; Inaoka, D.K.; Fukuda, K.; Kurasawa, H.; Iyoda, K.; Nakai, U.; Harada, S.; Balogun, E.O.; Mazet, M.; Millerioux, Y.; Bringaud, F.; Boshart, M.; Hirayama, K.; Kita, K.; Shiba, T.
Deposited on : 2023-01-18
Resolution : 2.79 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 : 2.36
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) : 2.36

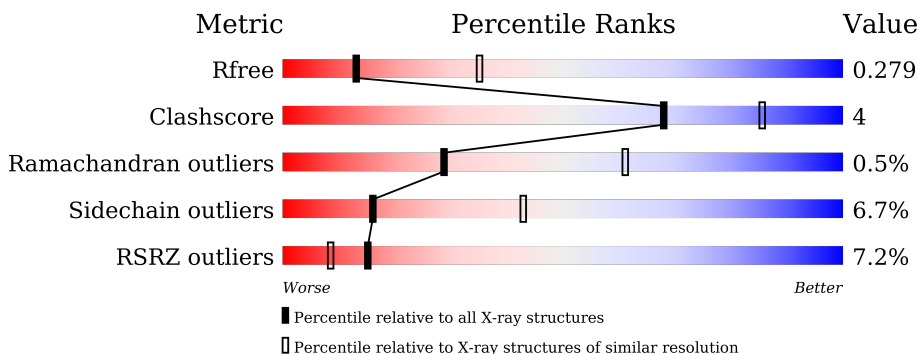
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	483	
1	B	483	
1	C	483	
1	D	483	

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
3	ACT	A	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14198 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.

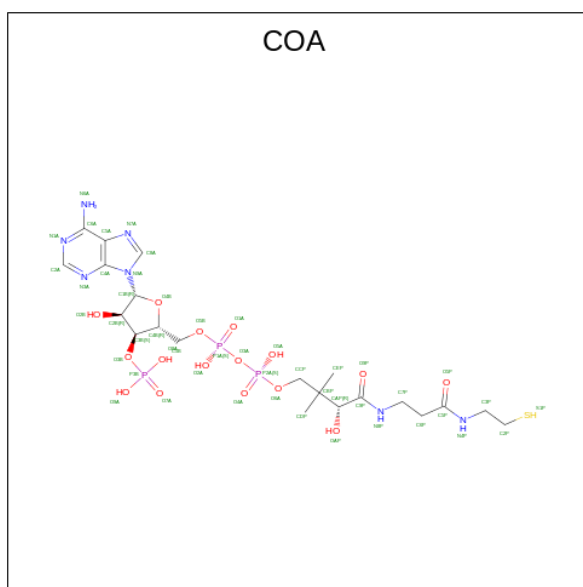
- Molecule 1 is a protein called Succinyl-CoA:3-ketoacid-coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	467	3514	2209	615	667	23	0	0	0
1	B	467	3515	2209	615	668	23	0	0	0
1	C	468	3520	2212	616	669	23	0	0	0
1	D	466	3511	2207	614	667	23	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

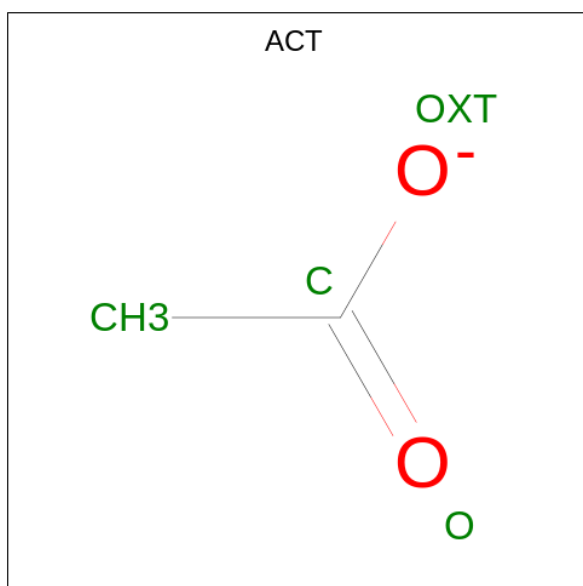
Chain	Residue	Modelled	Actual	Comment	Reference
A	419	ASN	SER	conflict	UNP Q386P1
B	419	ASN	SER	conflict	UNP Q386P1
C	419	ASN	SER	conflict	UNP Q386P1
D	419	ASN	SER	conflict	UNP Q386P1

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

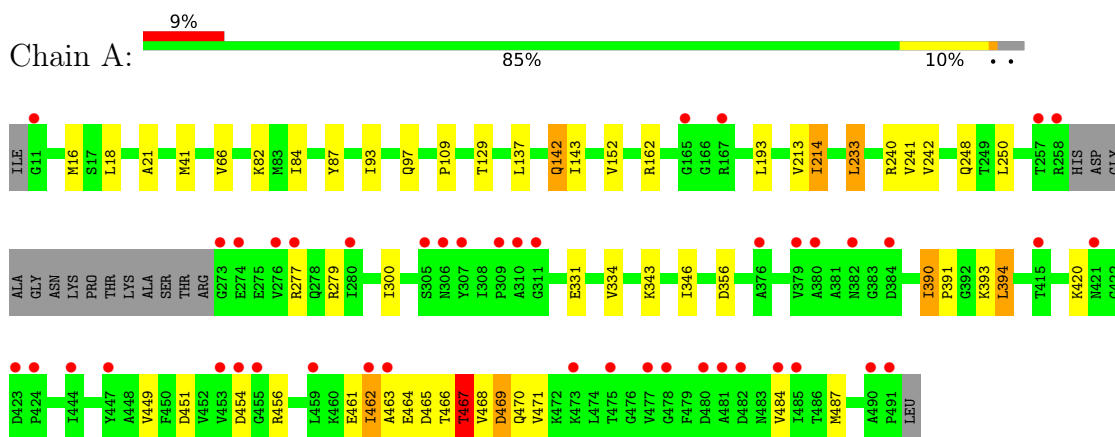
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	9	Total O 9 9	0	0
5	B	8	Total O 8 8	0	0
5	C	11	Total O 11 11	0	0
5	D	6	Total O 6 6	0	0

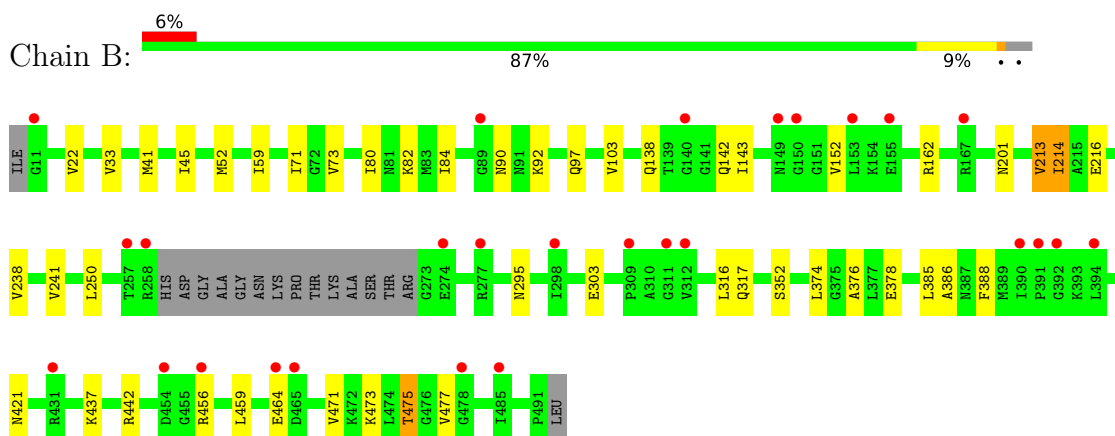
3 Residue-property plots [i](#)

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.

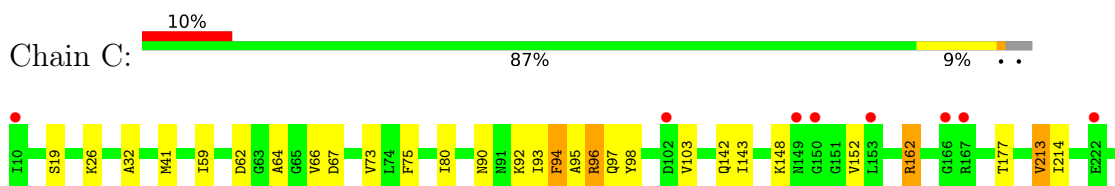
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase

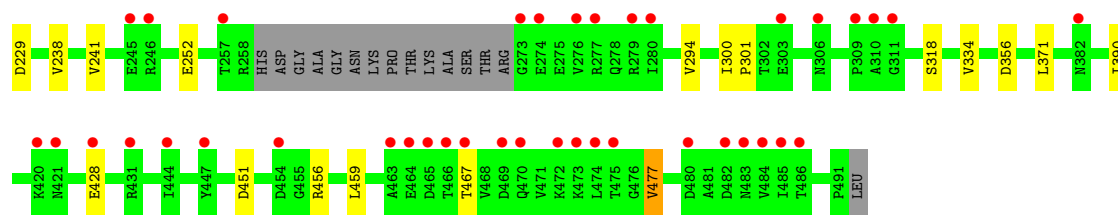


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase

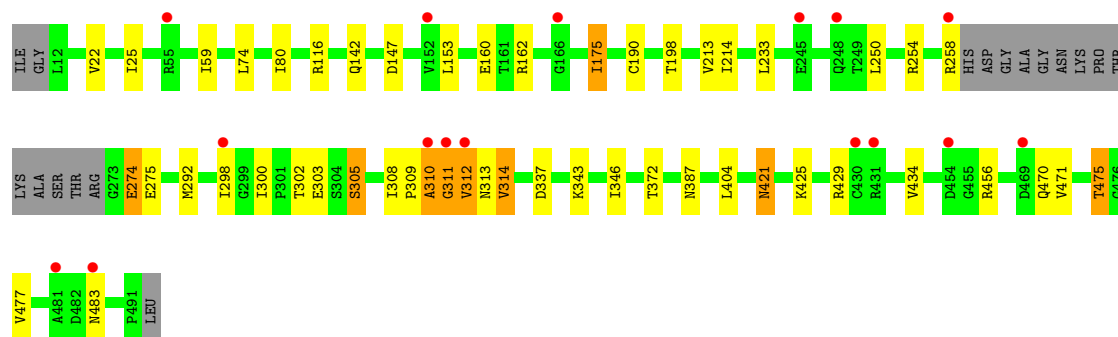
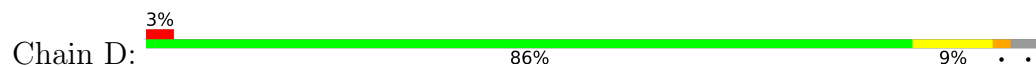


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase





● Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.79Å 165.15Å 188.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.79 19.90 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.90-2.79) 98.8 (19.90-2.79)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.79Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.223 , 0.284 0.224 , 0.279	Depositor DCC
R_{free} test set	2242 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtrriage
Anisotropy	0.070	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14198	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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: CA, ACT, 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	0.45	0/3571	0.68	1/4831 (0.0%)
1	B	0.40	0/3572	0.64	0/4833
1	C	0.43	0/3577	0.64	0/4840
1	D	0.46	0/3568	0.69	1/4828 (0.0%)
All	All	0.43	0/14288	0.66	2/19332 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	GLN	N-CA-C	-5.86	95.19	111.00
1	D	300	ILE	C-N-CD	5.01	138.93	128.40

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	3514	0	3527	53	0
1	B	3515	0	3527	14	0
1	C	3520	0	3529	21	0
1	D	3511	0	3524	20	0
2	A	48	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	32	0	0
3	A	4	0	3	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	9	0	0	0	0
5	B	8	0	0	0	0
5	C	11	0	0	0	0
5	D	6	0	0	0	0
All	All	14198	0	14173	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 4.

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:343:LYS:NZ	3:A:502:ACT:H1	1.53	1.22
1:A:466:THR:CG2	1:A:470:GLN:NE2	2.12	1.12
1:A:466:THR:HG21	1:A:470:GLN:CD	1.73	1.08
1:A:466:THR:HG21	1:A:470:GLN:NE2	1.69	1.08
1:A:343:LYS:HZ1	3:A:502:ACT:H1	1.23	0.98
1:A:466:THR:CG2	1:A:470:GLN:CB	2.42	0.98
1:A:143:ILE:HD13	1:A:152:VAL:HG22	1.43	0.97
1:A:466:THR:HG23	1:A:470:GLN:NE2	1.82	0.94
1:A:343:LYS:HZ2	3:A:502:ACT:H1	1.35	0.90
1:A:466:THR:HG22	1:A:470:GLN:HB3	1.55	0.88
1:A:466:THR:HG22	1:A:470:GLN:CB	2.03	0.88
1:A:466:THR:CG2	1:A:470:GLN:HB3	2.04	0.87
1:A:463:ALA:O	1:A:465:ASP:HA	1.75	0.85
1:A:466:THR:HG23	1:A:470:GLN:HE21	1.41	0.85
1:D:305:SER:O	1:D:308:ILE:HG13	1.78	0.84
1:A:394:LEU:HD23	1:A:394:LEU:O	1.81	0.81
1:A:468:VAL:HA	1:A:471:VAL:HG12	1.64	0.79
1:A:390:ILE:HG13	1:A:393:LYS:HB2	1.64	0.79
1:A:466:THR:HG21	1:A:470:GLN:CB	2.11	0.79
1:A:343:LYS:NZ	3:A:502:ACT:CH3	2.44	0.78
1:A:466:THR:CG2	1:A:470:GLN:HB2	2.12	0.78
1:A:343:LYS:HZ1	3:A:502:ACT:CH3	1.96	0.78
1:A:466:THR:CG2	1:A:470:GLN:HE21	1.95	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ILE:HD11	1:A:466:THR:O	1.87	0.75
1:C:66:VAL:HG23	1:C:90:ASN:O	1.87	0.74
1:A:390:ILE:HD12	1:A:391:PRO:N	2.04	0.73
1:A:21:ALA:HB1	1:A:214:ILE:HD12	1.76	0.68
1:A:466:THR:HG21	1:A:470:GLN:CG	2.23	0.67
1:A:449:VAL:HB	1:A:461:GLU:HB2	1.76	0.66
1:C:67:ASP:OD2	1:C:93:ILE:HG22	1.96	0.66
1:C:32:ALA:HB2	1:C:177:THR:HG21	1.79	0.65
1:A:464:GLU:HA	1:A:465:ASP:HB2	1.79	0.64
1:D:311:GLY:C	1:D:312:VAL:HG22	2.19	0.63
1:A:466:THR:HG22	1:A:470:GLN:HB2	1.75	0.63
1:C:66:VAL:HG22	1:C:67:ASP:N	2.14	0.63
1:D:311:GLY:O	1:D:312:VAL:CG2	2.48	0.62
1:D:309:PRO:O	1:D:310:ALA:HB3	2.00	0.61
1:A:143:ILE:CD1	1:A:152:VAL:HG22	2.23	0.61
1:A:390:ILE:HD12	1:A:391:PRO:CD	2.30	0.61
1:A:464:GLU:O	1:A:464:GLU:HG2	2.02	0.59
1:A:466:THR:HG21	1:A:470:GLN:HB3	1.80	0.58
1:D:311:GLY:O	1:D:312:VAL:HG23	2.03	0.58
1:D:311:GLY:C	1:D:312:VAL:CG2	2.73	0.57
1:D:302:THR:O	1:D:305:SER:OG	2.23	0.56
1:C:96:ARG:HG3	1:C:96:ARG:HH11	1.70	0.56
1:C:96:ARG:HG3	1:C:96:ARG:NH1	2.21	0.54
1:A:87:TYR:CD2	3:A:502:ACT:H2	2.43	0.54
1:B:376:ALA:HB2	1:B:385:LEU:HD11	1.90	0.54
1:D:372:THR:HG21	1:D:404:LEU:HB3	1.89	0.54
1:A:390:ILE:HD12	1:A:390:ILE:C	2.28	0.54
1:B:295:ASN:ND2	1:B:317:GLN:OE1	2.41	0.54
1:C:90:ASN:ND2	1:C:252:GLU:OE2	2.38	0.53
1:D:59:ILE:CD1	1:D:80:ILE:HD12	2.39	0.53
1:A:390:ILE:HD12	1:A:391:PRO:HD2	1.90	0.52
1:A:143:ILE:HD13	1:A:152:VAL:CG2	2.28	0.52
1:C:213:VAL:HG22	1:C:238:VAL:HA	1.93	0.51
1:A:193:LEU:HD12	1:A:233:LEU:HD12	1.92	0.50
1:B:33:VAL:HB	1:B:71:ILE:HD11	1.92	0.50
1:C:64:ALA:HB3	1:C:94:PHE:CD1	2.46	0.49
1:D:74:LEU:HB2	1:D:80:ILE:HD11	1.95	0.49
1:A:277:ARG:HG2	1:A:300:ILE:HD12	1.95	0.49
1:C:143:ILE:HD12	1:C:152:VAL:HG21	1.95	0.49
1:D:59:ILE:HD11	1:D:80:ILE:HD12	1.94	0.49
1:B:471:VAL:O	1:B:475:THR:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:VAL:CG2	1:C:67:ASP:N	2.75	0.49
1:D:309:PRO:O	1:D:310:ALA:CB	2.61	0.49
1:D:22:VAL:HG13	1:D:25:ILE:HD12	1.95	0.49
1:C:294:VAL:HG12	1:C:371:LEU:HB3	1.96	0.48
1:D:302:THR:O	1:D:302:THR:HG22	2.14	0.48
1:A:143:ILE:CD1	1:A:152:VAL:CG2	2.91	0.47
1:D:292:MET:HB2	1:D:314:VAL:HG23	1.97	0.46
1:C:75:PHE:HB3	1:C:93:ILE:HG12	1.97	0.46
1:B:45:ILE:HD13	1:B:214:ILE:HD11	1.97	0.46
1:C:97:GLN:HE21	1:C:103:VAL:HG23	1.80	0.46
1:D:116:ARG:HB3	1:D:175:ILE:HG22	1.96	0.46
1:B:22:VAL:HG12	1:B:52:MET:SD	2.56	0.46
1:A:82:LYS:HD2	1:A:84:ILE:HD11	1.98	0.45
1:C:162:ARG:NH2	1:D:160:GLU:OE2	2.48	0.45
1:A:462:ILE:O	1:A:487:MET:N	2.49	0.45
1:A:84:ILE:HD12	1:A:84:ILE:N	2.32	0.44
1:A:18:LEU:HD12	1:A:242:VAL:HG11	1.99	0.44
1:C:428:GLU:HA	1:C:477:VAL:HG11	2.00	0.44
1:B:213:VAL:CG2	1:B:238:VAL:HA	2.48	0.44
1:B:59:ILE:HD12	1:B:80:ILE:HD12	1.99	0.44
1:B:33:VAL:CB	1:B:71:ILE:HD11	2.48	0.44
1:D:471:VAL:O	1:D:475:THR:HG22	2.17	0.44
1:B:97:GLN:HE21	1:B:103:VAL:HG23	1.83	0.43
1:B:378:GLU:HB3	1:B:386:ALA:HB3	2.01	0.43
1:A:16:MET:SD	1:A:240:ARG:HD2	2.59	0.43
1:C:59:ILE:HD12	1:C:80:ILE:HD12	2.00	0.43
1:A:18:LEU:CD1	1:A:242:VAL:HG11	2.49	0.43
1:A:464:GLU:HA	1:A:465:ASP:CB	2.48	0.43
1:D:147:ASP:HB3	1:D:153:LEU:HD13	2.00	0.42
1:A:462:ILE:HG22	1:A:484:VAL:CG1	2.50	0.42
1:B:82:LYS:HD2	1:B:84:ILE:HD11	2.02	0.42
1:A:331:GLU:O	1:A:334:VAL:HG12	2.20	0.42
1:A:391:PRO:C	1:A:393:LYS:N	2.73	0.41
1:C:95:ALA:O	1:C:98:TYR:HB3	2.20	0.41
1:C:96:ARG:HH11	1:C:96:ARG:CG	2.33	0.41
1:A:467:THR:HB	1:A:469:ASP:HB2	2.02	0.41
1:A:462:ILE:CG2	1:A:484:VAL:CG1	2.99	0.41
1:B:45:ILE:HD11	1:B:216:GLU:HB3	2.02	0.41
1:C:143:ILE:HG23	1:C:152:VAL:HG13	2.03	0.41
1:B:143:ILE:HG23	1:B:152:VAL:HG13	2.01	0.41
1:D:425:LYS:HB3	1:D:425:LYS:HZ3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PRO:HD3	1:A:137:LEU:HD23	2.03	0.40
1:C:300:ILE:N	1:C:301:PRO:CD	2.85	0.40

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	463/483 (96%)	437 (94%)	25 (5%)	1 (0%)	47 78
1	B	463/483 (96%)	432 (93%)	28 (6%)	3 (1%)	25 56
1	C	464/483 (96%)	441 (95%)	23 (5%)	0	100 100
1	D	462/483 (96%)	436 (94%)	20 (4%)	6 (1%)	12 36
All	All	1852/1932 (96%)	1746 (94%)	96 (5%)	10 (0%)	29 61

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	421	ASN
1	B	201	ASN
1	B	388	PHE
1	D	274	GLU
1	D	311	GLY
1	D	312	VAL
1	D	313	ASN
1	A	467	THR
1	B	464	GLU
1	D	310	ALA

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	375/387 (97%)	350 (93%)	25 (7%)	16	43
1	B	375/387 (97%)	352 (94%)	23 (6%)	18	48
1	C	375/387 (97%)	351 (94%)	24 (6%)	17	45
1	D	375/387 (97%)	346 (92%)	29 (8%)	13	35
All	All	1500/1548 (97%)	1399 (93%)	101 (7%)	16	43

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	66	VAL
1	A	93	ILE
1	A	97	GLN
1	A	129	THR
1	A	142	GLN
1	A	162	ARG
1	A	213	VAL
1	A	214	ILE
1	A	233	LEU
1	A	241	VAL
1	A	248	GLN
1	A	250	LEU
1	A	279	ARG
1	A	346	ILE
1	A	356	ASP
1	A	390	ILE
1	A	394	LEU
1	A	420	LYS
1	A	451	ASP
1	A	454	ASP
1	A	456	ARG
1	A	462	ILE
1	A	467	THR

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Mol	Chain	Res	Type
1	A	469	ASP
1	B	41	MET
1	B	73	VAL
1	B	90	ASN
1	B	92	LYS
1	B	138	GLN
1	B	142	GLN
1	B	162	ARG
1	B	213	VAL
1	B	214	ILE
1	B	241	VAL
1	B	250	LEU
1	B	303	GLU
1	B	316	LEU
1	B	352	SER
1	B	374	LEU
1	B	421	ASN
1	B	437	LYS
1	B	442	ARG
1	B	456	ARG
1	B	459	LEU
1	B	473	LYS
1	B	475	THR
1	B	477	VAL
1	C	19	SER
1	C	26	LYS
1	C	41	MET
1	C	62	ASP
1	C	73	VAL
1	C	92	LYS
1	C	94	PHE
1	C	96	ARG
1	C	142	GLN
1	C	148	LYS
1	C	162	ARG
1	C	213	VAL
1	C	214	ILE
1	C	229	ASP
1	C	241	VAL
1	C	318	SER
1	C	334	VAL
1	C	356	ASP

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Mol	Chain	Res	Type
1	C	390	ILE
1	C	451	ASP
1	C	456	ARG
1	C	459	LEU
1	C	467	THR
1	C	477	VAL
1	D	142	GLN
1	D	162	ARG
1	D	175	ILE
1	D	190	CYS
1	D	198	THR
1	D	213	VAL
1	D	214	ILE
1	D	233	LEU
1	D	250	LEU
1	D	254	ARG
1	D	258	ARG
1	D	274	GLU
1	D	275	GLU
1	D	298	ILE
1	D	303	GLU
1	D	305	SER
1	D	314	VAL
1	D	337	ASP
1	D	343	LYS
1	D	346	ILE
1	D	387	ASN
1	D	421	ASN
1	D	429	ARG
1	D	434	VAL
1	D	456	ARG
1	D	470	GLN
1	D	475	THR
1	D	477	VAL
1	D	483	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	208	GLN
1	A	470	GLN

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Mol	Chain	Res	Type
1	B	47	GLN
1	B	77	ASN
1	B	97	GLN
1	B	208	GLN
1	B	306	ASN
1	C	77	ASN
1	C	97	GLN
1	C	208	GLN
1	C	248	GLN
1	D	97	GLN
1	D	110	GLN
1	D	278	GLN
1	D	290	ASN
1	D	306	ASN
1	D	344	GLN
1	D	382	ASN
1	D	421	ASN
1	D	470	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	COA	C	501	-	41,50,50	0.89	2 (4%)	52,75,75	1.13	3 (5%)
3	ACT	A	502	-	3,3,3	0.93	0	3,3,3	1.11	0
2	COA	A	501	1	41,50,50	0.92	3 (7%)	52,75,75	1.26	6 (11%)

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	COA	C	501	-	-	12/44/64/64	0/3/3/3
2	COA	A	501	1	-	11/44/64/64	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	COA	C5A-C4A	2.70	1.48	1.40
2	C	501	COA	C5A-C4A	2.68	1.48	1.40
2	A	501	COA	C2A-N3A	2.40	1.36	1.32
2	C	501	COA	C2A-N3A	2.22	1.35	1.32
2	A	501	COA	O4B-C1B	2.15	1.44	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	COA	N3A-C2A-N1A	-3.74	122.84	128.68
2	A	501	COA	N3A-C2A-N1A	-3.71	122.88	128.68
2	A	501	COA	C4A-C5A-N7A	-2.81	106.47	109.40
2	C	501	COA	C4A-C5A-N7A	-2.74	106.55	109.40
2	A	501	COA	C6P-C5P-N4P	2.62	120.83	116.42
2	A	501	COA	O6A-CCP-CBP	2.56	114.66	110.55
2	A	501	COA	P2A-O3A-P1A	-2.29	124.98	132.83
2	A	501	COA	C3B-C2B-C1B	2.16	104.67	99.89
2	C	501	COA	C2A-N1A-C6A	2.10	122.34	118.75

There are no chirality outliers.

All (23) torsion outliers are listed below:

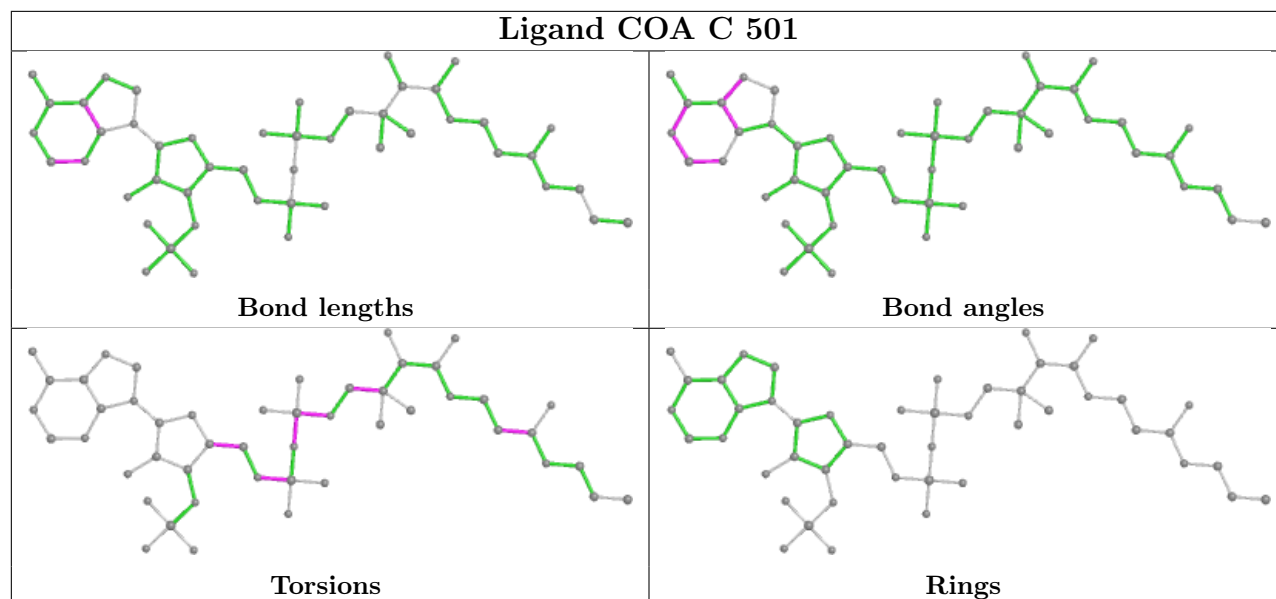
Mol	Chain	Res	Type	Atoms
2	A	501	COA	C5B-O5B-P1A-O2A
2	A	501	COA	C5B-O5B-P1A-O3A
2	A	501	COA	CCP-O6A-P2A-O3A
2	A	501	COA	S1P-C2P-C3P-N4P
2	C	501	COA	CCP-O6A-P2A-O3A
2	C	501	COA	CCP-O6A-P2A-O4A
2	C	501	COA	CCP-O6A-P2A-O5A
2	A	501	COA	C6P-C5P-N4P-C3P
2	A	501	COA	O5P-C5P-N4P-C3P
2	A	501	COA	C3B-C4B-C5B-O5B
2	A	501	COA	O4B-C4B-C5B-O5B
2	C	501	COA	CDP-CBP-CCP-O6A
2	C	501	COA	CEP-CBP-CCP-O6A
2	A	501	COA	P2A-O3A-P1A-O5B
2	C	501	COA	P1A-O3A-P2A-O6A
2	C	501	COA	P1A-O3A-P2A-O4A
2	A	501	COA	CCP-O6A-P2A-O5A
2	C	501	COA	CAP-CBP-CCP-O6A
2	A	501	COA	C4B-C5B-O5B-P1A
2	C	501	COA	O4B-C4B-C5B-O5B
2	C	501	COA	C5B-O5B-P1A-O3A
2	C	501	COA	C5B-O5B-P1A-O1A
2	C	501	COA	O5P-C5P-C6P-C7P

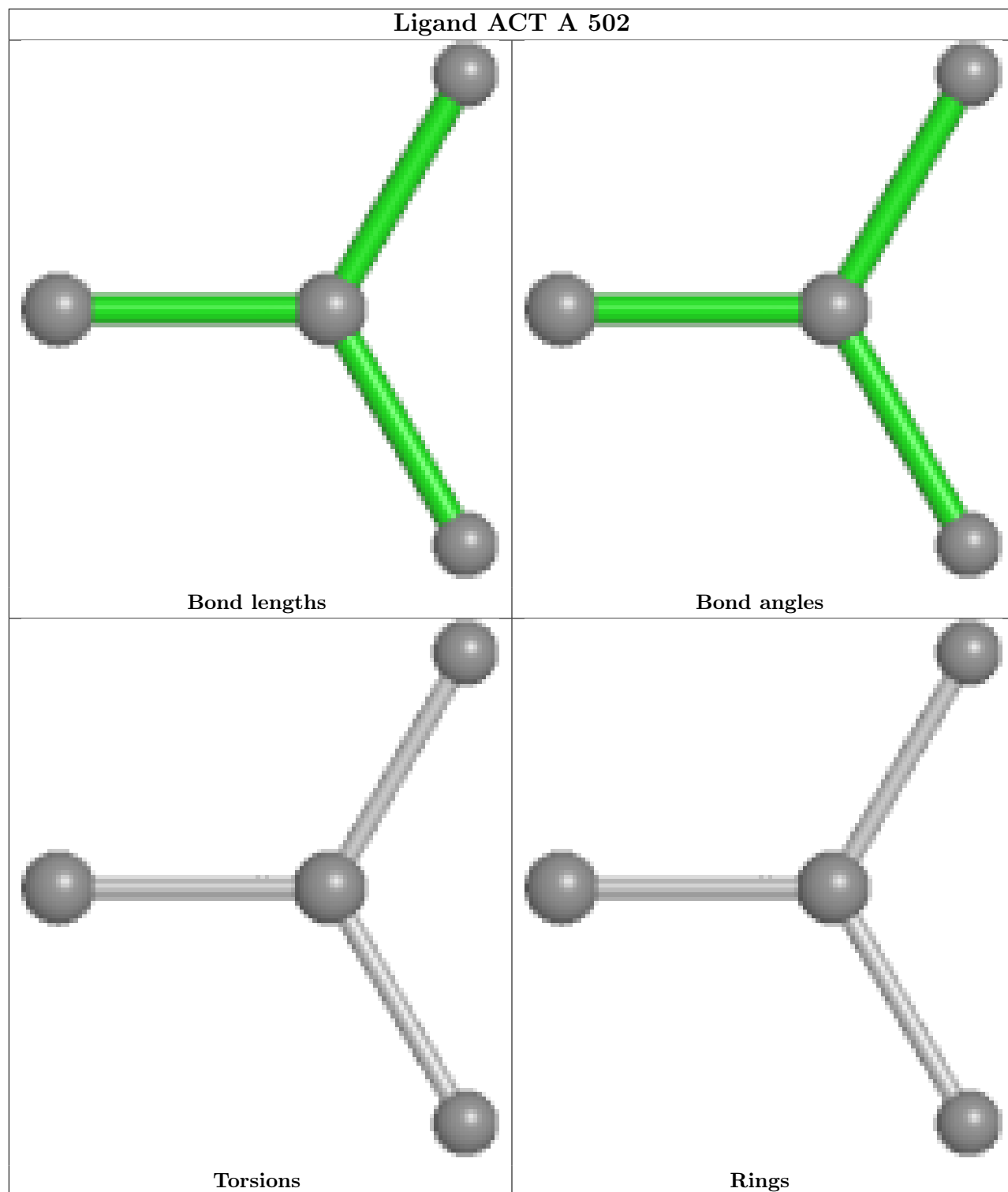
There are no ring outliers.

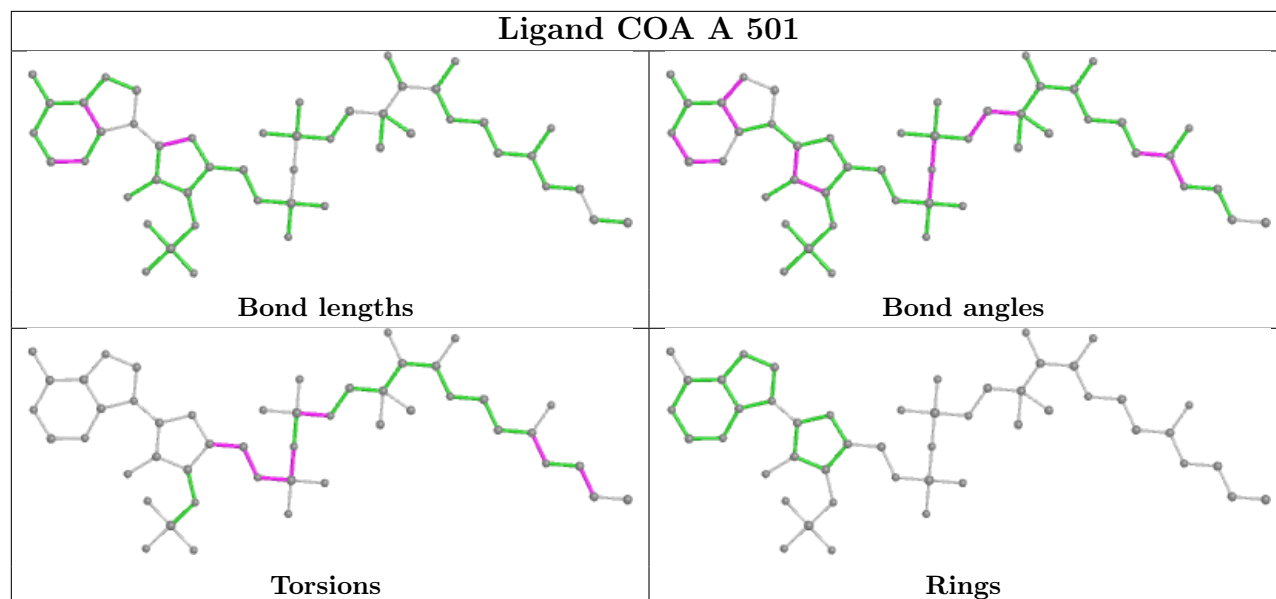
1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	ACT	6	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	467/483 (96%)	0.54	44 (9%) 8 4	27, 44, 93, 121	1 (0%)
1	B	467/483 (96%)	0.27	27 (5%) 23 15	26, 42, 64, 102	1 (0%)
1	C	468/483 (96%)	0.54	47 (10%) 7 4	25, 47, 86, 113	1 (0%)
1	D	466/483 (96%)	0.22	16 (3%) 45 35	29, 42, 62, 89	1 (0%)
All	All	1868/1932 (96%)	0.39	134 (7%) 15 8	25, 43, 85, 121	4 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	469	ASP	6.9
1	A	310	ALA	6.3
1	C	273	GLY	5.7
1	A	277	ARG	5.5
1	C	421	ASN	5.2
1	C	485	ILE	5.1
1	A	473	LYS	4.8
1	C	465	ASP	4.7
1	A	447	TYR	4.6
1	A	478	GLY	4.5
1	A	258	ARG	4.4
1	A	454	ASP	4.2
1	C	484	VAL	4.2
1	C	431	ARG	4.0
1	C	473	LYS	4.0
1	A	307	TYR	4.0
1	C	480	ASP	3.9
1	C	420	LYS	3.9
1	D	152	VAL	3.8
1	A	257	THR	3.8
1	C	475	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	311	GLY	3.8
1	C	277	ARG	3.7
1	B	485	ILE	3.7
1	C	483	ASN	3.7
1	D	312	VAL	3.7
1	B	312	VAL	3.7
1	C	245	GLU	3.6
1	B	153	LEU	3.6
1	C	482	ASP	3.6
1	A	455	GLY	3.5
1	C	470	GLN	3.5
1	A	11	GLY	3.5
1	C	464	GLU	3.4
1	B	149	ASN	3.4
1	A	380	ALA	3.3
1	D	310	ALA	3.3
1	C	166	GLY	3.3
1	A	306	ASN	3.3
1	C	447	TYR	3.3
1	D	258	ARG	3.3
1	B	89	GLY	3.2
1	A	280	ILE	3.2
1	C	310	ALA	3.2
1	A	475	THR	3.2
1	C	246	ARG	3.1
1	A	491	PRO	3.1
1	A	490	ALA	3.0
1	B	277	ARG	3.0
1	A	480	ASP	3.0
1	A	453	VAL	3.0
1	C	444	ILE	2.9
1	C	466	THR	2.9
1	C	274	GLU	2.9
1	A	311	GLY	2.9
1	C	428	GLU	2.9
1	B	258	ARG	2.9
1	A	421	ASN	2.9
1	B	311	GLY	2.9
1	B	394	LEU	2.9
1	C	474	LEU	2.8
1	C	463	ALA	2.8
1	B	274	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	485	ILE	2.8
1	C	306	ASN	2.8
1	D	166	GLY	2.8
1	C	257	THR	2.8
1	C	10	ILE	2.8
1	A	477	VAL	2.8
1	C	167	ARG	2.8
1	A	423	ASP	2.8
1	C	467	THR	2.7
1	B	454	ASP	2.7
1	D	298	ILE	2.7
1	A	274	GLU	2.7
1	B	11	GLY	2.7
1	B	391	PRO	2.6
1	B	392	GLY	2.6
1	C	276	VAL	2.6
1	C	222	GLU	2.6
1	A	167	ARG	2.6
1	C	279	ARG	2.6
1	D	454	ASP	2.6
1	A	376	ALA	2.6
1	B	456	ARG	2.6
1	A	276	VAL	2.6
1	C	149	ASN	2.6
1	A	459	LEU	2.6
1	A	462	ILE	2.5
1	C	311	GLY	2.5
1	A	415	THR	2.5
1	B	390	ILE	2.5
1	C	472	LYS	2.5
1	B	298	ILE	2.5
1	C	454	ASP	2.5
1	B	465	ASP	2.4
1	D	431	ARG	2.4
1	C	382	ASN	2.4
1	C	280	ILE	2.4
1	D	55	ARG	2.4
1	B	431	ARG	2.4
1	B	464	GLU	2.4
1	A	165	GLY	2.3
1	A	444	ILE	2.3
1	D	430	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	305	SER	2.3
1	A	481	ALA	2.3
1	C	153	LEU	2.3
1	C	486	THR	2.3
1	D	469	ASP	2.3
1	A	379	VAL	2.3
1	B	155	GLU	2.3
1	C	102	ASP	2.3
1	C	303	GLU	2.3
1	A	482	ASP	2.3
1	A	382	ASN	2.2
1	D	481	ALA	2.2
1	B	150	GLY	2.2
1	A	424	PRO	2.2
1	A	463	ALA	2.2
1	B	257	THR	2.2
1	A	384	ASP	2.2
1	A	484	VAL	2.1
1	B	309	PRO	2.1
1	B	140	GLY	2.1
1	B	478	GLY	2.1
1	C	309	PRO	2.1
1	D	245	GLU	2.1
1	A	273	GLY	2.1
1	D	248	GLN	2.0
1	A	309	PRO	2.0
1	D	483	ASN	2.0
1	C	150	GLY	2.0
1	B	167	ARG	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](#)

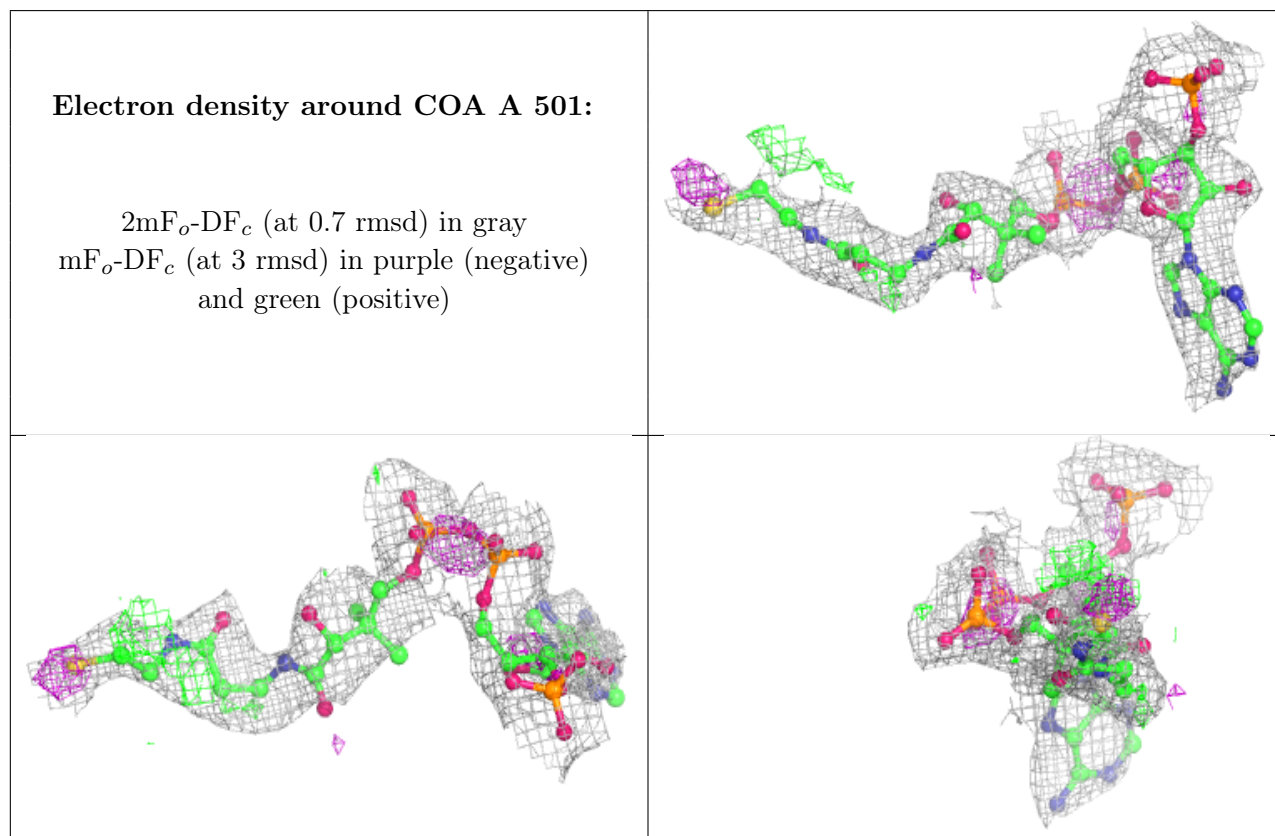
There are no monosaccharides in this entry.

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.

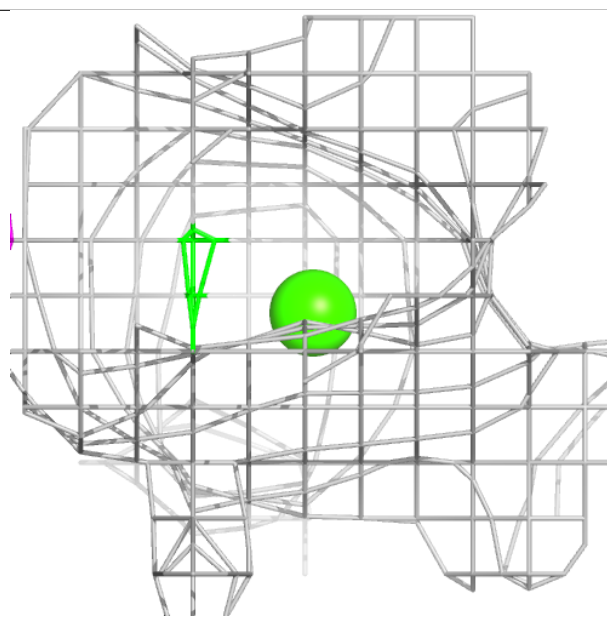
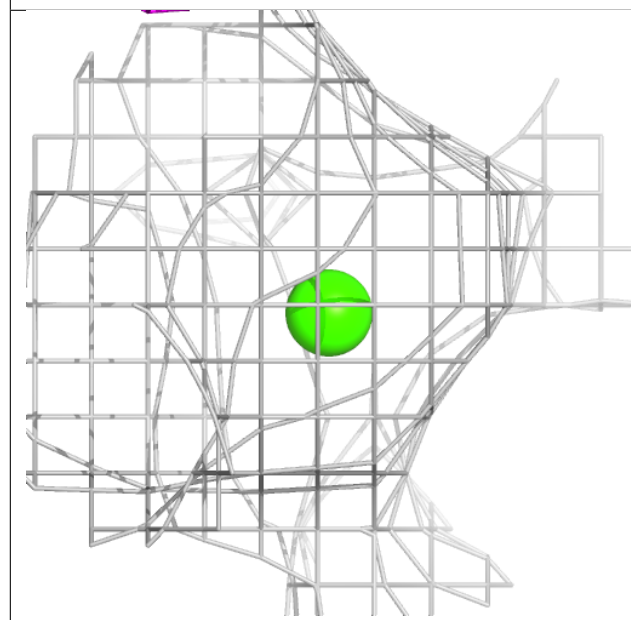
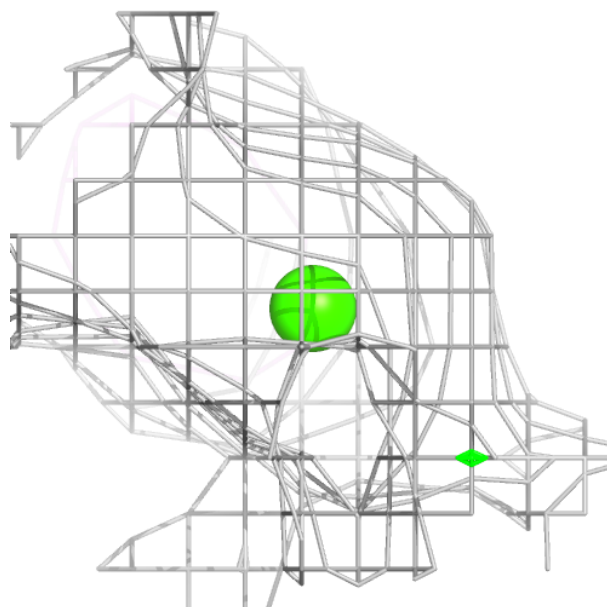
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COA	A	501	48/48	0.70	0.29	76,88,100,103	0
4	CA	D	701	1/1	0.74	0.17	83,83,83,83	0
2	COA	C	501	48/48	0.77	0.29	65,74,85,87	0
4	CA	B	701	1/1	0.80	0.12	74,74,74,74	0
4	CA	C	502	1/1	0.84	0.08	68,68,68,68	0
4	CA	A	503	1/1	0.88	0.12	77,77,77,77	0
3	ACT	A	502	4/4	0.88	0.20	59,62,62,63	0

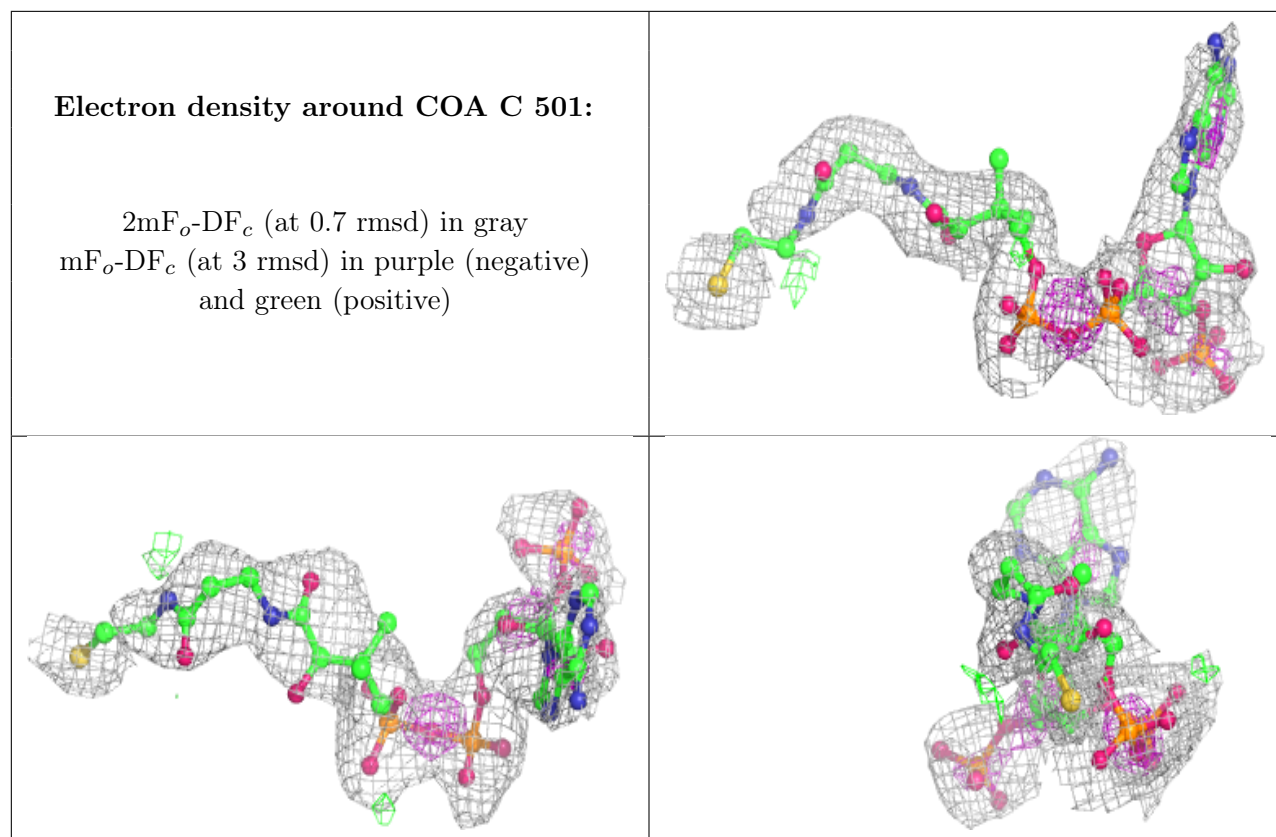
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around CA D 701:

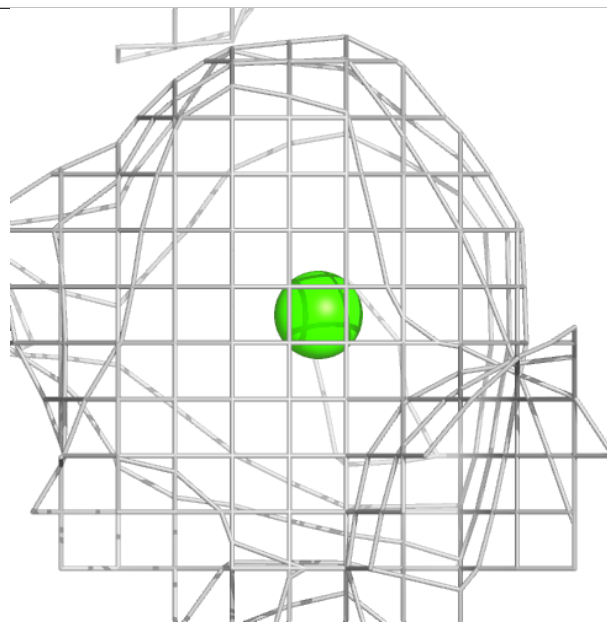
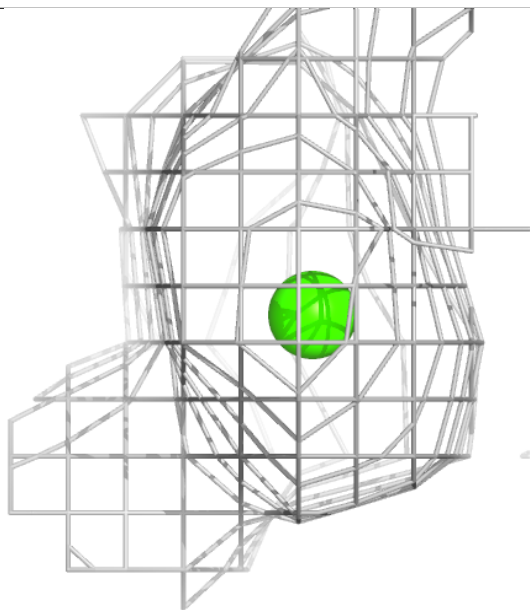
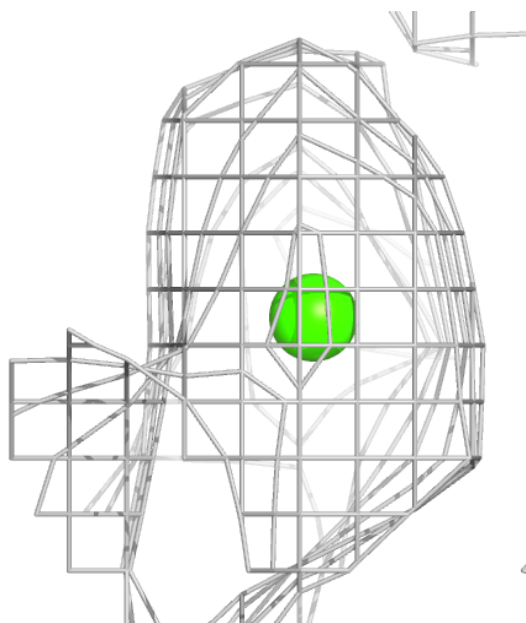
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





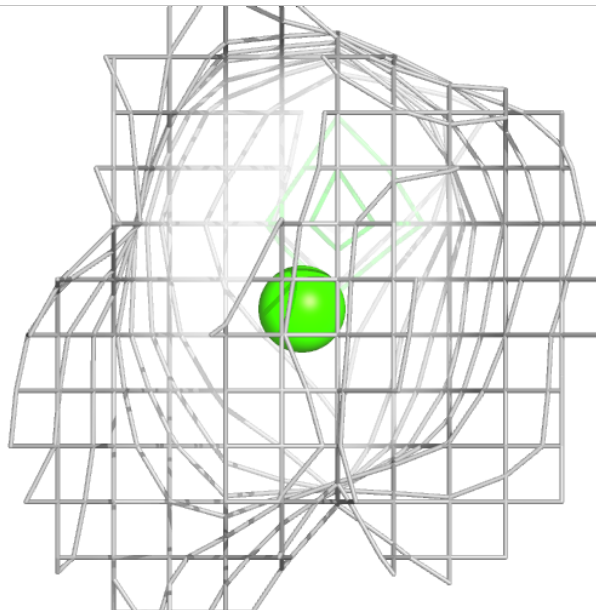
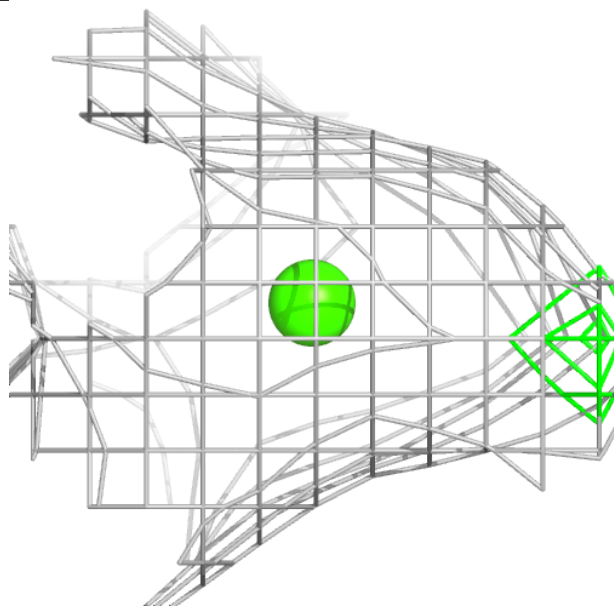
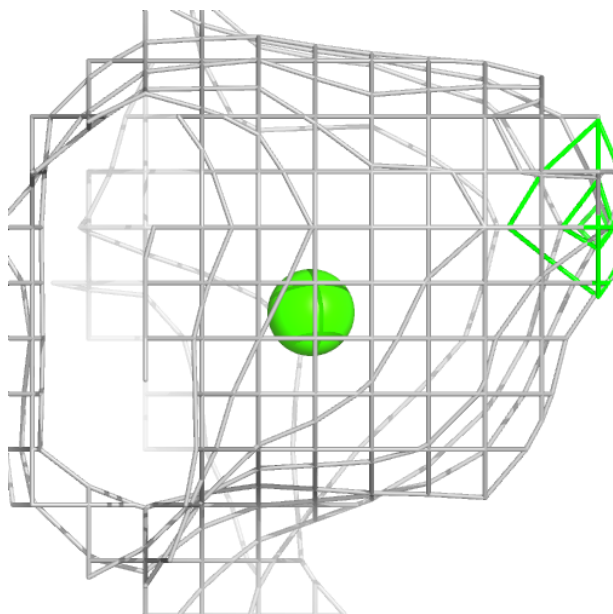
Electron density around CA B 701:

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



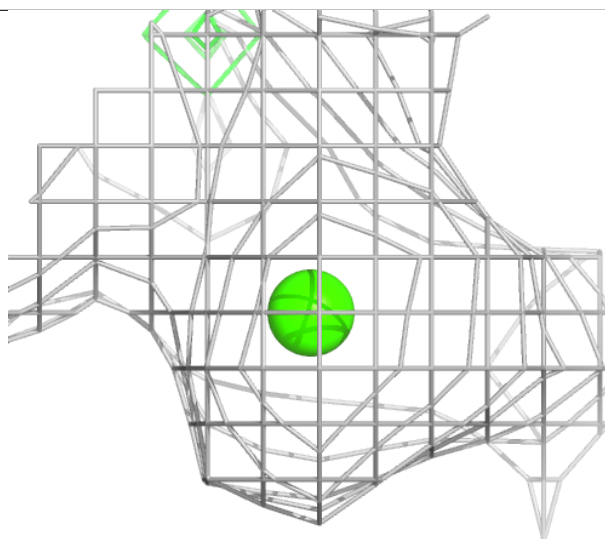
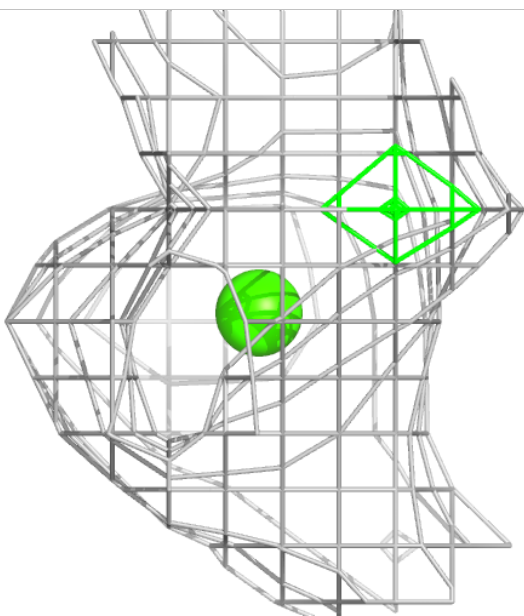
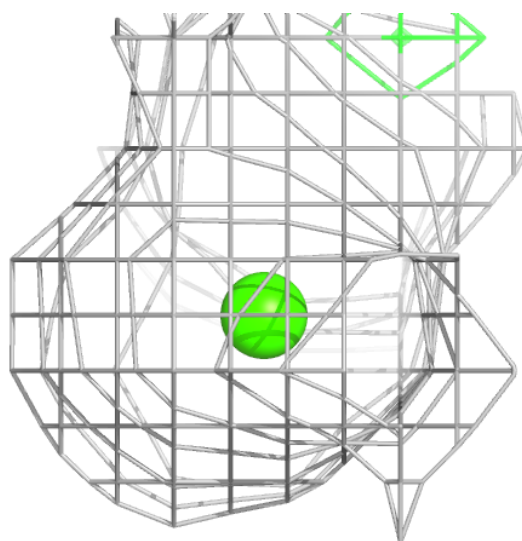
Electron density around CA C 502:

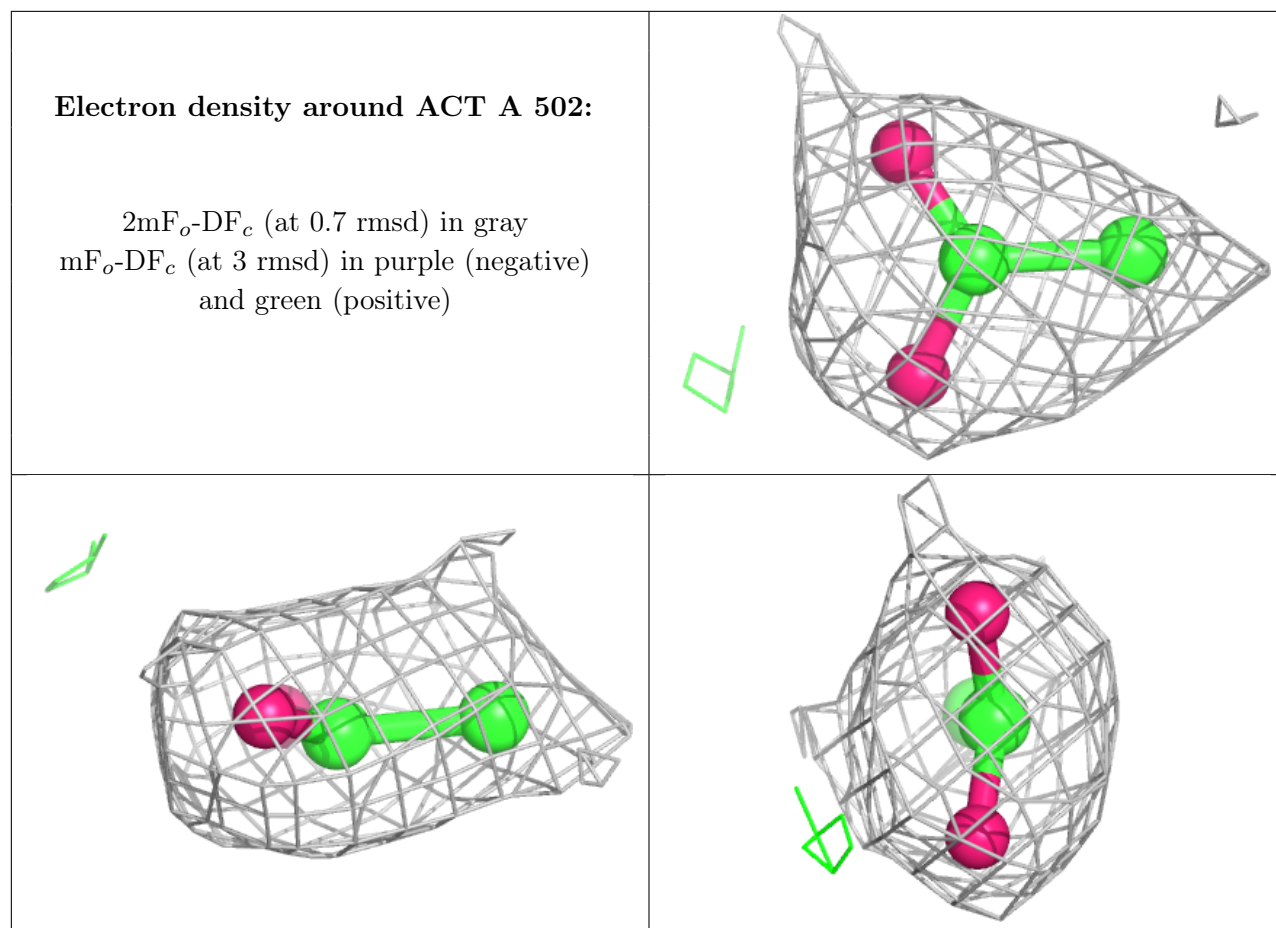
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.