Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 06:01 AM JST

PDB ID	:	6L2C
Title	:	Crystal structure of Aspergillus fumigatus mitochondrial acetyl-CoA acetyl-transferase in complex with CoA
Authors	:	Zhang, Y.; Wei, W.; Raimi, O.G.; Ferenbach, A.T.; Fang, W.
Deposited on	:	2019-10-03
Resolution	:	2.44 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:

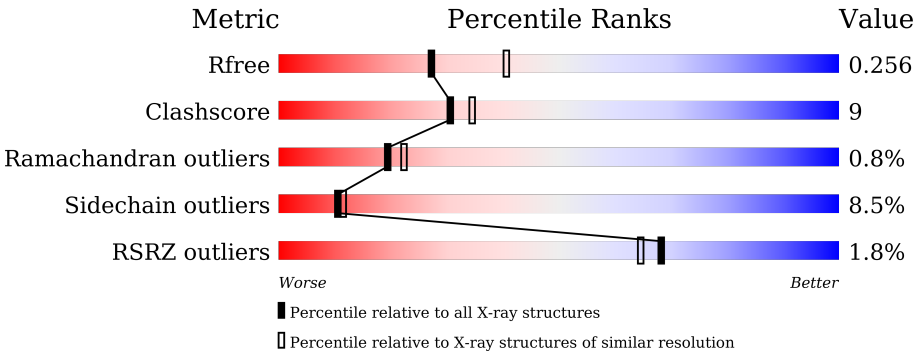
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	402	2% 80% 16% ·
1	B	402	2% 85% 12% · ·
1	C	402	3% 75% 21% · ·
1	D	402	85% 13% ··

2 Entry composition (i)

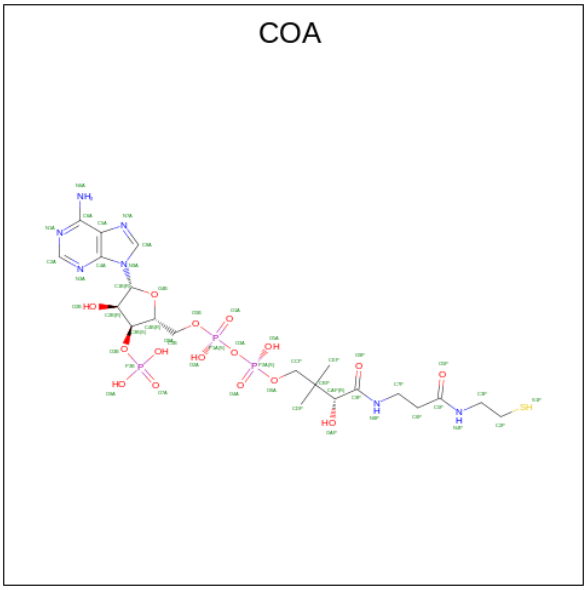
There are 3 unique types of molecules in this entry. The entry contains 12260 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetyl-CoA-acetyltransferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			2978	1872	521	573	12			
1	B	399	Total	C	N	O	S	0	0	0
			2959	1860	518	569	12			
1	C	398	Total	C	N	O	S	0	0	0
			2950	1854	516	568	12			
1	D	398	Total	C	N	O	S	0	0	0
			2950	1854	516	568	12			

- Molecule 2 is COENZYME A (three-letter code: 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	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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

- Molecule 3 is water.

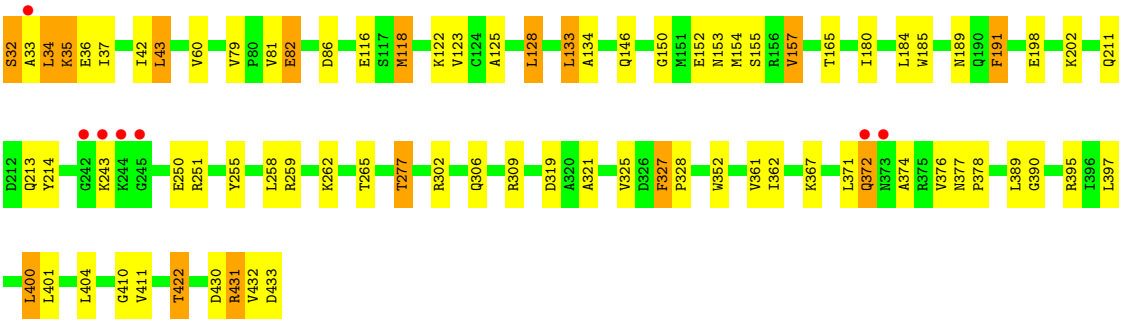
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total	O	0	0
			75	75		
3	B	82	Total	O	0	0
			82	82		
3	C	25	Total	O	0	0
			25	25		
3	D	49	Total	O	0	0
			49	49		

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.

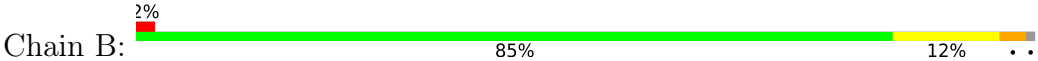
• Molecule 1: Acetyl-CoA-acetyltransferase, putative

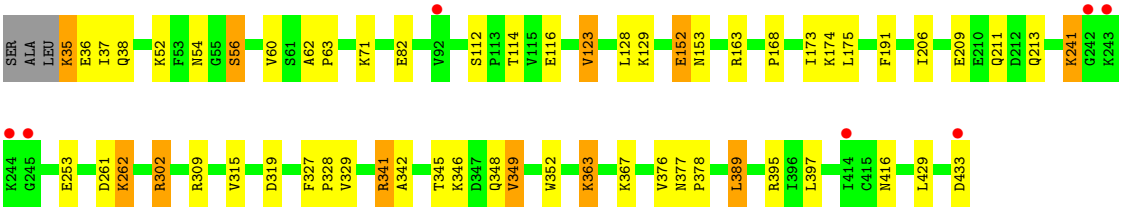
Chain A:



• Molecule 1: Acetyl-CoA-acetyltransferase, putative

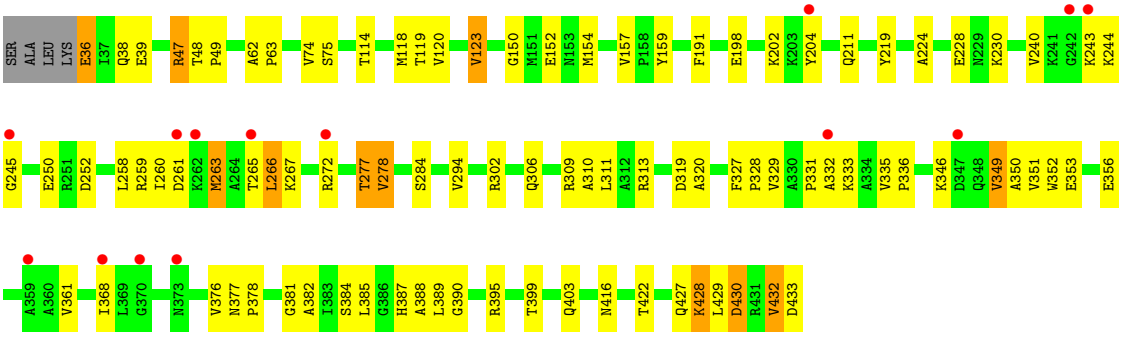
Chain B:





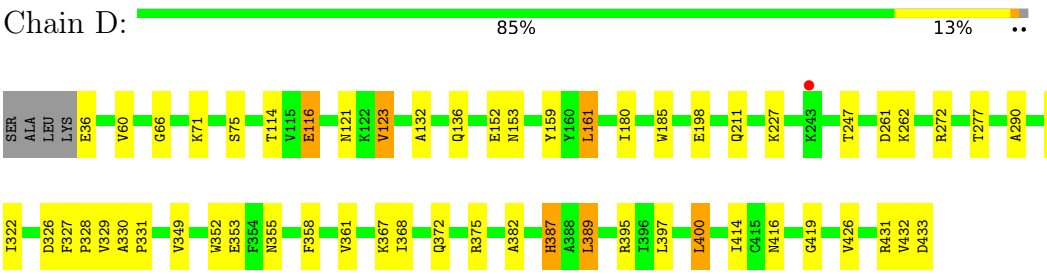
• Molecule 1: Acetyl-CoA-acetyltransferase, putative

Chain C:



• Molecule 1: Acetyl-CoA-acetyltransferase, putative

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.25Å 173.55Å 180.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 2.44 49.62 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.67-2.44) 99.2 (49.62-2.44)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.203 , 0.257 0.206 , 0.256	Depositor DCC
R_{free} test set	3736 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 30.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12260	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, 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	0.72	1/3016 (0.0%)	0.79	0/4084
1	B	0.76	1/2997 (0.0%)	0.76	0/4058
1	C	0.62	0/2988	0.76	0/4047
1	D	0.72	0/2988	0.76	0/4047
All	All	0.71	2/11989 (0.0%)	0.77	0/16236

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	GLU	CD-OE2	-5.20	1.20	1.25
1	A	152	GLU	CD-OE2	-5.09	1.20	1.25

There are no bond angle outliers.

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	2978	0	3016	62	0
1	B	2959	0	2995	41	0
1	C	2950	0	2982	89	0
1	D	2950	0	2982	35	0
2	A	48	0	32	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	32	2	0
2	C	48	0	32	8	0
2	D	48	0	32	2	0
3	A	75	0	0	0	0
3	B	82	0	0	0	0
3	C	25	0	0	0	0
3	D	49	0	0	3	0
All	All	12260	0	12103	221	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 (221) 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:C:428:LYS:C	1:C:429:LEU:HD23	1.52	1.29
1:C:211:GLN:NE2	1:C:277:THR:OG1	1.72	1.20
1:C:211:GLN:NE2	1:C:277:THR:HG1	1.45	1.12
1:C:39:GLU:OE1	1:C:313:ARG:NH1	1.82	1.11
1:C:284:SER:O	2:C:501:COA:O9P	1.67	1.10
1:C:427:GLN:HG2	1:C:429:LEU:HD21	1.29	1.08
1:C:356:GLU:CD	1:C:381:GLY:HA3	1.75	1.06
1:C:428:LYS:O	1:C:429:LEU:HD23	1.59	1.02
2:C:501:COA:H141	2:C:501:COA:HN8	1.23	1.02
1:B:209:GLU:O	1:B:213:GLN:HG3	1.63	0.98
1:C:198:GLU:OE2	1:C:278:VAL:HG12	1.64	0.97
1:C:346:LYS:O	1:C:349:VAL:HG13	1.63	0.97
1:C:302:ARG:HG3	1:C:432:VAL:HG11	1.50	0.92
1:C:47:ARG:HH11	1:C:47:ARG:HG3	1.36	0.91
2:A:501:COA:C8A	2:A:501:COA:H51A	2.00	0.90
2:A:501:COA:H51A	2:A:501:COA:H8A	1.53	0.90
1:C:263:MET:HA	1:C:266:LEU:HD22	1.54	0.89
1:C:356:GLU:OE2	1:C:381:GLY:HA3	1.74	0.88
1:C:427:GLN:HG2	1:C:429:LEU:CD2	2.03	0.87
1:C:349:VAL:HG21	1:C:352:TRP:CE2	2.11	0.86
1:C:356:GLU:OE2	1:C:381:GLY:CA	2.22	0.86
1:A:211:GLN:OE1	1:A:277:THR:CG2	2.24	0.86
1:C:211:GLN:HE21	1:C:277:THR:HG1	1.25	0.84
1:A:34:LEU:HD23	1:A:35:LYS:HE2	1.60	0.84
1:A:262:LYS:O	1:A:265:THR:OG1	1.95	0.83
1:D:262:LYS:NZ	3:D:601:HOH:O	1.90	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:PRO:O	1:C:335:VAL:HG13	1.80	0.81
1:C:306:GLN:HE22	1:C:432:VAL:H	1.26	0.78
1:A:302:ARG:HG2	1:A:432:VAL:CG2	2.13	0.78
1:C:428:LYS:O	1:C:429:LEU:CD2	2.30	0.77
1:B:262:LYS:NZ	2:B:501:COA:O8A	2.18	0.76
1:C:428:LYS:C	1:C:429:LEU:CD2	2.46	0.75
1:A:302:ARG:HG2	1:A:432:VAL:HG23	1.67	0.75
1:A:118:MET:HE1	1:B:129:LYS:HE3	1.69	0.74
1:A:328:PRO:HB3	1:A:361:VAL:HG22	1.68	0.74
2:A:501:COA:O2A	2:A:501:COA:H4B	1.88	0.72
1:A:34:LEU:O	1:B:37:ILE:HD12	1.89	0.72
1:A:122:LYS:HZ1	1:A:422:THR:HG22	1.55	0.72
1:A:211:GLN:OE1	1:A:277:THR:HG21	1.89	0.71
1:C:36:GLU:HA	1:C:36:GLU:OE1	1.90	0.71
1:C:429:LEU:HD23	1:C:429:LEU:N	2.02	0.71
1:C:356:GLU:CD	1:C:381:GLY:CA	2.58	0.71
2:A:501:COA:H8A	2:A:501:COA:C5B	2.20	0.70
1:A:211:GLN:OE1	1:A:277:THR:HG23	1.90	0.70
1:A:431:ARG:NH1	1:A:433:ASP:OD2	2.25	0.69
2:C:501:COA:HN8	2:C:501:COA:CEP	2.03	0.69
2:D:501:COA:OAP	2:D:501:COA:H72	1.92	0.69
1:C:335:VAL:N	1:C:336:PRO:HD2	2.08	0.68
1:C:198:GLU:OE1	1:C:277:THR:HG23	1.94	0.68
1:C:311:LEU:N	1:C:428:LYS:HZ2	1.92	0.67
1:A:367:LYS:HA	1:A:372:GLN:HE22	1.58	0.67
1:A:306:GLN:O	1:A:430:ASP:O	2.12	0.67
1:A:431:ARG:NH1	1:A:433:ASP:OD1	2.29	0.65
1:A:118:MET:CE	1:B:129:LYS:HE3	2.25	0.65
1:C:319:ASP:HB2	1:D:116:GLU:HG3	1.79	0.65
1:C:198:GLU:OE2	1:C:278:VAL:CG1	2.42	0.64
1:C:319:ASP:CB	1:D:116:GLU:HG3	2.28	0.64
1:C:432:VAL:HG12	1:C:433:ASP:N	2.12	0.64
1:B:60:VAL:O	1:B:153:ASN:ND2	2.30	0.63
1:A:122:LYS:NZ	1:A:422:THR:HG22	2.13	0.63
1:C:47:ARG:HG3	1:C:47:ARG:NH1	2.10	0.62
1:C:302:ARG:HA	1:C:306:GLN:OE1	1.99	0.62
1:D:306:GLN:OE1	1:D:431:ARG:HB2	1.99	0.62
1:B:377:ASN:N	1:B:378:PRO:HD3	2.13	0.62
1:A:157:VAL:O	1:B:163:ARG:NH2	2.33	0.62
1:B:168:PRO:HG2	1:B:173:ILE:HD11	1.82	0.62
1:C:349:VAL:CG2	1:C:352:TRP:CE2	2.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:SER:O	1:B:163:ARG:CD	2.48	0.61
1:D:329:VAL:HG12	1:D:329:VAL:O	2.01	0.61
1:C:266:LEU:HD21	2:C:501:COA:N3A	2.16	0.61
1:C:311:LEU:O	1:C:428:LYS:CD	2.49	0.61
1:A:371:LEU:O	1:A:374:ALA:N	2.32	0.60
1:A:155:SER:O	1:B:163:ARG:HD2	2.00	0.60
1:A:259:ARG:HH21	1:A:262:LYS:HD2	1.66	0.60
1:D:198:GLU:OE1	1:D:277:THR:HG22	2.01	0.60
1:B:345:THR:OG1	1:B:348:GLN:HG3	2.01	0.60
1:C:382:ALA:HB1	1:C:387:HIS:HB2	1.83	0.60
1:C:353:GLU:OE2	1:C:399:THR:HG22	2.02	0.60
1:C:198:GLU:CD	1:C:278:VAL:HG12	2.23	0.59
1:C:328:PRO:HB3	1:C:361:VAL:HG22	1.85	0.59
1:C:320:ALA:HB1	1:C:333:LYS:HG2	1.85	0.58
1:C:432:VAL:CG1	1:C:433:ASP:N	2.66	0.58
1:D:330:ALA:N	1:D:331:PRO:CD	2.67	0.58
2:A:501:COA:O5P	2:A:501:COA:N8P	2.35	0.57
1:B:173:ILE:HG12	1:D:159:TYR:CE2	2.40	0.56
1:B:241:LYS:O	1:B:241:LYS:HG3	2.04	0.56
1:C:311:LEU:O	1:C:428:LYS:HD3	2.05	0.56
2:C:501:COA:O5P	2:C:501:COA:H22	2.03	0.56
1:A:431:ARG:NH1	1:A:433:ASP:CG	2.58	0.56
1:C:311:LEU:N	1:C:428:LYS:NZ	2.53	0.56
1:A:400:LEU:O	1:A:400:LEU:HD22	2.05	0.55
1:A:431:ARG:HH11	1:A:433:ASP:CG	2.09	0.55
1:D:329:VAL:HG13	1:D:368:ILE:CD1	2.36	0.55
1:B:206:ILE:HG22	1:B:211:GLN:HG3	1.89	0.55
1:A:32:SER:N	1:B:341:ARG:HD3	2.21	0.55
1:B:206:ILE:HG12	1:B:363:LYS:HB3	1.89	0.55
1:B:327:PHE:N	1:B:328:PRO:CD	2.69	0.55
1:C:118:MET:HE2	1:C:120:VAL:HG22	1.89	0.54
1:C:309:ARG:O	1:C:428:LYS:NZ	2.34	0.54
1:D:302:ARG:NH1	1:D:433:ASP:O	2.40	0.54
2:B:501:COA:O6A	2:B:501:COA:OAP	2.22	0.54
1:B:168:PRO:CG	1:B:173:ILE:CD1	2.86	0.53
1:C:335:VAL:H	1:C:336:PRO:HD2	1.73	0.53
1:C:224:ALA:O	1:C:228:GLU:HG2	2.09	0.53
1:C:432:VAL:HG12	1:C:433:ASP:H	1.74	0.53
2:C:501:COA:H141	2:C:501:COA:N8P	2.03	0.53
1:D:329:VAL:CG1	1:D:368:ILE:CD1	2.87	0.52
1:B:123:VAL:HB	1:B:416:ASN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:PHE:CG	1:A:328:PRO:HD3	2.46	0.51
1:D:349:VAL:HG22	1:D:352:TRP:NE1	2.25	0.51
1:C:47:ARG:HD2	1:C:395:ARG:HG2	1.92	0.51
1:A:431:ARG:HD3	1:A:433:ASP:OD2	2.10	0.51
1:C:428:LYS:HD2	1:C:429:LEU:H	1.76	0.50
1:D:327:PHE:CD2	1:D:328:PRO:HD3	2.46	0.50
1:A:198:GLU:OE1	1:A:277:THR:HB	2.11	0.50
1:A:180:ILE:O	1:A:185:TRP:HB2	2.12	0.50
1:A:259:ARG:HH21	1:A:262:LYS:CD	2.24	0.50
1:D:400:LEU:HD22	1:D:400:LEU:O	2.12	0.50
1:D:116:GLU:HA	1:D:116:GLU:OE2	2.11	0.50
1:C:306:GLN:O	1:C:430:ASP:O	2.29	0.49
1:C:349:VAL:CG2	1:C:352:TRP:NE1	2.75	0.49
1:C:377:ASN:N	1:C:378:PRO:HD3	2.27	0.49
1:A:259:ARG:HE	1:A:262:LYS:HD2	1.76	0.49
1:B:302:ARG:NE	1:B:433:ASP:OD2	2.34	0.49
1:C:74:VAL:HA	1:C:294:VAL:HG21	1.94	0.49
1:C:349:VAL:HG22	1:C:352:TRP:NE1	2.26	0.49
2:D:501:COA:H131	3:D:607:HOH:O	2.13	0.49
1:C:219:TYR:CD1	1:C:384:SER:HB3	2.48	0.49
1:B:352:TRP:HB2	1:B:376:VAL:HG22	1.95	0.48
1:A:404:LEU:HD11	1:A:410:GLY:HA3	1.94	0.48
1:A:155:SER:O	1:B:163:ARG:HD3	2.12	0.48
1:C:428:LYS:HD2	1:C:429:LEU:N	2.28	0.48
1:C:118:MET:CE	1:C:120:VAL:HG22	2.43	0.48
1:C:150:GLY:HA3	1:C:390:GLY:O	2.14	0.48
1:C:349:VAL:HG22	1:C:349:VAL:O	2.14	0.48
1:B:315:VAL:HG11	1:B:342:ALA:HB1	1.95	0.48
1:D:375:ARG:HB2	3:D:611:HOH:O	2.14	0.48
1:A:125:ALA:HB1	1:A:422:THR:HG23	1.96	0.48
1:D:132:ALA:O	1:D:136:GLN:HG3	2.14	0.48
1:A:154:MET:O	1:A:157:VAL:HG13	2.13	0.48
2:A:501:COA:H141	2:A:501:COA:H71	1.95	0.48
1:C:356:GLU:OE2	1:C:381:GLY:C	2.52	0.48
1:B:168:PRO:HD2	1:B:173:ILE:HD12	1.96	0.47
1:C:74:VAL:CG2	1:C:75:SER:N	2.78	0.47
1:C:356:GLU:CG	1:C:381:GLY:HA3	2.44	0.47
1:A:118:MET:CE	1:B:129:LYS:CE	2.93	0.47
1:C:319:ASP:HB3	1:D:116:GLU:HG3	1.97	0.47
1:C:74:VAL:HG23	1:C:75:SER:N	2.29	0.46
1:D:60:VAL:O	1:D:153:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.75	0.46
1:B:62:ALA:HB3	1:B:63:PRO:HD3	1.97	0.46
1:C:119:THR:HB	1:D:121:ASN:HB3	1.96	0.46
1:C:311:LEU:O	1:C:428:LYS:HD2	2.16	0.46
1:B:168:PRO:CG	1:B:173:ILE:HD11	2.45	0.45
1:C:159:TYR:HB2	1:D:161:LEU:HB3	1.98	0.45
1:B:168:PRO:HD2	1:B:173:ILE:CD1	2.47	0.45
1:C:329:VAL:O	1:C:332:ALA:N	2.46	0.45
1:A:165:THR:HG21	1:B:54:ASN:CG	2.37	0.45
1:C:154:MET:HA	1:C:157:VAL:HG23	1.99	0.45
1:C:259:ARG:HA	1:C:259:ARG:HD3	1.68	0.44
1:C:310:ALA:C	1:C:428:LYS:HZ2	2.19	0.44
1:A:377:ASN:N	1:A:378:PRO:HD3	2.32	0.44
1:A:118:MET:HE2	1:B:129:LYS:CE	2.47	0.44
1:C:204:TYR:CZ	1:C:368:ILE:HD11	2.52	0.44
1:A:42:ILE:HG21	1:A:401:LEU:CD1	2.48	0.44
1:A:251:ARG:NH1	1:A:255:TYR:OH	2.50	0.44
1:B:56:SER:OG	1:B:253:GLU:OE1	2.28	0.44
1:A:60:VAL:O	1:A:153:ASN:ND2	2.50	0.44
1:A:352:TRP:CZ3	1:A:411:VAL:HG11	2.52	0.44
1:A:42:ILE:HD13	1:A:401:LEU:HD11	1.99	0.43
1:A:371:LEU:O	1:A:372:GLN:C	2.56	0.43
1:C:349:VAL:HG21	1:C:352:TRP:CZ2	2.51	0.43
1:D:180:ILE:O	1:D:185:TRP:HB2	2.18	0.43
1:A:86:ASP:OD1	1:A:116:GLU:HB3	2.19	0.43
1:B:152:GLU:HG2	1:B:389:LEU:HB2	2.01	0.43
1:C:263:MET:HA	1:C:263:MET:HE3	2.01	0.43
1:D:329:VAL:HG13	1:D:368:ILE:HD12	2.00	0.43
1:B:315:VAL:CG1	1:B:342:ALA:HB1	2.48	0.43
1:C:48:THR:HB	1:C:49:PRO:CD	2.48	0.43
1:A:319:ASP:OD1	1:A:422:THR:HB	2.18	0.43
1:D:123:VAL:HB	1:D:416:ASN:HB2	2.01	0.43
1:A:150:GLY:HA3	1:A:390:GLY:O	2.18	0.43
1:C:335:VAL:N	1:C:336:PRO:CD	2.79	0.43
1:C:252:ASP:OD2	1:C:385:LEU:HD22	2.19	0.42
1:C:378:PRO:HG2	1:C:403:GLN:OE1	2.19	0.42
1:A:189:ASN:HB3	1:A:191:PHE:CE2	2.54	0.42
1:A:321:ALA:O	1:B:114:THR:HA	2.19	0.42
1:A:37:ILE:HD12	1:B:35:LYS:HA	2.00	0.42
1:A:116:GLU:HG2	1:B:319:ASP:HB3	2.02	0.42
1:A:214:TYR:CZ	1:A:362:ILE:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:MET:HE3	1:C:266:LEU:CD2	2.50	0.42
1:A:367:LYS:HA	1:A:372:GLN:NE2	2.30	0.42
1:D:382:ALA:HB1	1:D:387:HIS:HB2	2.01	0.42
1:A:211:GLN:CD	1:A:277:THR:HG23	2.39	0.42
1:D:322:ILE:HD11	1:D:326:ASP:O	2.20	0.42
1:D:355:ASN:HB2	1:D:414:ILE:HD12	2.01	0.42
1:B:346:LYS:O	1:B:349:VAL:HG13	2.19	0.42
1:D:152:GLU:HG2	1:D:389:LEU:HB2	2.02	0.41
1:D:306:GLN:OE1	1:D:431:ARG:HA	2.20	0.41
1:D:358:PHE:O	1:D:361:VAL:HB	2.21	0.41
1:A:82:GLU:H	1:A:82:GLU:HG3	1.47	0.41
1:A:118:MET:HE2	1:B:129:LYS:HE2	2.01	0.41
1:B:128:LEU:HD12	1:B:128:LEU:HA	1.89	0.41
1:D:211:GLN:OE1	1:D:277:THR:CG2	2.69	0.41
1:A:43:LEU:HD23	1:A:79:VAL:HG11	2.03	0.41
1:B:327:PHE:N	1:B:328:PRO:HD3	2.35	0.41
1:C:62:ALA:HB3	1:C:63:PRO:HD3	2.03	0.41
1:C:356:GLU:O	1:C:382:ALA:HB3	2.20	0.41
1:C:356:GLU:OE2	1:C:381:GLY:N	2.53	0.41
1:D:349:VAL:CG2	1:D:352:TRP:CE2	3.04	0.41
1:A:134:ALA:O	1:A:146:GLN:HG3	2.21	0.40
2:C:501:COA:O9P	2:C:501:COA:H61	2.21	0.40
1:D:327:PHE:CB	1:D:419:GLY:HA2	2.52	0.40
1:C:152:GLU:HB3	1:C:388:ALA:HB1	2.02	0.40
1:C:320:ALA:CB	1:C:333:LYS:HG2	2.49	0.40
1:D:327:PHE:CG	1:D:328:PRO:HD3	2.56	0.40
1:C:266:LEU:HD12	1:C:266:LEU:HA	1.78	0.40
1:C:356:GLU:HB2	1:C:382:ALA:N	2.36	0.40
2:C:501:COA:CEP	2:C:501:COA:N8P	2.73	0.40
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.85	0.40
1:D:66:GLY:HA2	1:D:290:ALA:HB1	2.03	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	399/402 (99%)	381 (96%)	14 (4%)	4 (1%)	15 16
1	B	396/402 (98%)	385 (97%)	9 (2%)	2 (0%)	29 34
1	C	395/402 (98%)	360 (91%)	30 (8%)	5 (1%)	12 11
1	D	395/402 (98%)	378 (96%)	15 (4%)	2 (0%)	29 34
All	All	1585/1608 (99%)	1504 (95%)	68 (4%)	13 (1%)	19 22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	LEU
1	C	389	LEU
1	A	33	ALA
1	B	389	LEU
1	D	389	LEU
1	C	243	LYS
1	B	123	VAL
1	C	123	VAL
1	C	350	ALA
1	D	123	VAL
1	A	123	VAL
1	A	372	GLN
1	C	245	GLY

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	303/303 (100%)	275 (91%)	28 (9%)	9 9
1	B	301/303 (99%)	276 (92%)	25 (8%)	11 12
1	C	300/303 (99%)	270 (90%)	30 (10%)	7 7
1	D	300/303 (99%)	281 (94%)	19 (6%)	18 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1204/1212 (99%)	1102 (92%)	102 (8%)	10 11

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	34	LEU
1	A	35	LYS
1	A	36	GLU
1	A	43	LEU
1	A	81	VAL
1	A	82	GLU
1	A	118	MET
1	A	128	LEU
1	A	133	LEU
1	A	157	VAL
1	A	184	LEU
1	A	191	PHE
1	A	202	LYS
1	A	213	GLN
1	A	243	LYS
1	A	250	GLU
1	A	258	LEU
1	A	277	THR
1	A	309	ARG
1	A	325	VAL
1	A	327	PHE
1	A	376	VAL
1	A	395	ARG
1	A	397	LEU
1	A	400	LEU
1	A	422	THR
1	A	431	ARG
1	B	35	LYS
1	B	36	GLU
1	B	38	GLN
1	B	52	LYS
1	B	56	SER
1	B	71	LYS
1	B	82	GLU
1	B	112	SER
1	B	116	GLU

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Mol	Chain	Res	Type
1	B	174	LYS
1	B	175	LEU
1	B	191	PHE
1	B	241	LYS
1	B	261	ASP
1	B	262	LYS
1	B	302	ARG
1	B	309	ARG
1	B	329	VAL
1	B	341	ARG
1	B	349	VAL
1	B	363	LYS
1	B	367	LYS
1	B	395	ARG
1	B	397	LEU
1	B	429	LEU
1	C	36	GLU
1	C	38	GLN
1	C	47	ARG
1	C	114	THR
1	C	123	VAL
1	C	191	PHE
1	C	202	LYS
1	C	230	LYS
1	C	240	VAL
1	C	244	LYS
1	C	250	GLU
1	C	258	LEU
1	C	260	ILE
1	C	261	ASP
1	C	263	MET
1	C	265	THR
1	C	266	LEU
1	C	267	LYS
1	C	272	ARG
1	C	277	THR
1	C	278	VAL
1	C	327	PHE
1	C	349	VAL
1	C	351	VAL
1	C	376	VAL
1	C	416	ASN

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Mol	Chain	Res	Type
1	C	422	THR
1	C	428	LYS
1	C	430	ASP
1	C	432	VAL
1	D	36	GLU
1	D	71	LYS
1	D	75	SER
1	D	114	THR
1	D	116	GLU
1	D	161	LEU
1	D	227	LYS
1	D	247	THR
1	D	261	ASP
1	D	272	ARG
1	D	353	GLU
1	D	367	LYS
1	D	372	GLN
1	D	387	HIS
1	D	395	ARG
1	D	397	LEU
1	D	400	LEU
1	D	426	VAL
1	D	432	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
1	B	136	GLN
1	B	189	ASN
1	C	211	GLN
1	C	306	GLN
1	D	189	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSO	A	124	1	3,6,7	0.85	0	0,6,8	-	-
1	CSO	D	124	1	3,6,7	0.77	0	0,6,8	-	-
1	CSO	B	124	1	3,6,7	0.82	0	0,6,8	-	-
1	CSO	C	124	1	3,6,7	0.71	0	0,6,8	-	-

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
1	CSO	A	124	1	-	0/1/5/7	-
1	CSO	D	124	1	-	1/1/5/7	-
1	CSO	B	124	1	-	0/1/5/7	-
1	CSO	C	124	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	124	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	COA	B	501	-	41,50,50	0.67	0	52,75,75	0.80	2 (3%)
2	COA	D	501	-	41,50,50	0.69	0	52,75,75	0.74	1 (1%)
2	COA	A	501	-	41,50,50	0.73	1 (2%)	52,75,75	1.17	6 (11%)
2	COA	C	501	-	41,50,50	0.66	0	52,75,75	0.75	1 (1%)

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	B	501	-	-	12/44/64/64	0/3/3/3
2	COA	D	501	-	-	21/44/64/64	0/3/3/3
2	COA	A	501	-	-	15/44/64/64	0/3/3/3
2	COA	C	501	-	-	15/44/64/64	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	COA	C8A-N7A	-2.00	1.31	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	COA	C2B-C3B-C4B	-4.00	96.14	103.22
2	B	501	COA	C7P-C6P-C5P	-2.92	107.50	112.36
2	A	501	COA	P2A-O3A-P1A	-2.76	123.36	132.83
2	D	501	COA	C5A-C6A-N6A	2.70	124.46	120.35
2	A	501	COA	O2B-C2B-C1B	2.63	120.57	110.85
2	B	501	COA	C5A-C6A-N6A	2.42	124.03	120.35
2	C	501	COA	C5A-C6A-N6A	2.39	123.99	120.35
2	A	501	COA	O6A-CCP-CBP	-2.30	106.86	110.55
2	A	501	COA	P1A-O5B-C5B	-2.15	109.09	121.68
2	A	501	COA	C5A-C6A-N6A	2.14	123.61	120.35

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	COA	C3B-O3B-P3B-O9A
2	A	501	COA	CCP-O6A-P2A-O3A
2	A	501	COA	CCP-O6A-P2A-O4A
2	A	501	COA	CAP-C9P-N8P-C7P
2	A	501	COA	O9P-C9P-N8P-C7P
2	A	501	COA	C5P-C6P-C7P-N8P
2	A	501	COA	C6P-C5P-N4P-C3P
2	A	501	COA	O5P-C5P-N4P-C3P
2	A	501	COA	S1P-C2P-C3P-N4P
2	B	501	COA	OAP-CAP-CBP-CCP
2	B	501	COA	C9P-CAP-CBP-CCP
2	B	501	COA	OAP-CAP-CBP-CDP
2	B	501	COA	C9P-CAP-CBP-CDP
2	B	501	COA	OAP-CAP-CBP-CEP
2	B	501	COA	C9P-CAP-CBP-CEP
2	B	501	COA	C5P-C6P-C7P-N8P
2	C	501	COA	CCP-O6A-P2A-O4A
2	C	501	COA	CDP-CBP-CCP-O6A
2	C	501	COA	CEP-CBP-CCP-O6A
2	C	501	COA	CAP-CBP-CCP-O6A
2	C	501	COA	O9P-C9P-CAP-CBP
2	C	501	COA	N8P-C9P-CAP-CBP
2	C	501	COA	N8P-C9P-CAP-OAP
2	C	501	COA	C2P-C3P-N4P-C5P
2	D	501	COA	C5B-O5B-P1A-O1A
2	D	501	COA	C5B-O5B-P1A-O3A
2	D	501	COA	CAP-CBP-CCP-O6A
2	D	501	COA	OAP-CAP-CBP-CCP

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Mol	Chain	Res	Type	Atoms
2	D	501	COA	C9P-CAP-CBP-CCP
2	D	501	COA	OAP-CAP-CBP-CDP
2	D	501	COA	C9P-CAP-CBP-CDP
2	D	501	COA	OAP-CAP-CBP-CEP
2	D	501	COA	C9P-CAP-CBP-CEP
2	D	501	COA	N8P-C9P-CAP-OAP
2	D	501	COA	CAP-C9P-N8P-C7P
2	D	501	COA	O9P-C9P-N8P-C7P
2	C	501	COA	C6P-C7P-N8P-C9P
2	A	501	COA	C4B-C5B-O5B-P1A
2	D	501	COA	CDP-CBP-CCP-O6A
2	D	501	COA	CEP-CBP-CCP-O6A
2	D	501	COA	C3B-C4B-C5B-O5B
2	C	501	COA	O5P-C5P-C6P-C7P
2	C	501	COA	N4P-C5P-C6P-C7P
2	A	501	COA	O4B-C4B-C5B-O5B
2	D	501	COA	O4B-C4B-C5B-O5B
2	D	501	COA	O9P-C9P-CAP-OAP
2	A	501	COA	C3B-C4B-C5B-O5B
2	D	501	COA	O9P-C9P-CAP-CBP
2	B	501	COA	C5B-O5B-P1A-O3A
2	C	501	COA	CCP-O6A-P2A-O3A
2	D	501	COA	CCP-O6A-P2A-O3A
2	C	501	COA	CAP-C9P-N8P-C7P
2	D	501	COA	C5B-O5B-P1A-O2A
2	D	501	COA	CCP-O6A-P2A-O5A
2	C	501	COA	O9P-C9P-N8P-C7P
2	A	501	COA	CDP-CBP-CCP-O6A
2	B	501	COA	C3B-O3B-P3B-O7A
2	B	501	COA	C3B-O3B-P3B-O8A
2	B	501	COA	CCP-O6A-P2A-O3A
2	B	501	COA	P1A-O3A-P2A-O5A
2	C	501	COA	P1A-O3A-P2A-O5A
2	A	501	COA	C5B-O5B-P1A-O1A
2	A	501	COA	CCP-O6A-P2A-O5A

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	COA	2	0
2	D	501	COA	2	0

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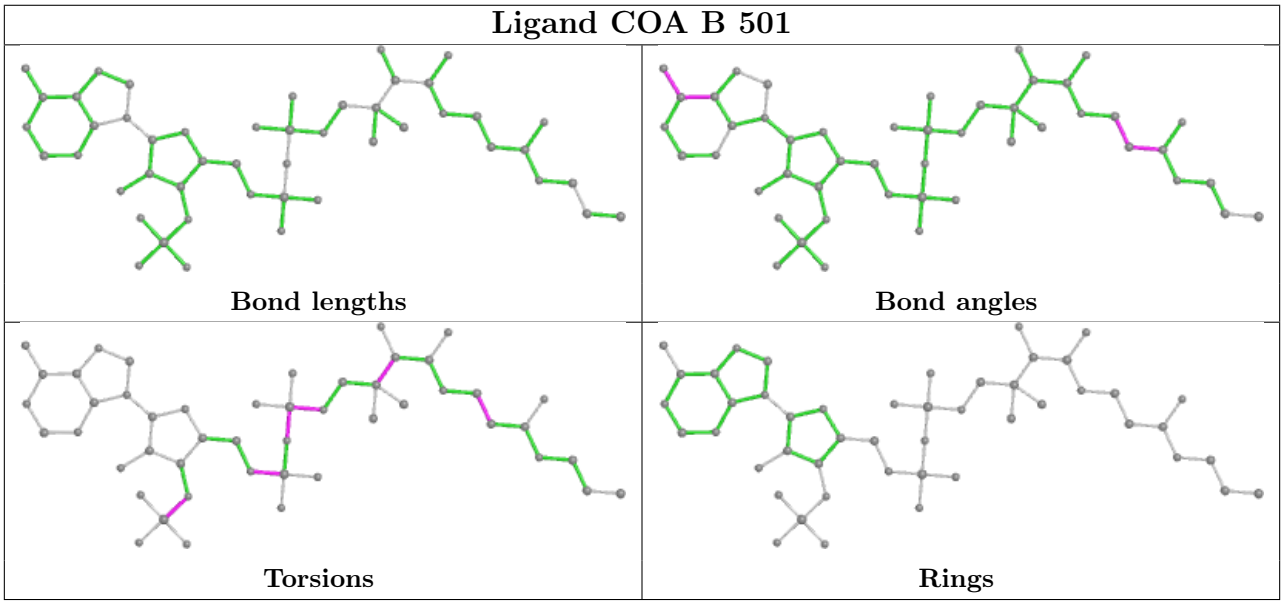
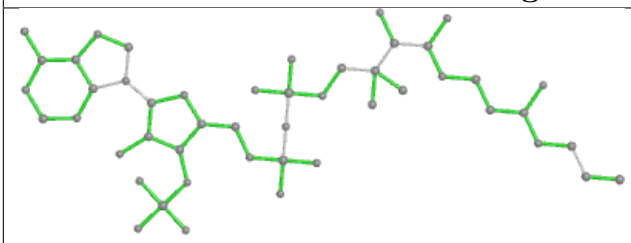
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	COA	6	0
2	C	501	COA	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

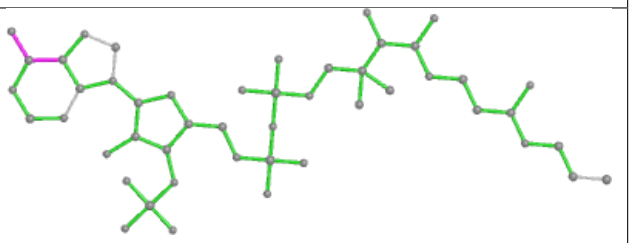
Ligand COA B 501



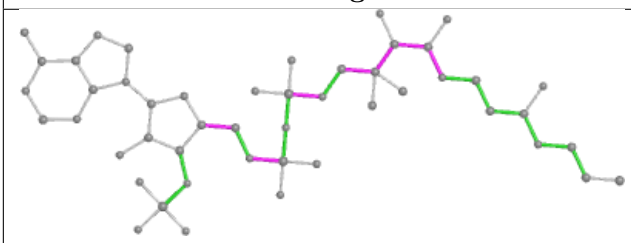
Ligand COA D 501



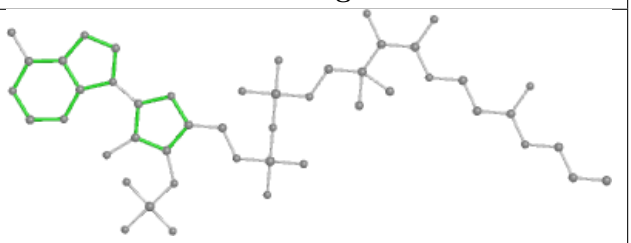
Bond lengths



Bond angles

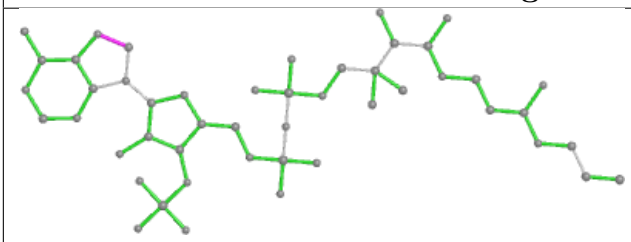


Torsions

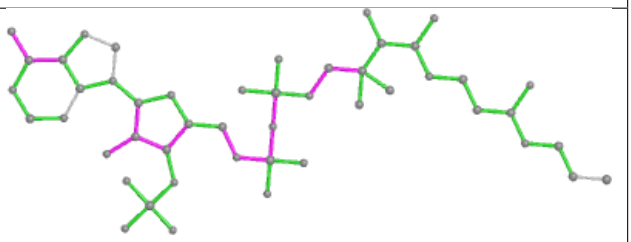


Rings

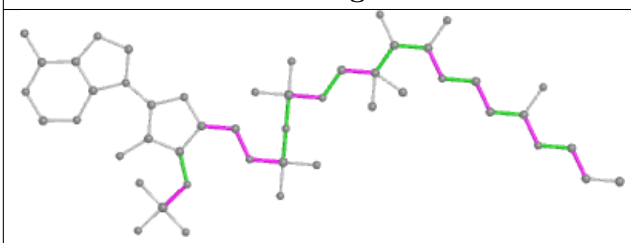
Ligand COA A 501



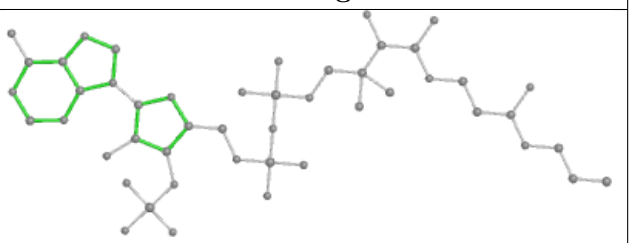
Bond lengths



Bond angles

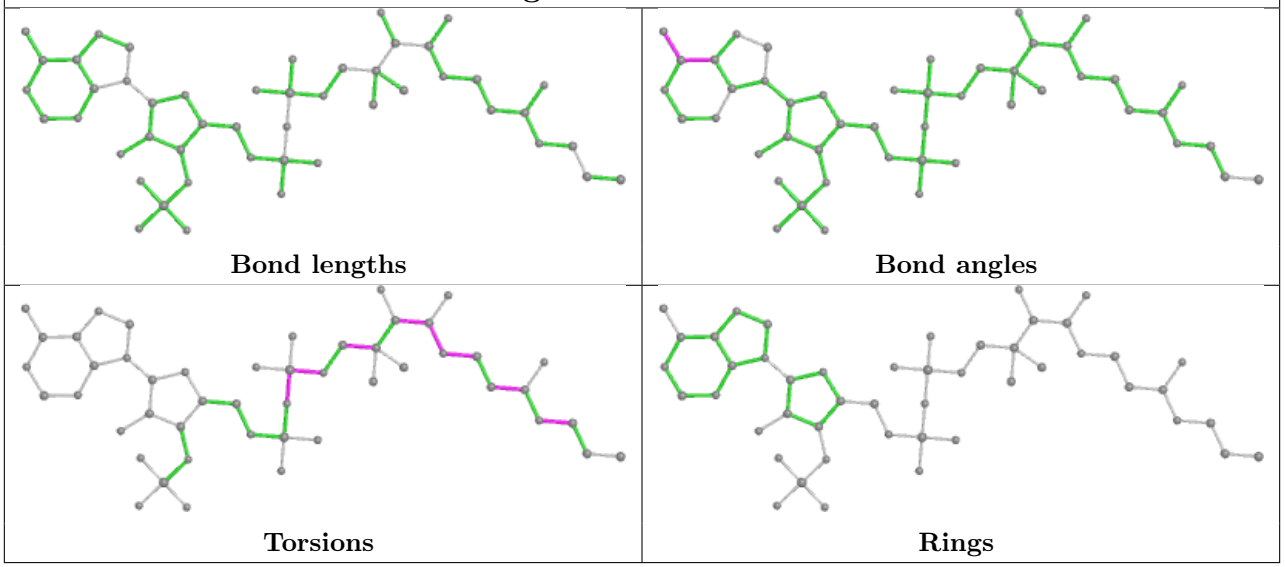


Torsions



Rings

Ligand COA C 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	401/402 (99%)	-0.30	7 (1%)	70	66	30, 46, 72, 137	0
1	B	398/402 (99%)	-0.13	7 (1%)	68	64	29, 42, 73, 124	0
1	C	397/402 (98%)	0.05	14 (3%)	44	40	37, 67, 102, 137	0
1	D	397/402 (98%)	-0.38	1 (0%)	94	94	31, 49, 74, 127	0
All	All	1593/1608 (99%)	-0.19	29 (1%)	68	64	29, 50, 90, 137	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	ASN	5.5
1	A	372	GLN	4.1
1	B	243	LYS	4.1
1	A	243	LYS	3.9
1	A	33	ALA	3.8
1	A	244	LYS	3.7
1	C	261	ASP	3.5
1	D	243	LYS	3.5
1	C	368	ILE	3.2
1	A	242	GLY	3.2
1	B	433	ASP	3.1
1	C	245	GLY	3.0
1	C	373	ASN	2.9
1	C	265	THR	2.9
1	C	243	LYS	2.8
1	C	242	GLY	2.8
1	C	332	ALA	2.8
1	C	359	ALA	2.8
1	B	92	VAL	2.7
1	B	244	LYS	2.7
1	C	204	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	262	LYS	2.6
1	B	245	GLY	2.6
1	B	242	GLY	2.6
1	A	245	GLY	2.4
1	C	347	ASP	2.3
1	B	414	ILE	2.2
1	C	272	ARG	2.2
1	C	370	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	CSO	A	124	7/8	0.94	0.14	38,40,48,56	0
1	CSO	B	124	7/8	0.95	0.29	32,34,51,53	0
1	CSO	D	124	7/8	0.95	0.18	41,45,53,64	0
1	CSO	C	124	7/8	0.96	0.12	54,57,62,71	0

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, 95^{th} 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.

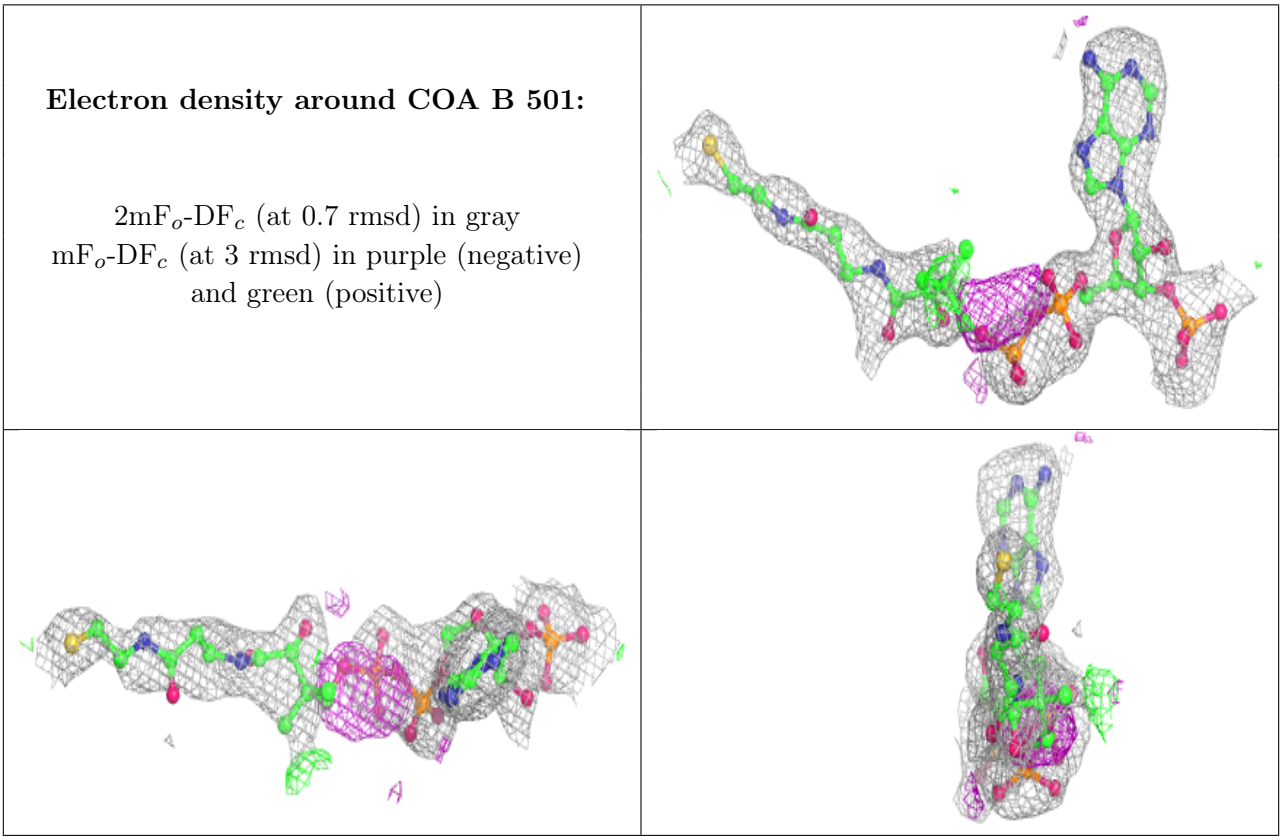
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	COA	B	501	48/48	0.77	0.29	65,92,113,118	0
2	COA	D	501	48/48	0.78	0.32	78,98,119,121	0
2	COA	C	501	48/48	0.81	0.26	78,109,123,137	0
2	COA	A	501	48/48	0.87	0.24	57,80,92,97	0

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.

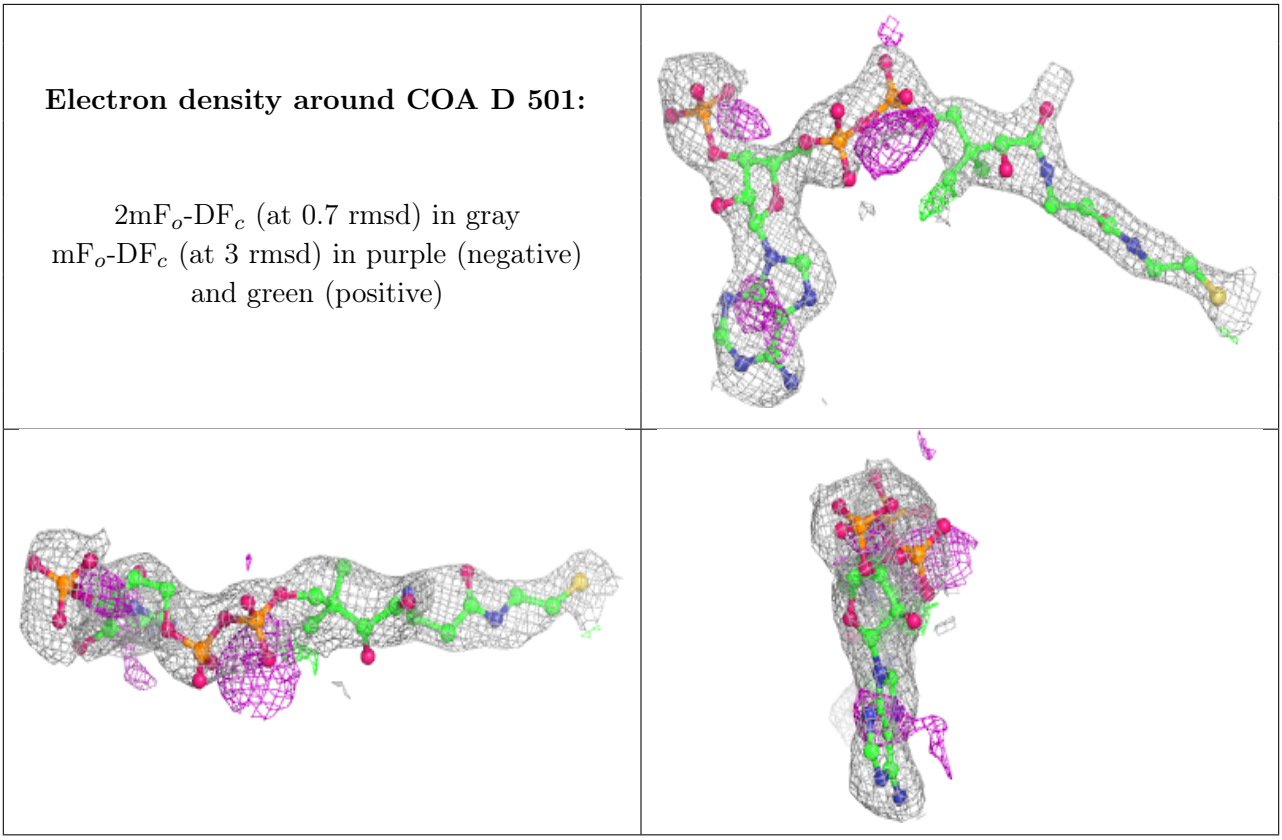
Electron density around COA B 501:

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



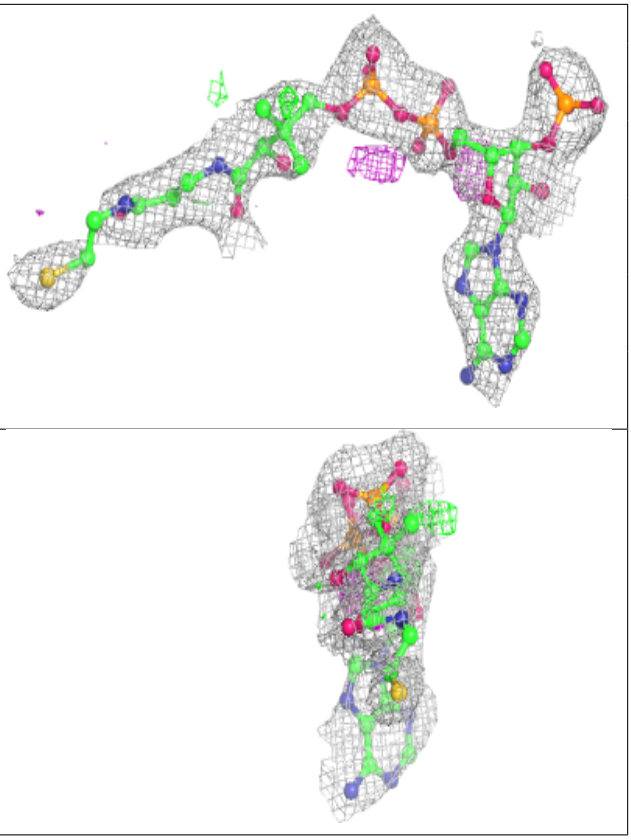
Electron density around COA D 501:

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



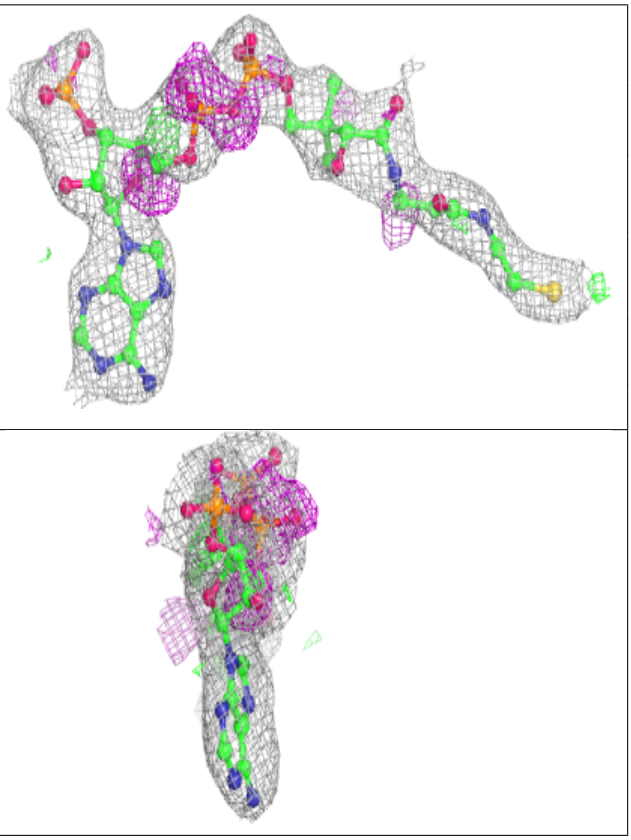
Electron density around COA C 501:

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



Electron density around COA A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.