Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 07:14 PM EDT

PDB ID	:	3B7K
Title	:	Human Acyl-coenzyme A thioesterase 12
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Deposited on	:	2007-10-31
Resolution	:	2.70 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:

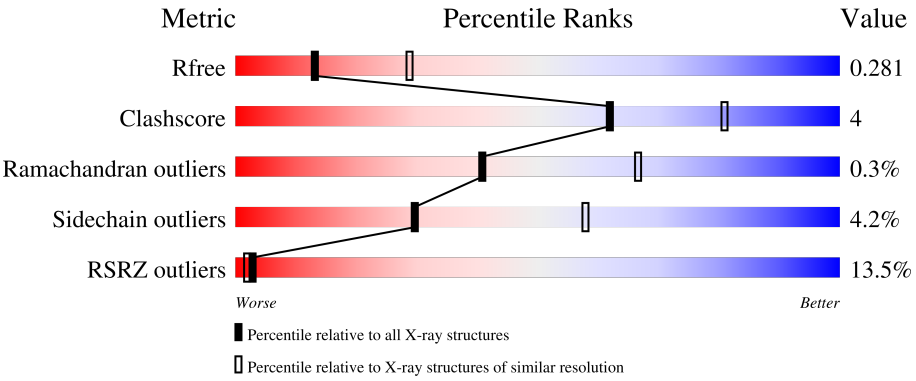
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	333	8% 70% 10% 20%
1	B	333	11% 64% 10% 26%

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CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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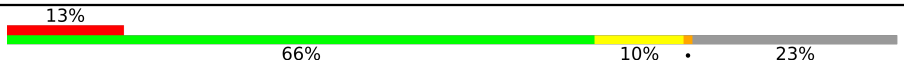
Mol	Chain	Length	Quality of chain
1	C	333	

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
2	COA	B	317	X	-	-	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6061 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 Acyl-coenzyme A thioesterase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2050	1291	362	384	13			
1	B	247	Total	C	N	O	S	0	0	0
			1901	1201	338	350	12			
1	C	255	Total	C	N	O	S	0	0	0
			1966	1243	349	361	13			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP Q8WYK0
A	-15	HIS	-	expression tag	UNP Q8WYK0
A	-14	HIS	-	expression tag	UNP Q8WYK0
A	-13	HIS	-	expression tag	UNP Q8WYK0
A	-12	HIS	-	expression tag	UNP Q8WYK0
A	-11	HIS	-	expression tag	UNP Q8WYK0
A	-10	HIS	-	expression tag	UNP Q8WYK0
A	-9	SER	-	expression tag	UNP Q8WYK0
A	-8	SER	-	expression tag	UNP Q8WYK0
A	-7	GLY	-	expression tag	UNP Q8WYK0
A	-6	VAL	-	expression tag	UNP Q8WYK0
A	-5	ASP	-	expression tag	UNP Q8WYK0
A	-4	LEU	-	expression tag	UNP Q8WYK0
A	-3	GLY	-	expression tag	UNP Q8WYK0
A	-2	THR	-	expression tag	UNP Q8WYK0
A	-1	GLU	-	expression tag	UNP Q8WYK0
A	0	ASN	-	expression tag	UNP Q8WYK0
A	1	LEU	-	expression tag	UNP Q8WYK0
A	2	TYR	-	expression tag	UNP Q8WYK0
A	3	PHE	-	expression tag	UNP Q8WYK0
A	4	GLN	-	expression tag	UNP Q8WYK0
A	5	SER	-	expression tag	UNP Q8WYK0
A	6	MET	-	expression tag	UNP Q8WYK0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	expression tag	UNP Q8WYK0
B	-15	HIS	-	expression tag	UNP Q8WYK0
B	-14	HIS	-	expression tag	UNP Q8WYK0
B	-13	HIS	-	expression tag	UNP Q8WYK0
B	-12	HIS	-	expression tag	UNP Q8WYK0
B	-11	HIS	-	expression tag	UNP Q8WYK0
B	-10	HIS	-	expression tag	UNP Q8WYK0
B	-9	SER	-	expression tag	UNP Q8WYK0
B	-8	SER	-	expression tag	UNP Q8WYK0
B	-7	GLY	-	expression tag	UNP Q8WYK0
B	-6	VAL	-	expression tag	UNP Q8WYK0
B	-5	ASP	-	expression tag	UNP Q8WYK0
B	-4	LEU	-	expression tag	UNP Q8WYK0
B	-3	GLY	-	expression tag	UNP Q8WYK0
B	-2	THR	-	expression tag	UNP Q8WYK0
B	-1	GLU	-	expression tag	UNP Q8WYK0
B	0	ASN	-	expression tag	UNP Q8WYK0
B	1	LEU	-	expression tag	UNP Q8WYK0
B	2	TYR	-	expression tag	UNP Q8WYK0
B	3	PHE	-	expression tag	UNP Q8WYK0
B	4	GLN	-	expression tag	UNP Q8WYK0
B	5	SER	-	expression tag	UNP Q8WYK0
B	6	MET	-	expression tag	UNP Q8WYK0
C	-16	MET	-	expression tag	UNP Q8WYK0
C	-15	HIS	-	expression tag	UNP Q8WYK0
C	-14	HIS	-	expression tag	UNP Q8WYK0
C	-13	HIS	-	expression tag	UNP Q8WYK0
C	-12	HIS	-	expression tag	UNP Q8WYK0
C	-11	HIS	-	expression tag	UNP Q8WYK0
C	-10	HIS	-	expression tag	UNP Q8WYK0
C	-9	SER	-	expression tag	UNP Q8WYK0
C	-8	SER	-	expression tag	UNP Q8WYK0
C	-7	GLY	-	expression tag	UNP Q8WYK0
C	-6	VAL	-	expression tag	UNP Q8WYK0
C	-5	ASP	-	expression tag	UNP Q8WYK0
C	-4	LEU	-	expression tag	UNP Q8WYK0
C	-3	GLY	-	expression tag	UNP Q8WYK0
C	-2	THR	-	expression tag	UNP Q8WYK0
C	-1	GLU	-	expression tag	UNP Q8WYK0
C	0	ASN	-	expression tag	UNP Q8WYK0
C	1	LEU	-	expression tag	UNP Q8WYK0
C	2	TYR	-	expression tag	UNP Q8WYK0

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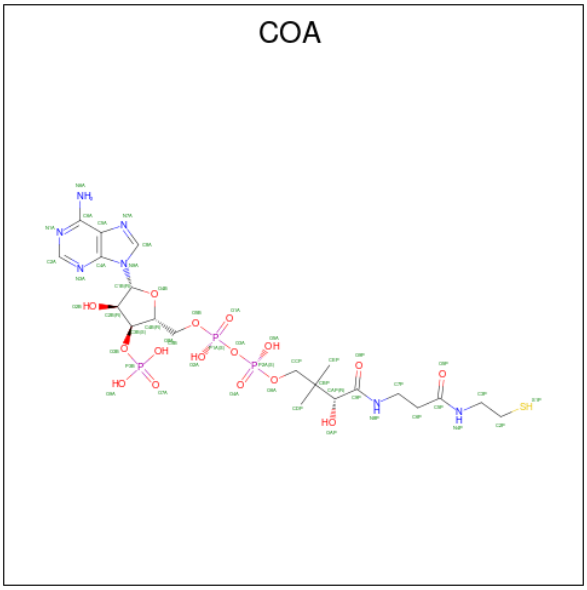
Chain	Residue	Modelled	Actual	Comment	Reference
C	3	PHE	-	expression tag	UNP Q8WYK0
C	4	GLN	-	expression tag	UNP Q8WYK0
C	5	SER	-	expression tag	UNP Q8WYK0
C	6	MET	-	expression tag	UNP Q8WYK0

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



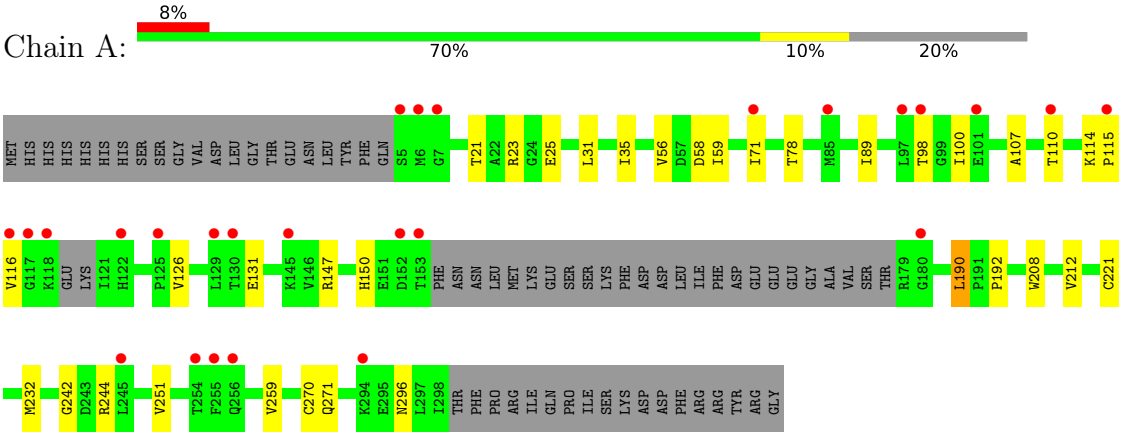
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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.

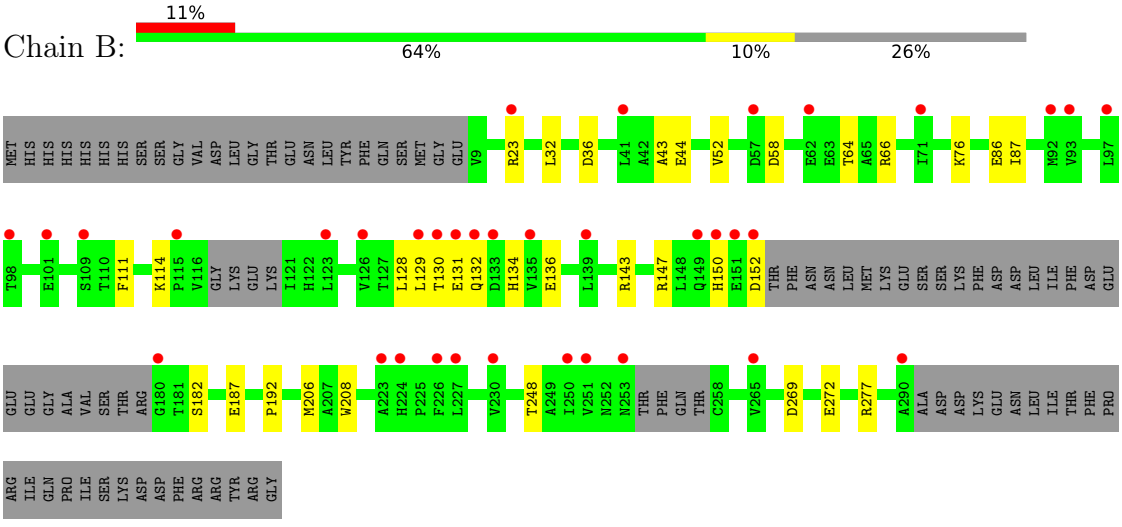
• Molecule 1: Acyl-coenzyme A thioesterase 12

Chain A:



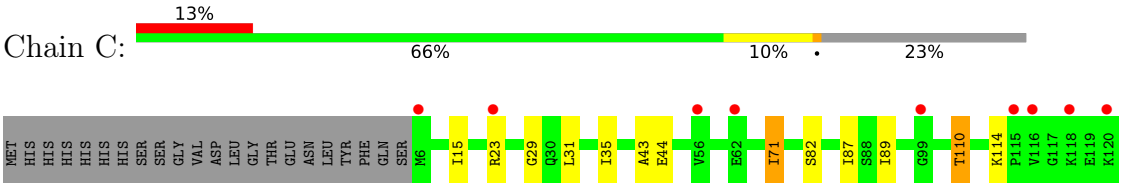
• Molecule 1: Acyl-coenzyme A thioesterase 12

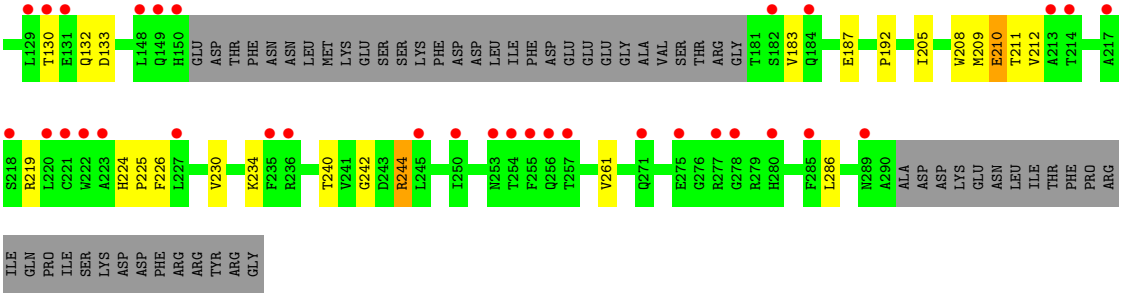
Chain B:



• Molecule 1: Acyl-coenzyme A thioesterase 12

Chain C:




L129 T130 E131 Q132 D133 L148 Q149 H150 GLU ASP THR PHE ASN ASN LEU MET LYS GLU SER SER LYS PHE ASP ASP LEU ILE PHE ASP GLU GLU GLU GLY ALA VAL SER THR ARG GLY T181 S182 V183 Q184 E187 P192 I205 W208 M209 E210 T211 V212 A213 T214 A217
S218 R219 L220 C221 W222 A223 H224 P225 F226 L227 V230 K234 F235 R236 T240 V241 G242 D243 R244 L245 I250 N253 T254 F255 Q256 T257 V261 Q271 E275 G276 R277 G278 R279 H280 P285 L286 N289 A290 ALA ASP ASP LYS GLU ASN LEU ILE THR PHE PRO ARG
ILE GLN PRO ILE SER LYS ASP ASP PHE ARG ARG TYR ARG GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	82.70Å 126.05Å 185.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.70 19.74 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.89-2.70) 99.6 (19.74-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.234 , 0.285 0.231 , 0.281	Depositor DCC
R_{free} test set	1339 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6061	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 4.56% 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: 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	0.43	0/2086	0.58	0/2825
1	B	0.40	0/1935	0.52	0/2621
1	C	0.38	0/2003	0.52	0/2713
All	All	0.40	0/6024	0.54	0/8159

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2050	0	2046	20	0
1	B	1901	0	1906	16	0
1	C	1966	0	1979	20	0
2	A	48	0	32	2	0
2	B	48	0	32	1	0
2	C	48	0	32	3	0
All	All	6061	0	6027	53	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 (53) 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:147:ARG:HA	1:A:232:MET:HE1	1.52	0.89
1:A:147:ARG:HA	1:A:232:MET:CE	2.10	0.82
1:C:242:GLY:O	1:C:244:ARG:NH1	2.19	0.75
1:C:31:LEU:HD13	1:C:71:ILE:HD12	1.69	0.74
1:A:35:ILE:HG23	1:A:89:ILE:HG21	1.74	0.69
1:A:192:PRO:HG3	1:C:192:PRO:HB3	1.76	0.67
1:A:242:GLY:O	1:A:244:ARG:NH1	2.28	0.67
1:A:21:THR:HG23	1:A:23:ARG:H	1.62	0.65
1:B:187:GLU:HG2	1:B:208:TRP:CE2	2.32	0.64
1:B:52:VAL:HB	2:B:317:COA:HN4	1.63	0.63
1:B:36:ASP:OD1	1:B:111:PHE:HZ	1.82	0.61
1:C:187:GLU:HG2	1:C:208:TRP:CE2	2.35	0.61
1:B:23:ARG:O	1:B:66:ARG:NH2	2.34	0.60
1:A:208:TRP:O	1:A:212:VAL:HG23	2.02	0.58
1:A:190:LEU:HB3	1:A:192:PRO:HD2	1.91	0.53
1:C:205:ILE:O	1:C:209:MET:HB2	2.09	0.53
1:C:23:ARG:HH22	1:C:226:PHE:HB3	1.74	0.53
1:C:234:LYS:HD2	2:C:317:COA:H62A	1.74	0.52
1:A:110:THR:HG21	2:A:317:COA:H2A	1.95	0.49
1:B:152:ASP:N	1:B:152:ASP:OD1	2.44	0.49
1:A:98:THR:HB	1:A:100:ILE:HG22	1.95	0.48
1:C:130:THR:HG22	1:C:132:GLN:H	1.79	0.48
2:C:317:COA:H131	2:C:317:COA:N8P	2.28	0.48
1:A:244:ARG:NH2	1:C:44:GLU:OE1	2.44	0.48
1:C:35:ILE:HG23	1:C:89:ILE:HG21	1.95	0.48
1:A:59:ILE:HD12	1:A:107:ALA:HB1	1.96	0.48
1:B:44:GLU:OE1	1:C:244:ARG:NH2	2.46	0.47
1:A:192:PRO:HB3	1:B:192:PRO:HG3	1.97	0.46
1:B:32:LEU:HD13	1:B:206:MET:HB3	1.98	0.46
1:B:136:GLU:HG3	1:B:143:ARG:HH22	1.81	0.46
1:C:43:ALA:HB2	1:C:87:ILE:HD11	1.97	0.45
1:B:36:ASP:OD1	1:B:111:PHE:CZ	2.68	0.45
1:A:147:ARG:HA	1:A:232:MET:HE3	1.95	0.44
1:B:130:THR:HG22	1:B:132:GLN:H	1.82	0.44
1:B:277:ARG:HD2	1:B:277:ARG:O	2.17	0.44
1:A:23:ARG:HE	1:A:25:GLU:CD	2.21	0.44
1:A:251:VAL:HG13	1:A:259:VAL:HG23	1.99	0.44
1:A:56:VAL:HG12	1:A:59:ILE:HD11	2.00	0.44
1:C:208:TRP:O	1:C:212:VAL:HG23	2.18	0.43
1:C:15:ILE:HD11	1:C:71:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ASP:HB2	1:B:272:GLU:CG	2.49	0.42
1:C:183:VAL:HG22	1:C:219:ARG:NH1	2.34	0.42
1:C:29:GLY:N	1:C:210:GLU:HG2	2.34	0.42
1:C:110:THR:HG21	2:C:317:COA:H2A	2.02	0.42
1:C:230:VAL:HG22	1:C:286:LEU:HD22	2.02	0.42
1:A:110:THR:HG21	2:A:317:COA:C2A	2.50	0.41
1:B:86:GLU:HG3	1:B:147:ARG:HH22	1.85	0.41
1:B:128:LEU:HD23	1:B:134:HIS:CD2	2.55	0.41
1:C:130:THR:O	1:C:133:ASP:HB2	2.20	0.41
1:B:43:ALA:HB2	1:B:87:ILE:HD11	2.02	0.41
1:A:114:LYS:HA	1:A:115:PRO:HD2	1.73	0.41
1:A:221:CYS:HA	1:A:296:ASN:O	2.21	0.41
1:C:224:HIS:HA	1:C:225:PRO:HD3	1.91	0.41

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	261/333 (78%)	247 (95%)	13 (5%)	1 (0%)	34	60
1	B	239/333 (72%)	228 (95%)	10 (4%)	1 (0%)	34	60
1	C	251/333 (75%)	237 (94%)	14 (6%)	0	100	100
All	All	751/999 (75%)	712 (95%)	37 (5%)	2 (0%)	41	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	HIS
1	A	150	HIS

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	222/284 (78%)	212 (96%)	10 (4%)	27	55
1	B	206/284 (72%)	198 (96%)	8 (4%)	32	61
1	C	213/284 (75%)	204 (96%)	9 (4%)	30	58
All	All	641/852 (75%)	614 (96%)	27 (4%)	30	58

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	58	ASP
1	A	71	ILE
1	A	78	THR
1	A	116	VAL
1	A	126	VAL
1	A	131	GLU
1	A	190	LEU
1	A	270	CYS
1	A	271	GLN
1	B	58	ASP
1	B	64	THR
1	B	76	LYS
1	B	114	LYS
1	B	129	LEU
1	B	131	GLU
1	B	182	SER
1	B	248	THR
1	C	71	ILE
1	C	82	SER
1	C	110	THR
1	C	114	LYS
1	C	210	GLU
1	C	211	THR
1	C	240	THR
1	C	244	ARG

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Mol	Chain	Res	Type
1	C	261	VAL

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

Mol	Chain	Res	Type
1	A	132	GLN
1	A	271	GLN
1	B	134	HIS
1	B	184	GLN
1	C	184	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)

3 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	A	317	-	41,50,50	1.69	3 (7%)	52,75,75	1.15	4 (7%)
2	COA	C	317	-	41,50,50	1.71	3 (7%)	52,75,75	1.20	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	COA	B	317	-	41,50,50	1.73	3 (7%)	52,75,75	1.11	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	A	317	-	-	17/44/64/64	0/3/3/3
2	COA	C	317	-	-	12/44/64/64	0/3/3/3
2	COA	B	317	-	1/1/11/13	20/44/64/64	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	317	COA	O9P-C9P	9.32	1.41	1.23
2	C	317	COA	O9P-C9P	8.98	1.41	1.23
2	A	317	COA	O9P-C9P	8.96	1.41	1.23
2	C	317	COA	C2A-N3A	4.12	1.38	1.32
2	B	317	COA	C2A-N3A	4.05	1.38	1.32
2	A	317	COA	C2A-N3A	3.89	1.38	1.32
2	C	317	COA	C2A-N1A	2.67	1.38	1.33
2	B	317	COA	C2A-N1A	2.50	1.38	1.33
2	A	317	COA	C2A-N1A	2.34	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	317	COA	N3A-C2A-N1A	-5.61	119.90	128.68
2	B	317	COA	N3A-C2A-N1A	-5.37	120.28	128.68
2	A	317	COA	N3A-C2A-N1A	-5.04	120.81	128.68
2	C	317	COA	P2A-O3A-P1A	-3.64	120.35	132.83
2	A	317	COA	P2A-O3A-P1A	-3.09	122.24	132.83
2	C	317	COA	C1B-N9A-C4A	-2.54	122.18	126.64
2	A	317	COA	CEP-CBP-CAP	2.07	112.41	108.82
2	A	317	COA	O4B-C1B-C2B	-2.04	103.94	106.93

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	317	COA	CAP

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	317	COA	C5B-O5B-P1A-O2A
2	A	317	COA	P2A-O3A-P1A-O5B
2	A	317	COA	CCP-O6A-P2A-O3A
2	A	317	COA	CCP-O6A-P2A-O4A
2	A	317	COA	CCP-O6A-P2A-O5A
2	A	317	COA	CAP-C9P-N8P-C7P
2	A	317	COA	C5P-C6P-C7P-N8P
2	B	317	COA	C5B-O5B-P1A-O3A
2	B	317	COA	CCP-O6A-P2A-O3A
2	B	317	COA	C9P-CAP-CBP-CCP
2	B	317	COA	C9P-CAP-CBP-CDP
2	B	317	COA	C9P-CAP-CBP-CEP
2	B	317	COA	CAP-C9P-N8P-C7P
2	B	317	COA	C5P-C6P-C7P-N8P
2	B	317	COA	C6P-C5P-N4P-C3P
2	B	317	COA	O5P-C5P-N4P-C3P
2	C	317	COA	O4B-C4B-C5B-O5B
2	C	317	COA	C5B-O5B-P1A-O3A
2	C	317	COA	CCP-O6A-P2A-O3A
2	C	317	COA	CCP-O6A-P2A-O4A
2	C	317	COA	CCP-O6A-P2A-O5A
2	C	317	COA	O9P-C9P-CAP-CBP
2	C	317	COA	N8P-C9P-CAP-OAP
2	B	317	COA	O9P-C9P-N8P-C7P
2	A	317	COA	O9P-C9P-N8P-C7P
2	A	317	COA	O4B-C4B-C5B-O5B
2	C	317	COA	C3B-C4B-C5B-O5B
2	A	317	COA	C3B-C4B-C5B-O5B
2	B	317	COA	C3B-C4B-C5B-O5B
2	B	317	COA	O4B-C4B-C5B-O5B
2	A	317	COA	C6P-C7P-N8P-C9P
2	C	317	COA	O9P-C9P-CAP-OAP
2	C	317	COA	N8P-C9P-CAP-CBP
2	A	317	COA	C3B-O3B-P3B-O9A
2	A	317	COA	C5B-O5B-P1A-O3A
2	B	317	COA	CBP-CCP-O6A-P2A
2	A	317	COA	C5B-O5B-P1A-O1A
2	B	317	COA	C5B-O5B-P1A-O1A
2	B	317	COA	C5B-O5B-P1A-O2A
2	B	317	COA	CCP-O6A-P2A-O4A
2	B	317	COA	CCP-O6A-P2A-O5A
2	C	317	COA	C5B-O5B-P1A-O1A

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Mol	Chain	Res	Type	Atoms
2	B	317	COA	O9P-C9P-CAP-OAP
2	B	317	COA	C4B-C5B-O5B-P1A
2	A	317	COA	O5P-C5P-C6P-C7P
2	A	317	COA	S1P-C2P-C3P-N4P
2	B	317	COA	N8P-C9P-CAP-OAP
2	A	317	COA	N4P-C5P-C6P-C7P
2	C	317	COA	C3B-O3B-P3B-O9A

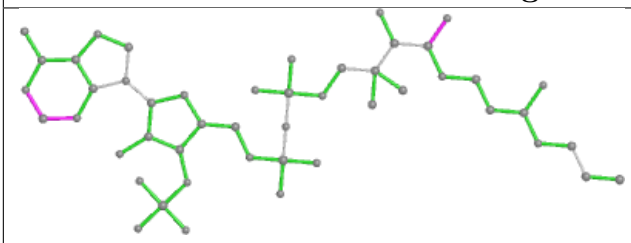
There are no ring outliers.

3 monomers are involved in 6 short contacts:

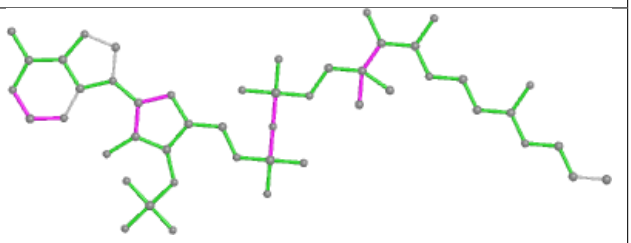
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	317	COA	2	0
2	C	317	COA	3	0
2	B	317	COA	1	0

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

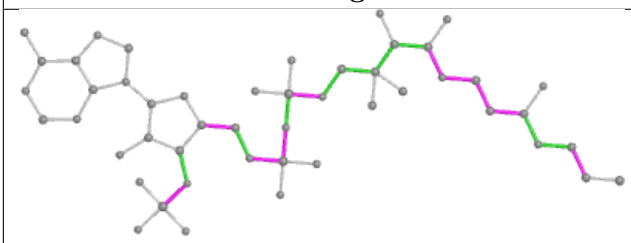
Ligand COA A 317



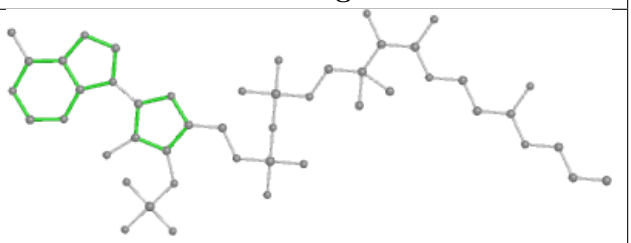
Bond lengths



Bond angles

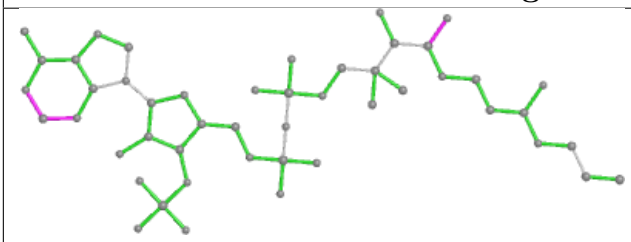


Torsions

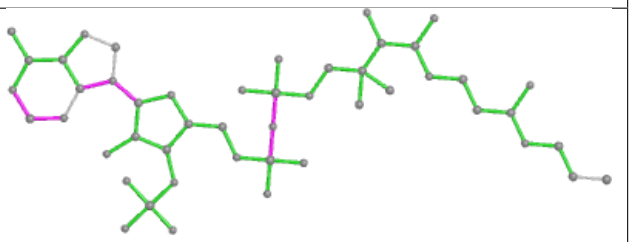


Rings

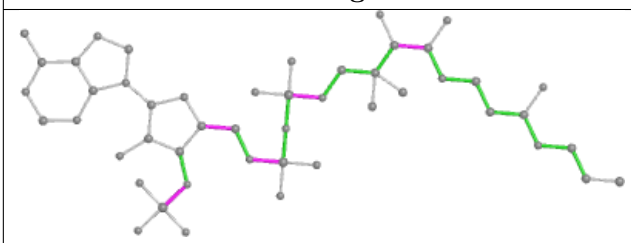
Ligand COA C 317



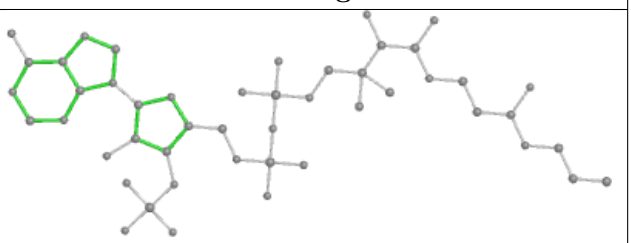
Bond lengths



Bond angles

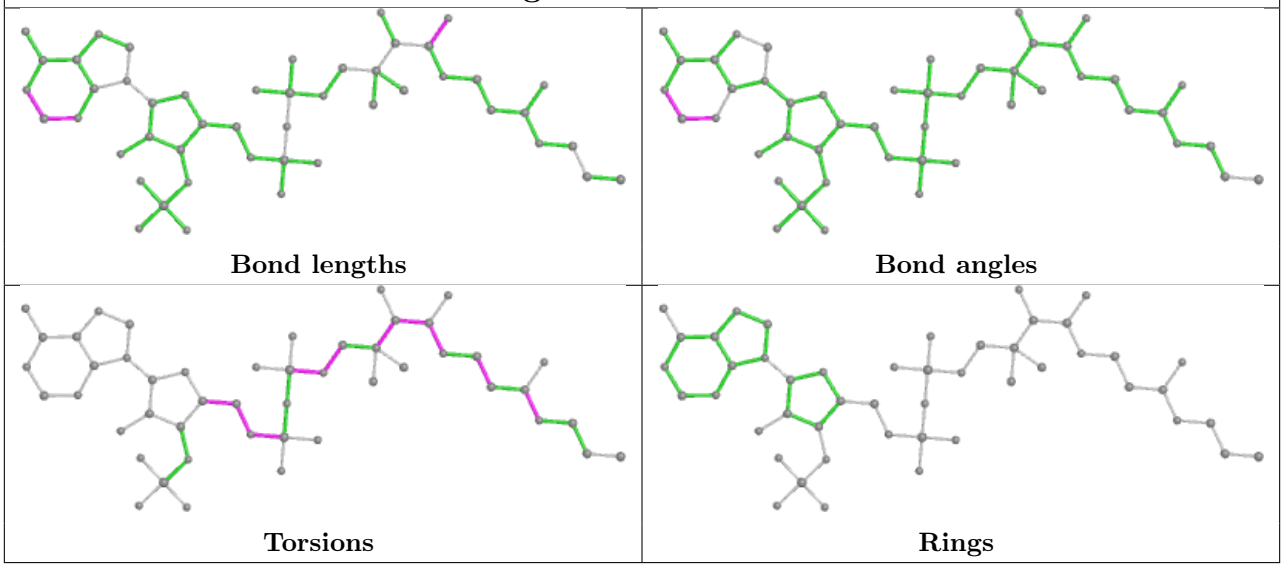


Torsions



Rings

Ligand COA B 317



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	267/333 (80%)	0.63	26 (9%)	7 6	47, 54, 60, 66	0
1	B	247/333 (74%)	0.98	36 (14%)	2 1	47, 56, 63, 66	0
1	C	255/333 (76%)	0.81	42 (16%)	1 1	48, 56, 61, 67	0
All	All	769/999 (76%)	0.80	104 (13%)	3 2	47, 55, 61, 67	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	257	THR	6.4
1	A	153	THR	5.7
1	C	256	GLN	5.3
1	A	122	HIS	5.2
1	C	149	GLN	5.0
1	A	6	MET	5.0
1	A	115	PRO	4.8
1	C	130	THR	4.7
1	A	5	SER	4.4
1	B	151	GLU	4.4
1	C	255	PHE	4.3
1	C	6	MET	4.2
1	B	152	ASP	4.1
1	C	150	HIS	4.1
1	B	132	GLN	4.0
1	C	289	ASN	4.0
1	B	253	ASN	3.9
1	C	254	THR	3.9
1	B	290	ALA	3.8
1	C	221	CYS	3.8
1	A	256	GLN	3.7
1	B	115	PRO	3.7
1	B	135	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	97	LEU	3.7
1	B	23	ARG	3.5
1	B	97	LEU	3.4
1	C	131	GLU	3.4
1	B	62	GLU	3.4
1	A	117	GLY	3.4
1	C	222	TRP	3.4
1	A	130	THR	3.3
1	B	109	SER	3.3
1	A	255	PHE	3.3
1	A	152	ASP	3.2
1	B	133	ASP	3.2
1	A	245	LEU	3.2
1	B	251	VAL	3.2
1	C	116	VAL	3.2
1	B	129	LEU	3.1
1	C	253	ASN	3.0
1	B	224	HIS	3.0
1	B	92	MET	2.9
1	C	99	GLY	2.8
1	B	130	THR	2.8
1	C	148	LEU	2.8
1	B	131	GLU	2.8
1	A	98	THR	2.7
1	B	139	LEU	2.7
1	B	93	VAL	2.6
1	C	182	SER	2.6
1	A	294	LYS	2.6
1	A	180	GLY	2.6
1	C	250	ILE	2.6
1	C	245	LEU	2.6
1	C	277	ARG	2.6
1	A	129	LEU	2.5
1	C	275	GLU	2.5
1	B	149	GLN	2.5
1	A	85	MET	2.5
1	C	120	LYS	2.5
1	B	101	GLU	2.4
1	B	180	GLY	2.4
1	B	123	LEU	2.4
1	B	223	ALA	2.4
1	A	71	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	57	ASP	2.3
1	A	125	PRO	2.3
1	C	220	LEU	2.3
1	B	126	VAL	2.2
1	C	271	GLN	2.2
1	C	235	PHE	2.2
1	A	118	LYS	2.2
1	B	265	VAL	2.2
1	C	115	PRO	2.2
1	A	110	THR	2.2
1	B	41	LEU	2.2
1	B	98	THR	2.2
1	C	118	LYS	2.2
1	B	150	HIS	2.2
1	C	129	LEU	2.2
1	C	184	GLN	2.2
1	C	213	ALA	2.2
1	B	226	PHE	2.2
1	C	56	VAL	2.1
1	C	62	GLU	2.1
1	A	116	VAL	2.1
1	B	230	VAL	2.1
1	A	254	THR	2.1
1	C	23	ARG	2.1
1	C	236	ARG	2.1
1	C	278	GLY	2.1
1	C	285	PHE	2.1
1	C	214	THR	2.1
1	A	7	GLY	2.1
1	A	101	GLU	2.1
1	B	227	LEU	2.1
1	C	217	ALA	2.1
1	C	223	ALA	2.0
1	C	280	HIS	2.0
1	B	71	ILE	2.0
1	B	250	ILE	2.0
1	C	218	SER	2.0
1	C	227	LEU	2.0
1	A	145	LYS	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)

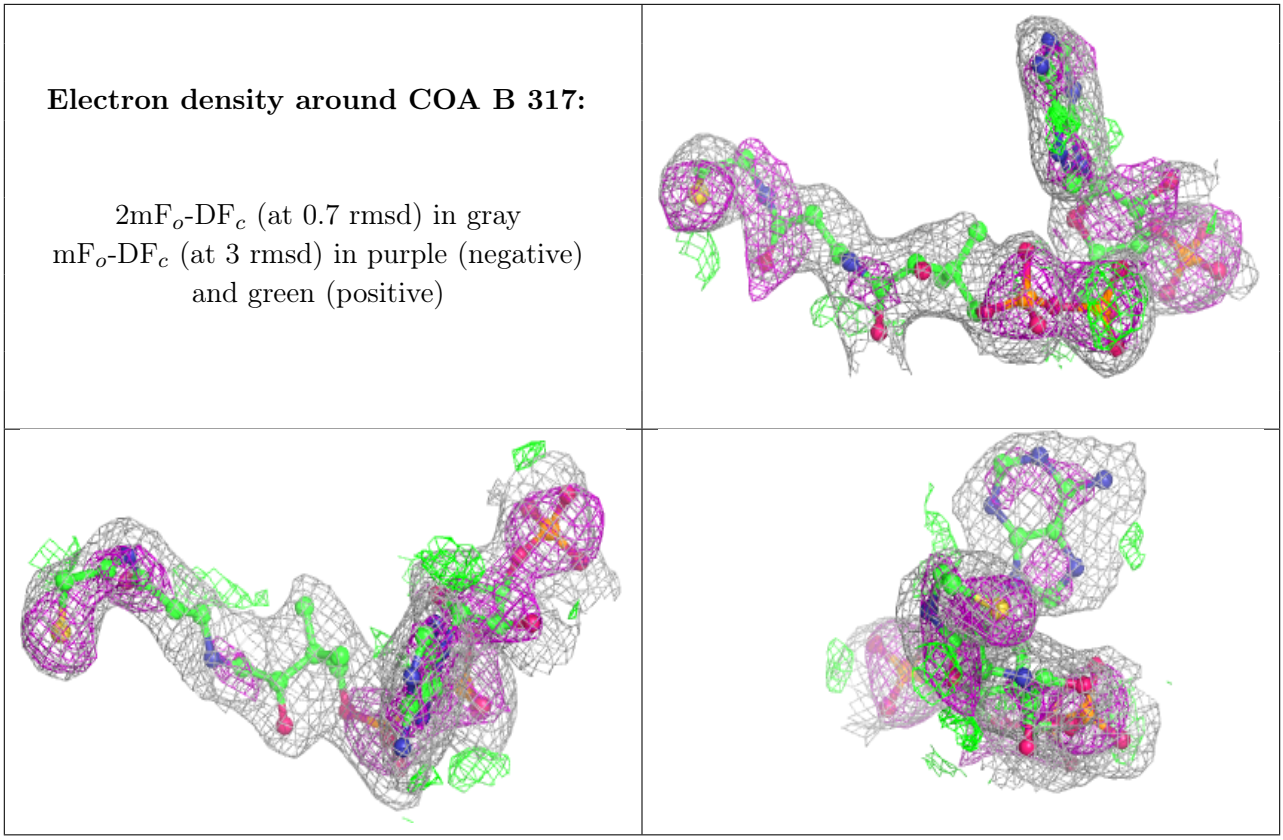
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	317	48/48	0.90	0.28	45,53,57,58	0
2	COA	C	317	48/48	0.91	0.23	44,55,59,59	0
2	COA	A	317	48/48	0.94	0.22	31,41,44,46	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.

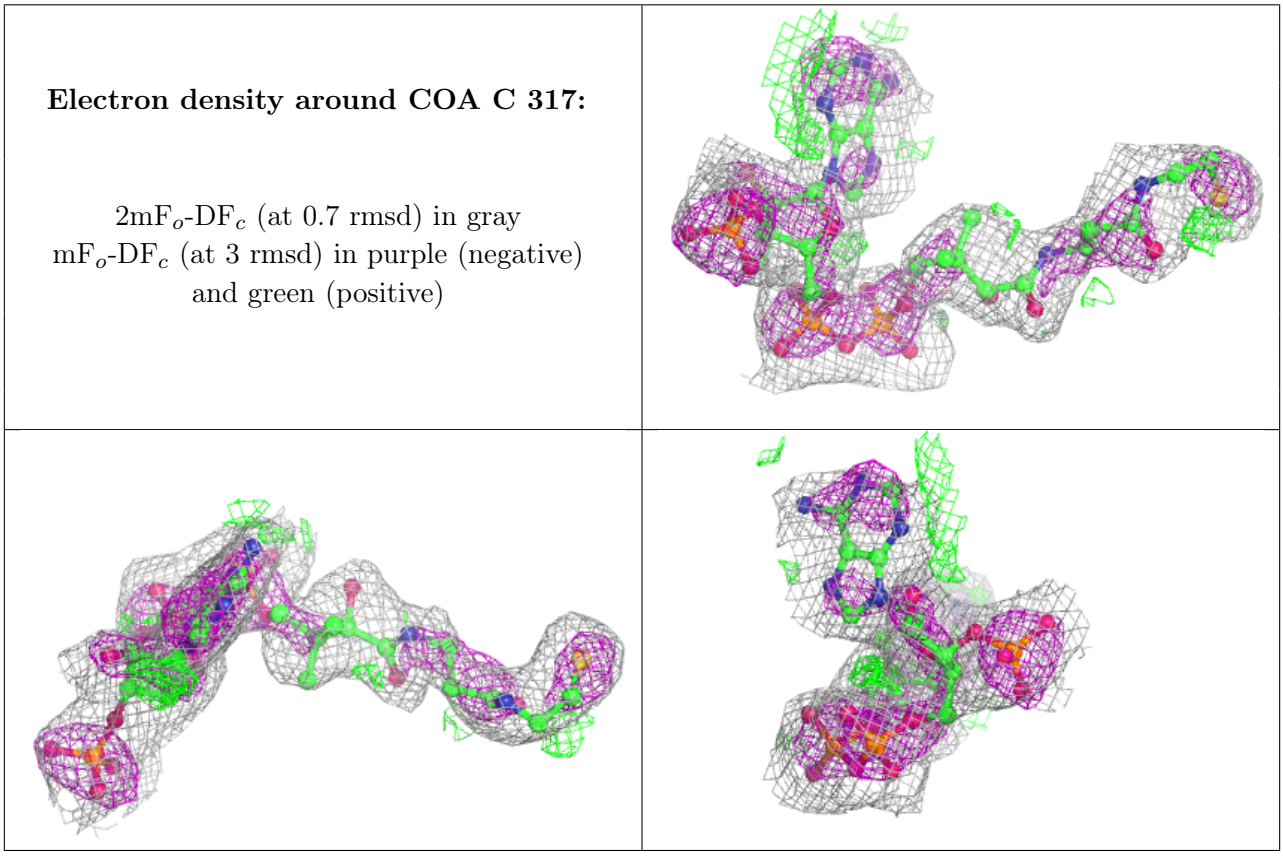
Electron density around COA B 317:

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



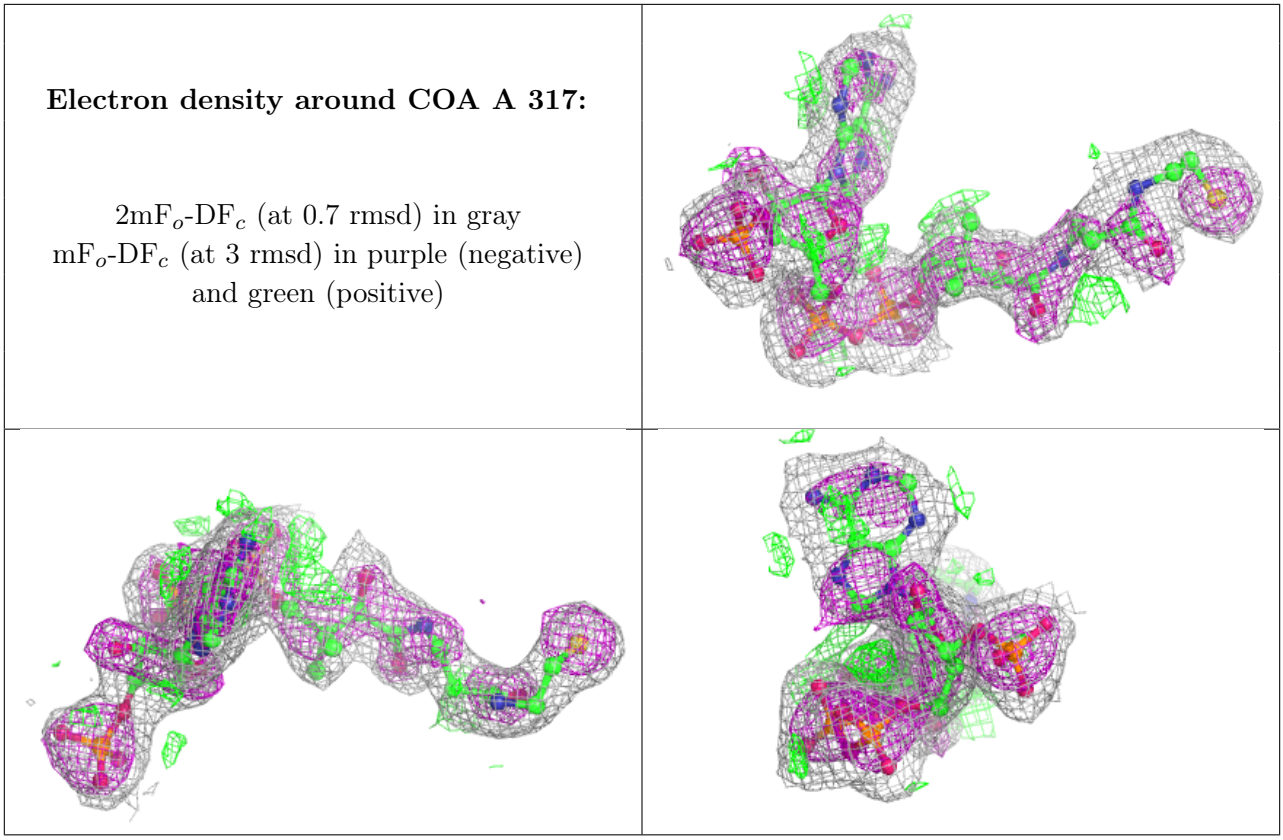
Electron density around COA C 317:

$2mF_o$-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 317:

$2mF_o$-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.