



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:11 PM UTC

PDB ID : 8I40 / pdb_00008i40
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.; Millerieux, 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	:	4-5-2 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

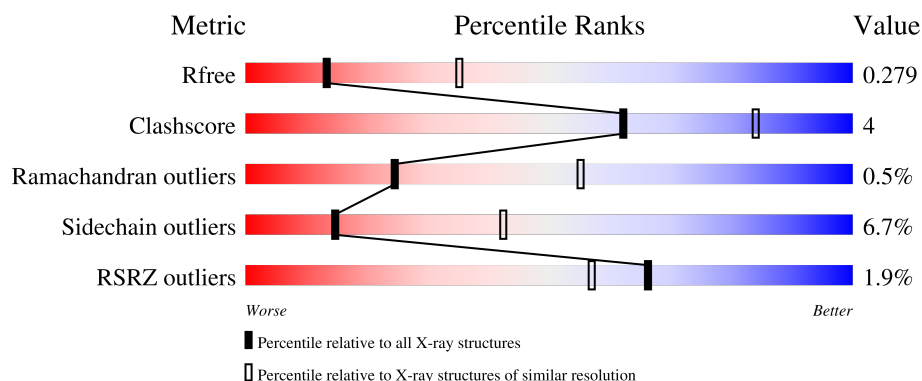
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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
1	A	467	Total	C	N	O	S	0	0	0
			3514	2209	615	667	23			
1	B	467	Total	C	N	O	S	0	0	0
			3515	2209	615	668	23			
1	C	468	Total	C	N	O	S	0	0	0
			3520	2212	616	669	23			
1	D	466	Total	C	N	O	S	0	0	0
			3511	2207	614	667	23			

There are 4 discrepancies between the modelled and reference sequences:

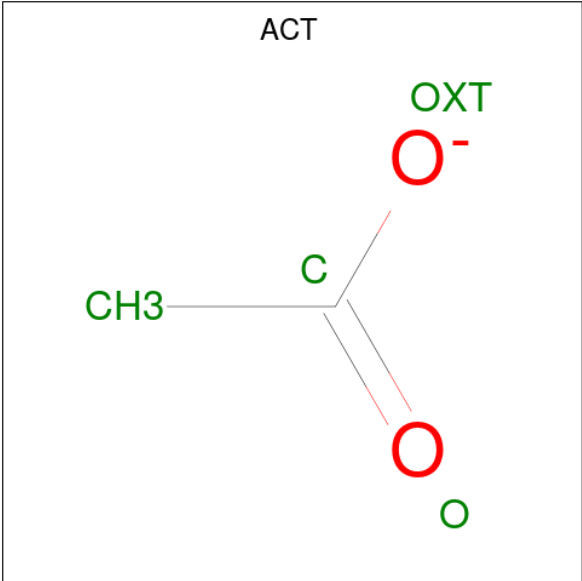
Chain	Residue	Modelled	Actual	Comment	Reference
A	419	ASN	SER	conflict	UNP Q386P1
B	419	ASN	SER	conflict	UNP Q386P1
C	419	ASN	SER	conflict	UNP Q386P1
D	419	ASN	SER	conflict	UNP Q386P1

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is CALCIUM ION (CCD ID: 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

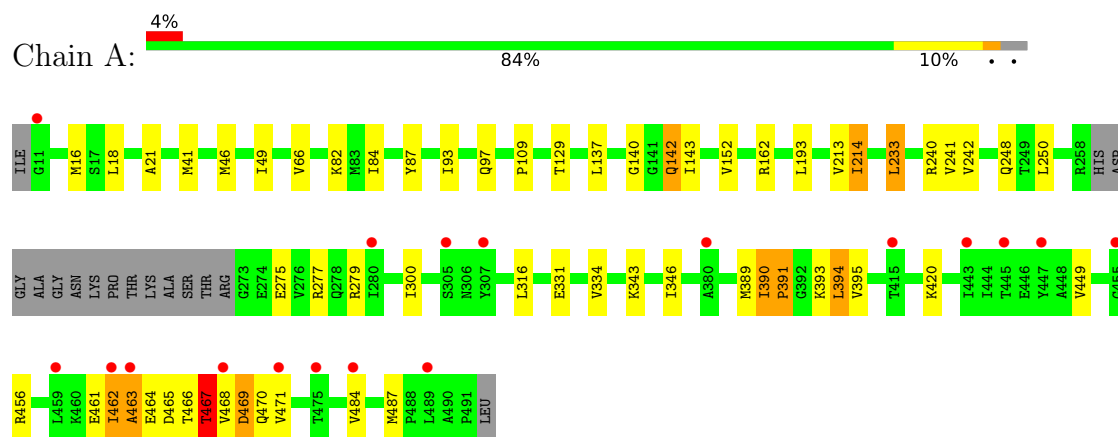
- Molecule 5 is water.

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

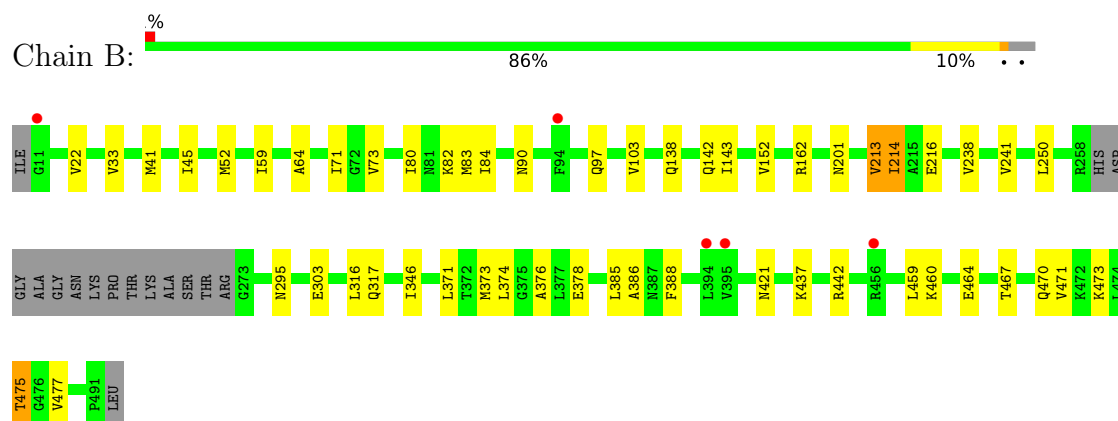
3 Residue-property plots [i](#)

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.

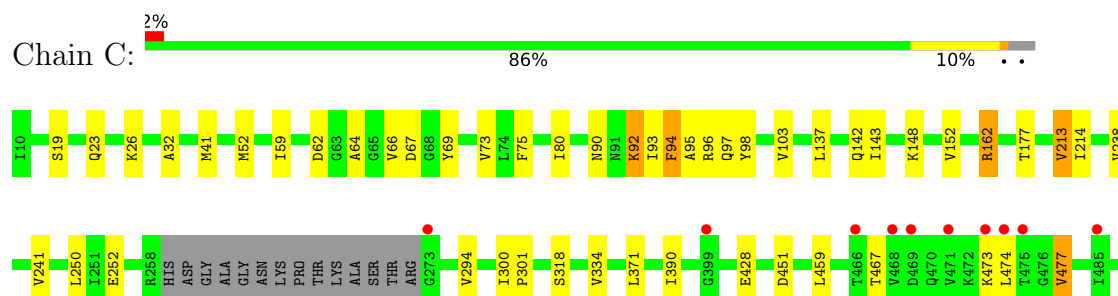
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase



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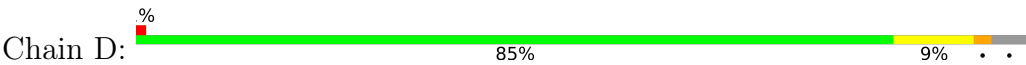


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase



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



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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) 98.5 (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)	Xtriage
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 (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CA, 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	0.67	0/3571	0.88	6/4831 (0.1%)
1	B	0.60	0/3572	0.82	1/4833 (0.0%)
1	C	0.65	0/3577	0.84	3/4840 (0.1%)
1	D	0.66	1/3568 (0.0%)	0.87	2/4828 (0.0%)
All	All	0.64	1/14288 (0.0%)	0.85	12/19332 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	300	ILE	CA-CB	-5.12	1.50	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	GLN	N-CA-C	-9.30	95.19	110.17
1	A	463	ALA	N-CA-C	8.48	123.01	109.86
1	B	467	THR	N-CA-C	7.99	122.35	110.52
1	A	389	MET	N-CA-C	7.55	120.06	108.42
1	D	314	VAL	N-CA-C	6.26	118.48	108.85
1	A	391	PRO	N-CA-C	6.21	121.38	111.26
1	C	92	LYS	N-CA-C	6.19	118.02	111.28
1	C	69	TYR	N-CA-C	5.67	116.70	107.23
1	A	395	VAL	N-CA-C	5.59	114.41	106.53
1	A	140	GLY	N-CA-C	-5.38	105.65	112.65
1	C	94	PHE	N-CA-C	-5.05	105.68	111.14
1	D	93	ILE	N-CA-CB	5.03	116.09	110.51

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	3514	0	3527	56	0
1	B	3515	0	3527	18	0
1	C	3520	0	3529	23	0
1	D	3511	0	3524	21	0
2	A	48	0	31	0	0
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	117	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 (117) 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:HG21	1:A:470:GLN:CD	1.73	1.13
1:A:466:THR:CG2	1:A:470:GLN:NE2	2.12	1.12
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:311:GLY:C	1:D:312:VAL:HG22	2.19	0.68
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:B:41:MET:HE1	1:B:71:ILE:HD12	1.79	0.65
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: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:D:311:GLY:C	1:D:312:VAL:CG2	2.73	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:A:390:ILE:HD12	1:A:390:ILE:C	2.28	0.58
1:D:355:PHE:CE2	1:D:363:MET:HE1	2.39	0.58
1:B:64:ALA:HB2	1:B:83:MET:HE2	1.87	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:391:PRO:C	1:A:393:LYS:N	2.73	0.46
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:B:371:LEU:HD21	1:B:373:MET:HE2	1.98	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:46:MET:HE2	1:A:49:ILE:HD12	1.98	0.45
1:A:84:ILE:HD12	1:A:84:ILE:N	2.32	0.44
1:C:94:PHE:C	1:C:94:PHE:CD2	2.93	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:A:394:LEU:HD23	1:A:394:LEU:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:HA	1:C:52:MET:HE3	2.00	0.43
1:A:463:ALA:C	1:A:465:ASP:HA	2.39	0.43
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:D:355:PHE:CZ	1:D:363:MET:HE1	2.54	0.42
1:B:41:MET:HE1	1:B:71:ILE:CD1	2.46	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: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%)	43 72
1	B	463/483 (96%)	432 (93%)	28 (6%)	3 (1%)	21 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	464/483 (96%)	441 (95%)	23 (5%)	0	100	100
1	D	462/483 (96%)	436 (94%)	20 (4%)	6 (1%)	9	31
All	All	1852/1932 (96%)	1746 (94%)	96 (5%)	10 (0%)	24	55

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 ⓘ

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%)	351 (94%)	24 (6%)	16	44
1	B	375/387 (97%)	353 (94%)	22 (6%)	18	48
1	C	375/387 (97%)	352 (94%)	23 (6%)	17	46
1	D	375/387 (97%)	344 (92%)	31 (8%)	10	32
All	All	1500/1548 (97%)	1400 (93%)	100 (7%)	15	42

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	66	VAL

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Mol	Chain	Res	Type
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	275	GLU
1	A	279	ARG
1	A	316	LEU
1	A	346	ILE
1	A	390	ILE
1	A	394	LEU
1	A	420	LYS
1	A	456	ARG
1	A	462	ILE
1	A	467	THR
1	A	469	ASP
1	B	73	VAL
1	B	90	ASN
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	346	ILE
1	B	374	LEU
1	B	421	ASN
1	B	437	LYS
1	B	442	ARG
1	B	459	LEU
1	B	460	LYS
1	B	470	GLN
1	B	473	LYS

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Mol	Chain	Res	Type
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	137	LEU
1	C	142	GLN
1	C	148	LYS
1	C	162	ARG
1	C	213	VAL
1	C	214	ILE
1	C	241	VAL
1	C	250	LEU
1	C	318	SER
1	C	334	VAL
1	C	390	ILE
1	C	451	ASP
1	C	459	LEU
1	C	467	THR
1	C	473	LYS
1	C	474	LEU
1	C	477	VAL
1	D	26	LYS
1	D	66	VAL
1	D	93	ILE
1	D	142	GLN
1	D	162	ARG
1	D	175	ILE
1	D	198	THR
1	D	213	VAL
1	D	214	ILE
1	D	233	LEU
1	D	241	VAL
1	D	250	LEU
1	D	254	ARG
1	D	274	GLU
1	D	275	GLU
1	D	296	LEU
1	D	298	ILE

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Mol	Chain	Res	Type
1	D	303	GLU
1	D	305	SER
1	D	314	VAL
1	D	343	LYS
1	D	346	ILE
1	D	387	ASN
1	D	389	MET
1	D	421	ASN
1	D	429	ARG
1	D	434	VAL
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 (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	77	ASN
1	A	306	ASN
1	A	382	ASN
1	A	470	GLN
1	B	47	GLN
1	B	77	ASN
1	B	97	GLN
1	B	208	GLN
1	B	232	HIS
1	B	248	GLN
1	B	306	ASN
1	B	419	ASN
1	C	77	ASN
1	C	97	GLN
1	C	208	GLN
1	C	248	GLN
1	C	306	ASN
1	C	382	ASN
1	C	438	HIS
1	D	97	GLN
1	D	110	GLN
1	D	208	GLN
1	D	248	GLN

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Mol	Chain	Res	Type
1	D	278	GLN
1	D	290	ASN
1	D	306	ASN
1	D	344	GLN
1	D	382	ASN
1	D	387	ASN
1	D	419	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 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	A	501	1	47,50,50	1.35	6 (12%)	69,75,75	1.63	11 (15%)
3	ACT	A	502	-	3,3,3	0.98	0	3,3,3	1.10	0
2	COA	C	501	-	47,50,50	1.38	6 (12%)	69,75,75	1.60	11 (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
2	COA	A	501	1	-	11/48/64/64	0/3/3/3
2	COA	C	501	-	-	10/48/64/64	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	COA	C5A-C4A	5.03	1.48	1.39
2	C	501	COA	C5A-C4A	5.00	1.48	1.39
2	C	501	COA	P1A-O3A	3.48	1.63	1.59
2	C	501	COA	P2A-O3A	3.38	1.63	1.59
2	A	501	COA	P2A-O3A	3.11	1.62	1.59
2	A	501	COA	P1A-O3A	2.97	1.62	1.59
2	C	501	COA	C5A-C6A	2.97	1.49	1.41
2	A	501	COA	C5A-C6A	2.92	1.49	1.41
2	C	501	COA	C8A-N7A	2.48	1.36	1.31
2	A	501	COA	C8A-N7A	2.37	1.36	1.31
2	A	501	COA	C5A-N7A	-2.36	1.34	1.39
2	C	501	COA	C5A-N7A	-2.29	1.34	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	COA	C5A-C4A-N3A	-6.02	118.43	126.72
2	C	501	COA	C5A-C4A-N3A	-5.65	118.93	126.72
2	A	501	COA	N3A-C4A-N9A	4.72	135.19	127.17
2	C	501	COA	N3A-C4A-N9A	4.68	135.12	127.17
2	A	501	COA	C2A-N3A-C4A	3.97	121.52	111.83
2	C	501	COA	C2A-N3A-C4A	3.84	121.21	111.83
2	C	501	COA	N3A-C2A-N1A	-3.80	122.84	128.58
2	A	501	COA	N3A-C2A-N1A	-3.77	122.88	128.58
2	A	501	COA	C4A-C5A-N7A	-3.60	106.47	110.58
2	C	501	COA	C4A-C5A-N7A	-3.53	106.55	110.58
2	C	501	COA	C4A-N9A-C8A	3.16	109.06	105.74
2	C	501	COA	C5A-N7A-C8A	2.79	107.84	103.45
2	A	501	COA	C5A-N7A-C8A	2.72	107.72	103.45
2	A	501	COA	O6A-CCP-CBP	2.56	114.66	110.55
2	A	501	COA	C6P-C5P-N4P	2.47	120.83	116.34
2	A	501	COA	C4A-N9A-C8A	2.43	108.29	105.74
2	C	501	COA	N9A-C8A-N7A	-2.34	110.62	113.94
2	C	501	COA	O4B-C1B-N9A	2.31	112.53	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	COA	C2A-N1A-C6A	2.20	122.34	118.73
2	A	501	COA	C3B-C2B-C1B	2.17	104.67	99.89
2	C	501	COA	C6A-C5A-N7A	2.17	136.27	132.09
2	A	501	COA	C6A-C5A-N7A	2.13	136.20	132.09

There are no chirality outliers.

All (21) 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	CCP-O6A-P2A-O5A
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	C	501	COA	CDP-CBP-CCP-O6A
2	C	501	COA	CEP-CBP-CCP-O6A
2	A	501	COA	C6P-C5P-N4P-C3P
2	A	501	COA	O5P-C5P-N4P-C3P
2	A	501	COA	O4B-C4B-C5B-O5B
2	A	501	COA	C3B-C4B-C5B-O5B
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	C	501	COA	CAP-CBP-CCP-O6A
2	C	501	COA	C5B-O5B-P1A-O1A
2	C	501	COA	O4B-C4B-C5B-O5B
2	A	501	COA	C4B-C5B-O5B-P1A

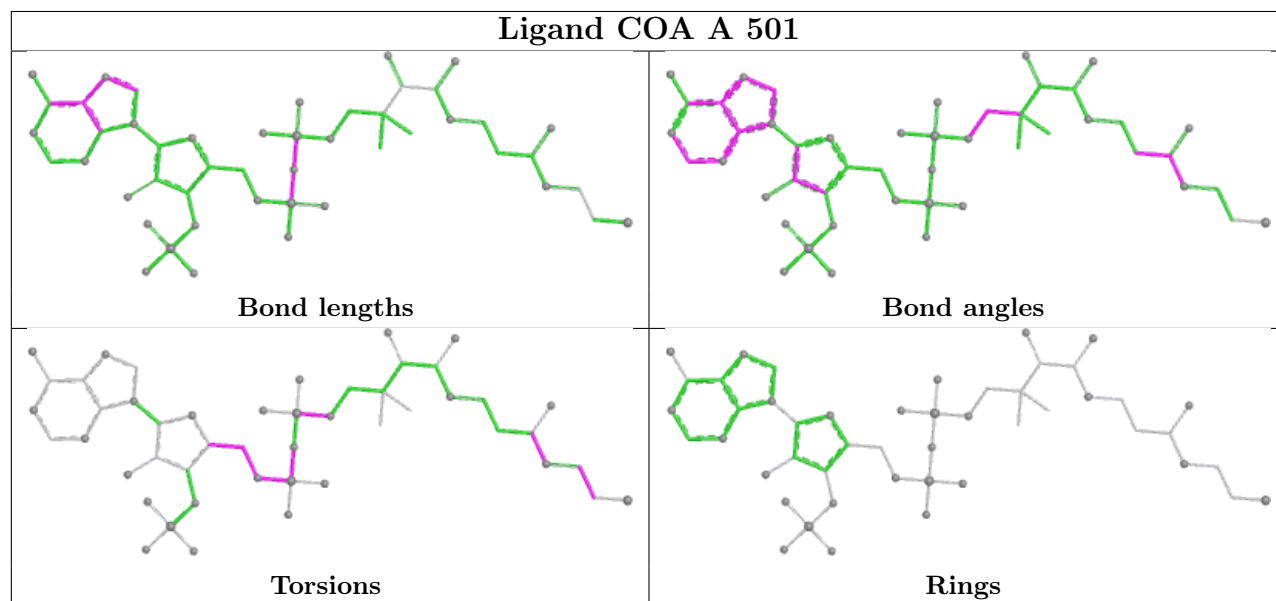
There are no ring outliers.

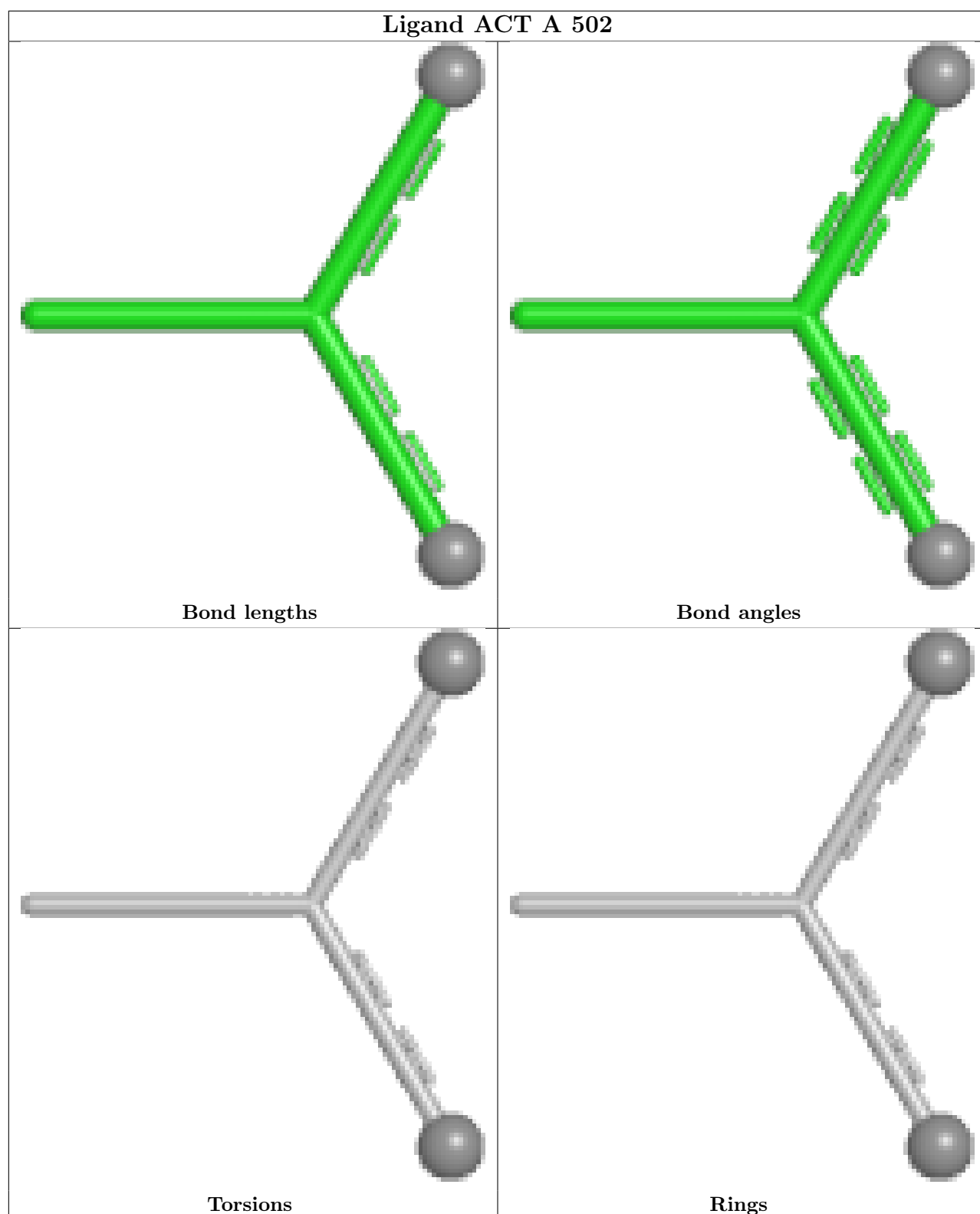
1 monomer is involved in 6 short contacts:

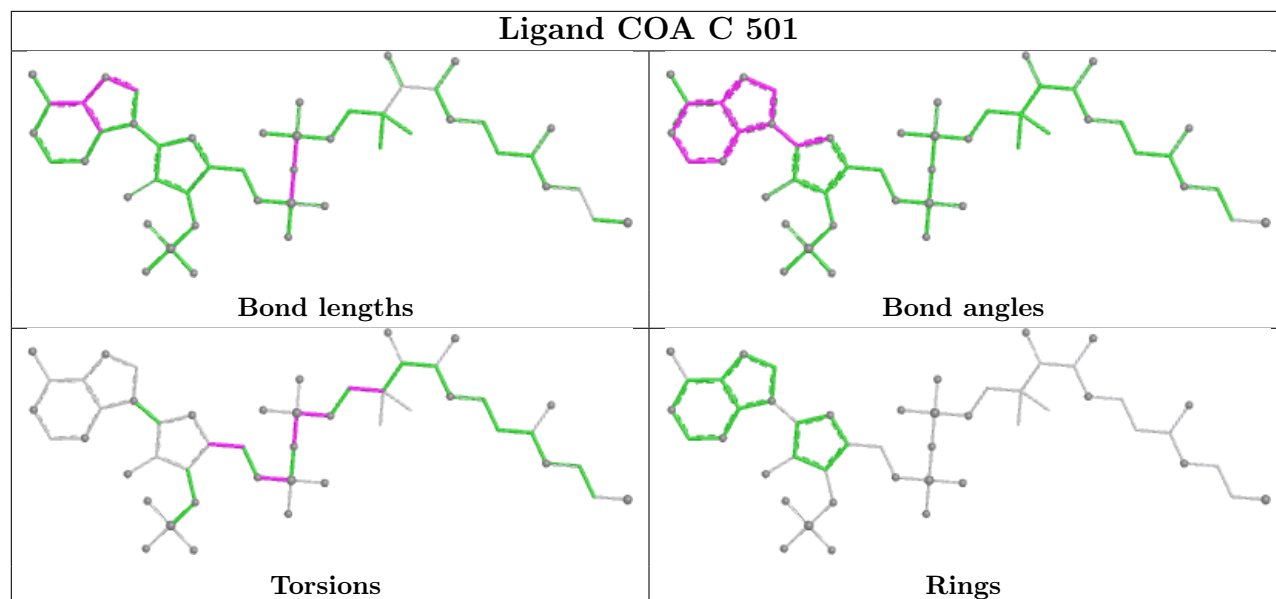
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	ACT	6	0

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%)	0.23	18 (3%) 43 34	27, 44, 93, 121	1 (0%)
1	B	467/483 (96%)	-0.04	5 (1%) 78 70	26, 42, 64, 102	1 (0%)
1	C	468/483 (96%)	0.16	10 (2%) 63 54	25, 47, 86, 113	1 (0%)
1	D	466/483 (96%)	-0.01	3 (0%) 85 80	29, 42, 62, 89	1 (0%)
All	All	1868/1932 (96%)	0.08	36 (1%) 66 57	25, 43, 85, 121	4 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	GLY	3.1
1	A	280	ILE	3.1
1	C	468	VAL	3.1
1	C	475	THR	3.0
1	B	395	VAL	2.9
1	C	473	LYS	2.9
1	A	380	ALA	2.8
1	A	415	THR	2.8
1	A	462	ILE	2.7
1	D	273	GLY	2.6
1	C	466	THR	2.6
1	C	474	LEU	2.6
1	B	11	GLY	2.5
1	A	475	THR	2.5
1	C	485	ILE	2.5
1	C	469	ASP	2.5
1	D	466	THR	2.4
1	A	459	LEU	2.4
1	A	447	TYR	2.4
1	A	471	VAL	2.4
1	A	489	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	305	SER	2.3
1	A	468	VAL	2.3
1	C	399	GLY	2.3
1	C	273	GLY	2.3
1	A	443	ILE	2.2
1	A	445	THR	2.2
1	D	312	VAL	2.2
1	B	394	LEU	2.2
1	B	94	PHE	2.2
1	A	463	ALA	2.1
1	A	455	GLY	2.1
1	C	471	VAL	2.1
1	B	456	ARG	2.1
1	A	484	VAL	2.1
1	A	307	TYR	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](#)

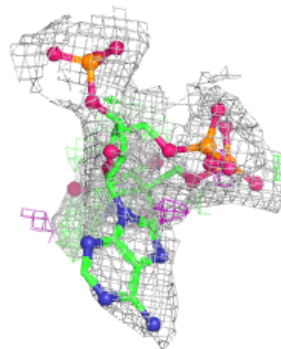
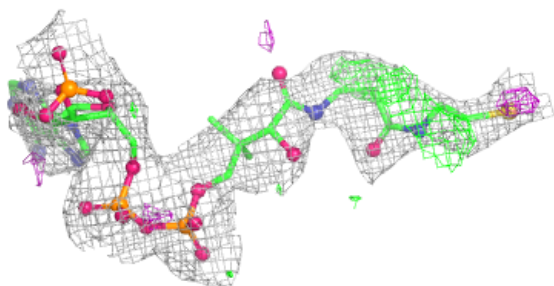
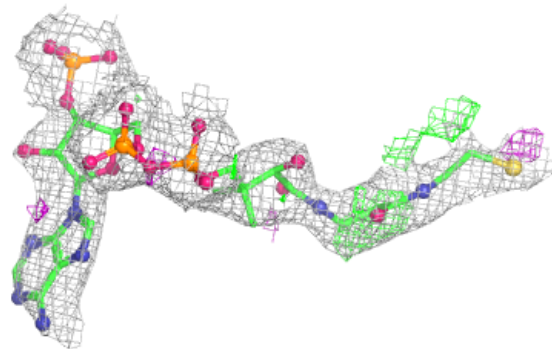
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	COA	A	501	48/48	0.69	0.14	76,88,100,103	0
3	ACT	A	502	4/4	0.76	0.14	59,62,62,63	0
2	COA	C	501	48/48	0.80	0.12	65,74,85,87	0
4	CA	D	701	1/1	0.82	0.12	83,83,83,83	0
4	CA	B	701	1/1	0.84	0.09	74,74,74,74	0
4	CA	A	503	1/1	0.89	0.11	77,77,77,77	0
4	CA	C	502	1/1	0.91	0.14	68,68,68,68	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.

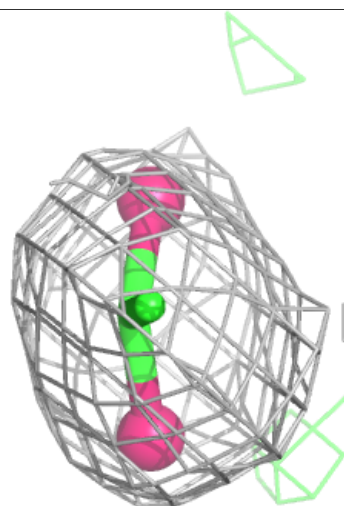
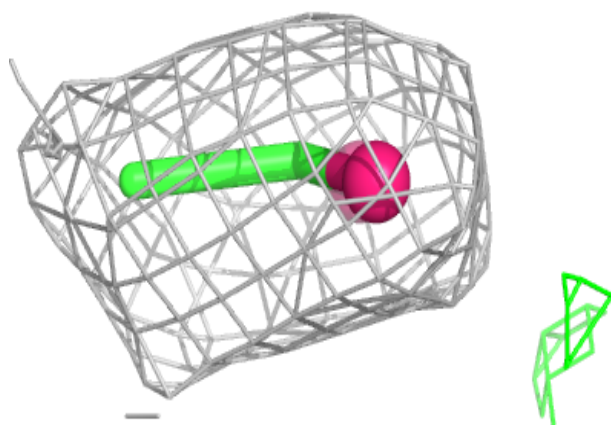
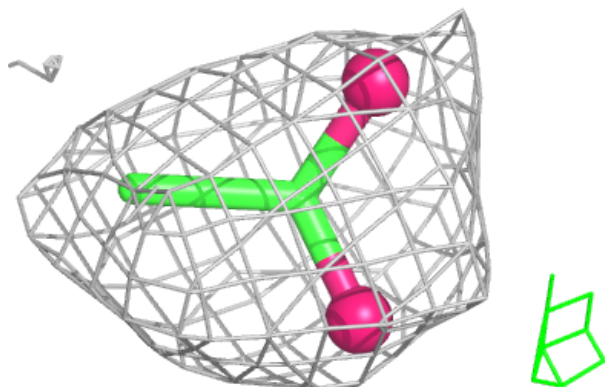
Electron density around COA A 501:

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



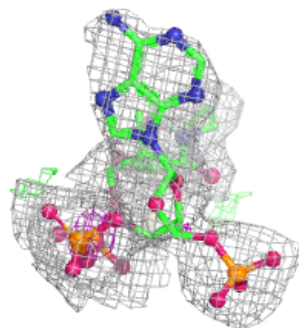
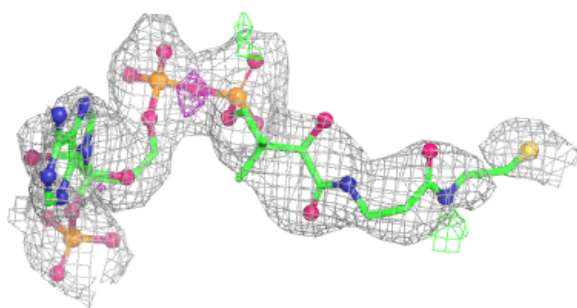
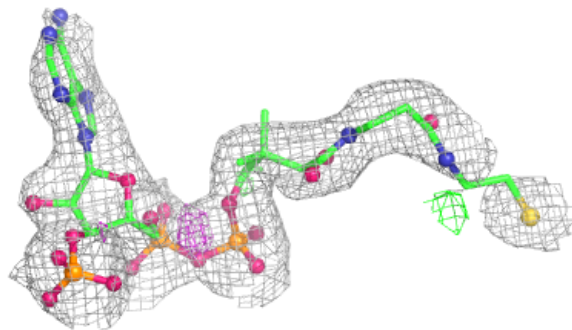
Electron density around ACT A 502:

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



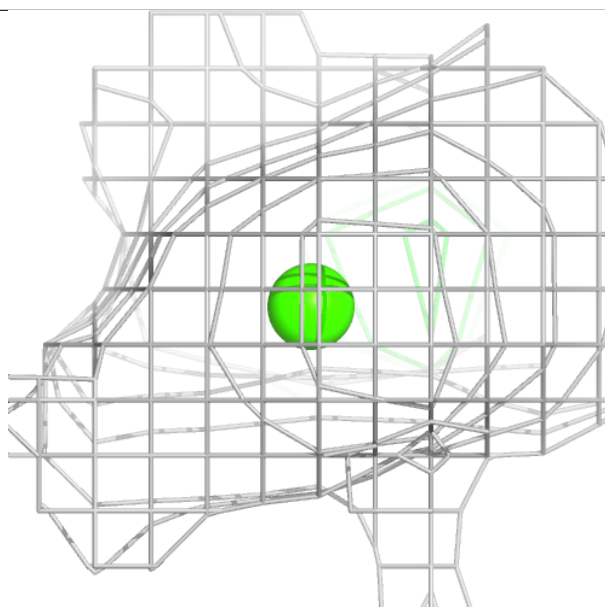
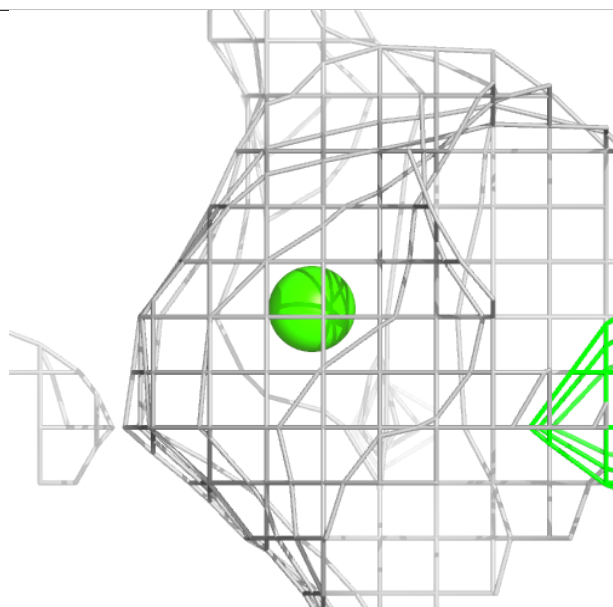
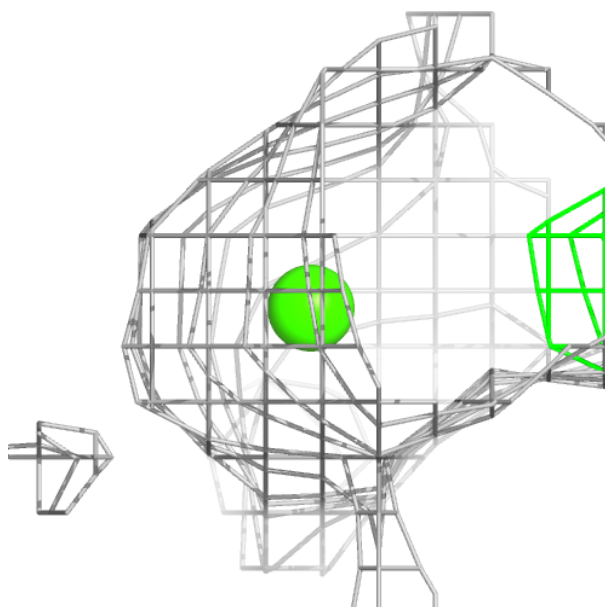
Electron density around COA C 501:

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



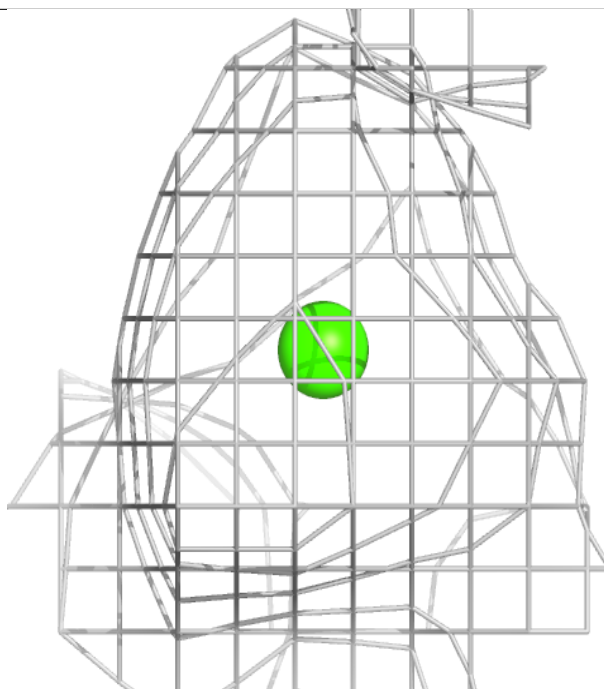
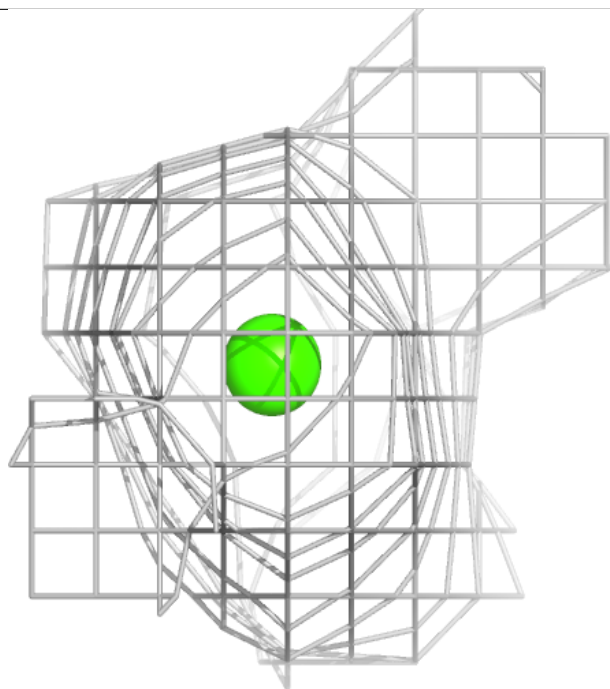
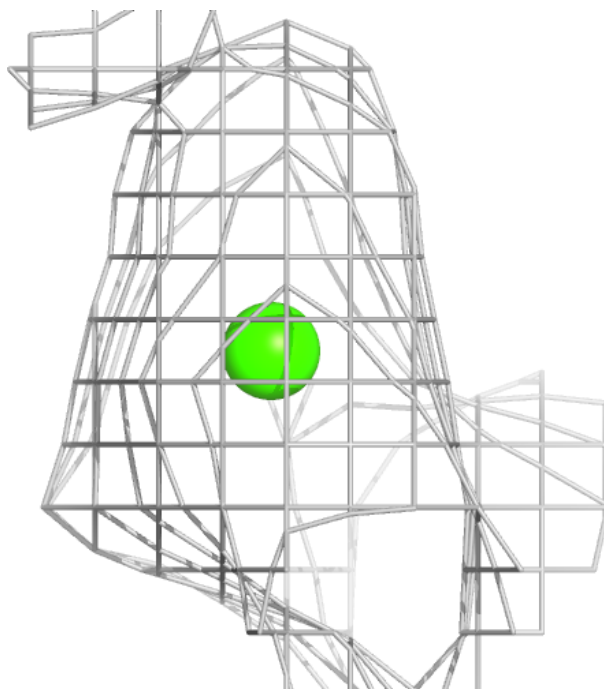
Electron density around CA D 701:

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



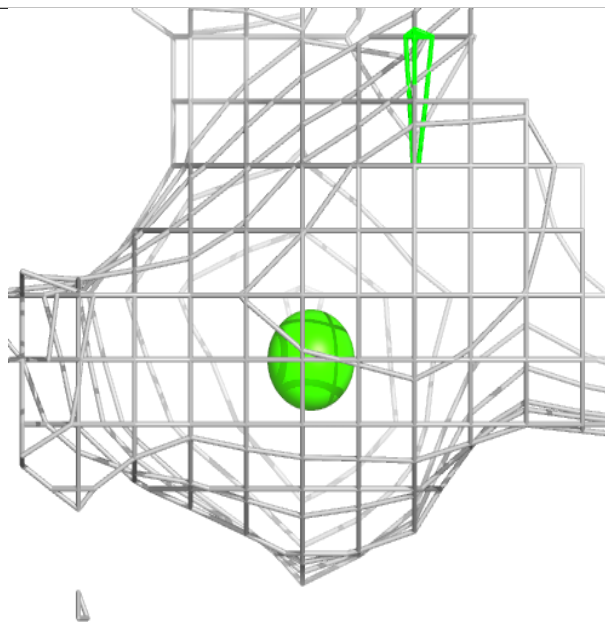
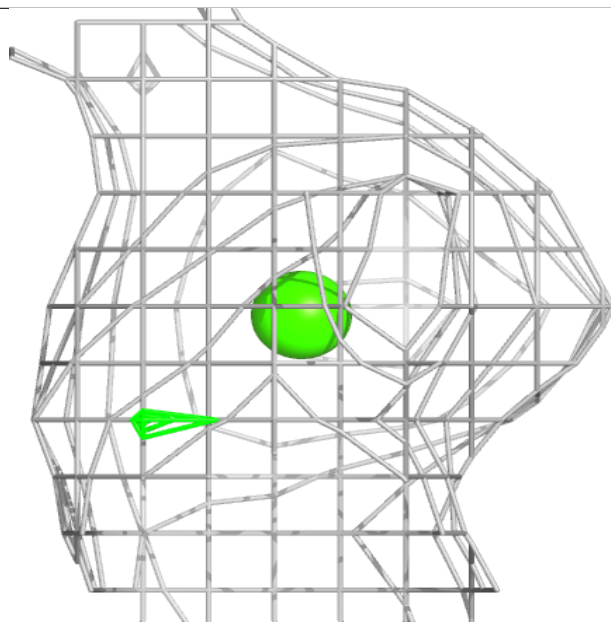
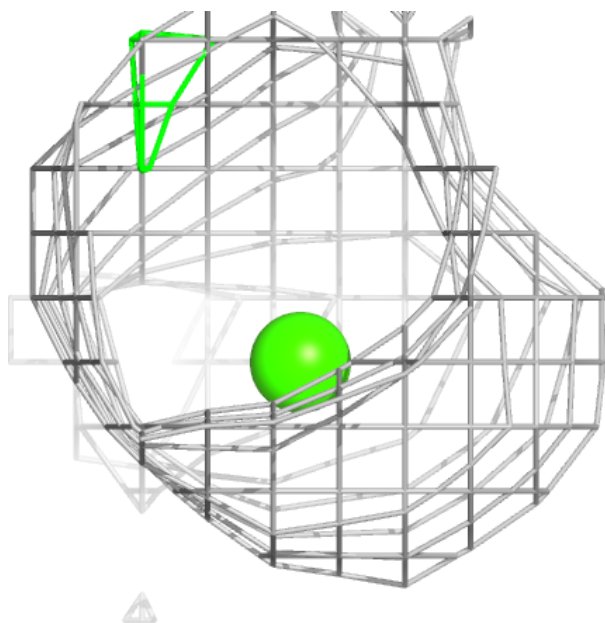
Electron density around CA B 701:

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



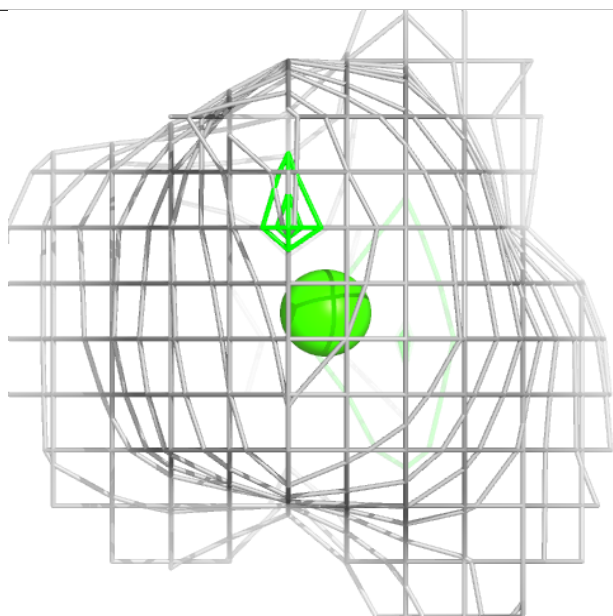
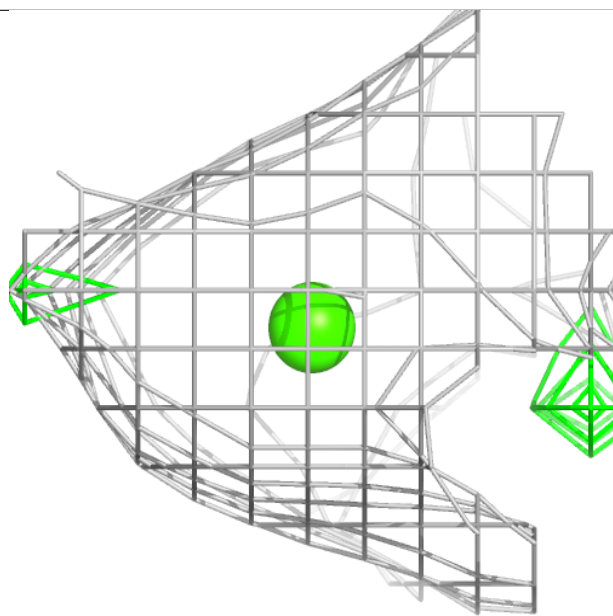
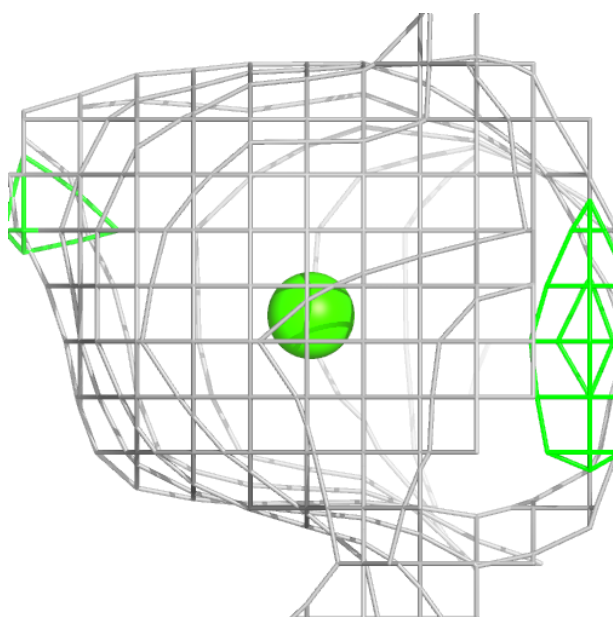
Electron density around CA A 503:

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



Electron density around 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.