



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 09:59 PM BST

PDB ID : 6ESQ  
Title : Structure of the acetoacetyl-CoA thiolase/HMG-CoA synthase complex from Methanothermococcus thermolithotrophicus soaked with acetyl-CoA  
Authors : Voegeli, B.; Engilberge, S.; Girard, E.; Riobe, F.; Maury, O.; Erb, J.T.; Shima, S.; Wagner, T.  
Deposited on : 2017-10-24  
Resolution : 2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

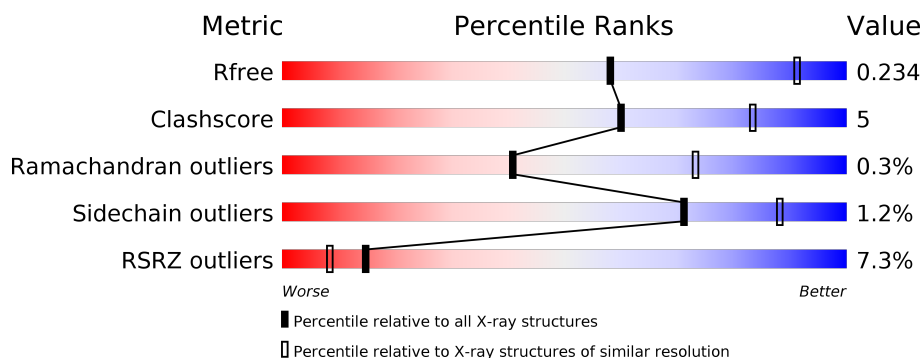
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	392	<div> <div>14%</div> <div>85%</div> <div>15%</div> </div>
1	B	392	<div> <div>2%</div> <div>88%</div> <div>12%</div> </div>
1	C	392	<div> <div>16%</div> <div>87%</div> <div>13%</div> </div>
1	D	392	<div> <div>88%</div> <div>13%</div> </div>
2	E	130	<div> <div>2%</div> <div>92%</div> <div>5%</div> </div>
2	F	130	<div> <div>3%</div> <div>96%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	130	
2	H	130	
3	I	349	
3	J	349	
3	K	349	
3	L	349	

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
7	CL	F	202	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 52823 atoms, of which 26256 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 acetoacetyl-CoA thiolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	392	Total	C	H	N	O	S	0	0	0
			5800	1836	2873	495	577	19			
1	B	392	Total	C	H	N	O	S	0	0	0
			5815	1839	2884	496	577	19			
1	C	392	Total	C	H	N	O	S	0	0	0
			5814	1839	2883	496	577	19			
1	D	392	Total	C	H	N	O	S	0	0	0
			5815	1839	2884	496	577	19			

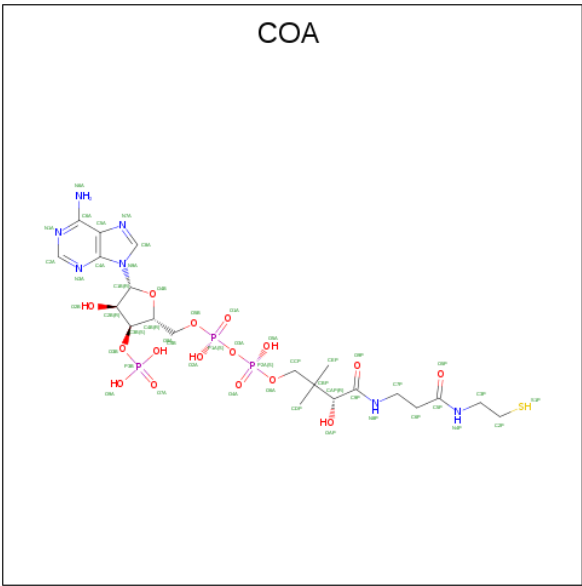
- Molecule 2 is a protein called Pfam DUF35.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	127	Total	C	H	N	O	S	0	0	0
			2066	658	1045	175	182	6			
2	F	129	Total	C	H	N	O	S	0	0	0
			2095	667	1058	177	187	6			
2	G	128	Total	C	H	N	O	S	0	0	0
			2081	662	1053	176	184	6			
2	H	128	Total	C	H	N	O	S	0	0	0
			2080	662	1052	176	184	6			

- Molecule 3 is a protein called HydroxyMethylGlutaryl-CoA synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	I	347	Total	C	H	N	O	S	0	0	0
			5219	1671	2599	435	505	9			
3	J	348	Total	C	H	N	O	S	0	0	0
			5253	1680	2621	437	506	9			
3	K	347	Total	C	H	N	O	S	0	0	0
			5234	1674	2610	436	505	9			
3	L	347	Total	C	H	N	O	S	0	0	0
			5234	1674	2610	436	505	9			

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			61	16	21	6	15	3		
4	B	1	Total	C	H	N	O	P	0	0
			61	16	21	6	15	3		
4	C	1	Total	C	H	N	O	P	0	0
			61	16	21	6	15	3		
4	D	1	Total	C	H	N	O	P	0	0
			61	16	21	6	15	3		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	K	0	0
			2	2		
5	I	1	Total	K	0	0
			1	1		
5	L	1	Total	K	0	0
			1	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Zn	0	0
			1	1		
6	G	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total 1	Zn 1	0	0
6	E	1	Total 1	Zn 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total 1	Cl 1	0	0
7	F	1	Total 1	Cl 1	0	0
7	E	1	Total 1	Cl 1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	K	1	Total 1	Na 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 1	O 1	0	0
9	B	7	Total 7	O 7	0	0
9	C	6	Total 6	O 6	0	0
9	D	9	Total 9	O 9	0	0
9	E	2	Total 2	O 2	0	0
9	F	4	Total 4	O 4	0	0
9	G	6	Total 6	O 6	0	0
9	H	2	Total 2	O 2	0	0
9	I	11	Total 11	O 11	0	0

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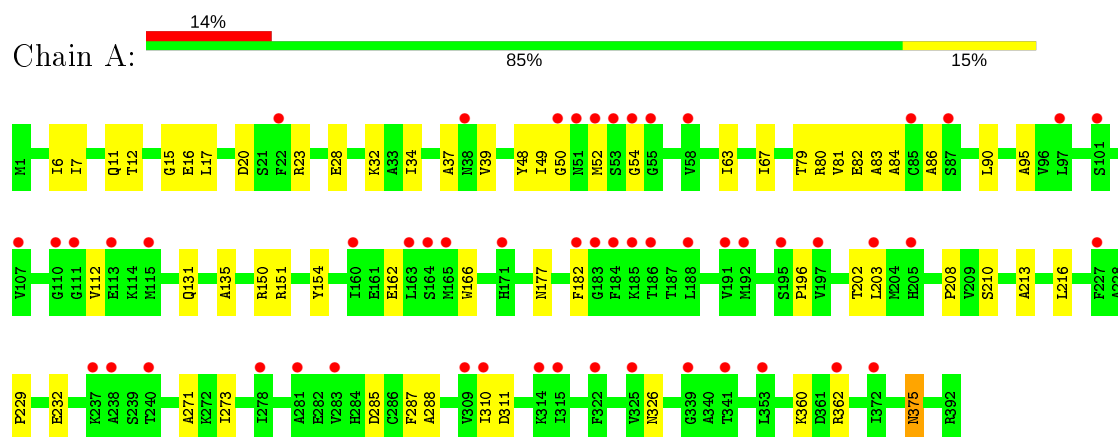
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	3	Total 3	O 3	0	0
9	K	3	Total 3	O 3	0	0
9	L	7	Total 7	O 7	0	0

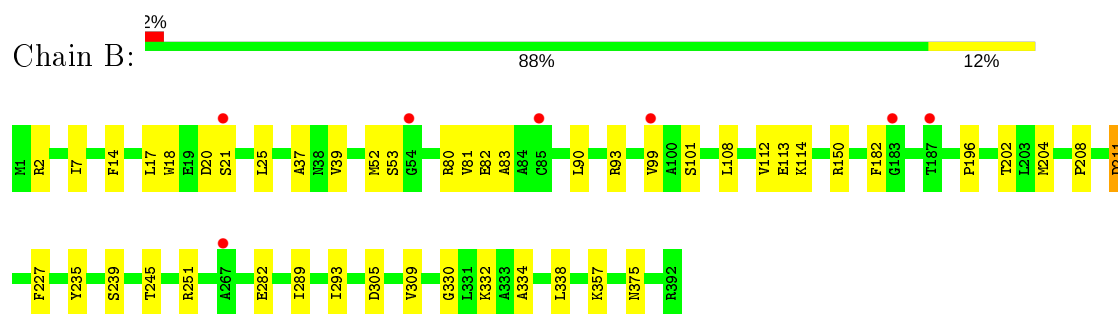
### 3 Residue-property plots [i](#)

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.

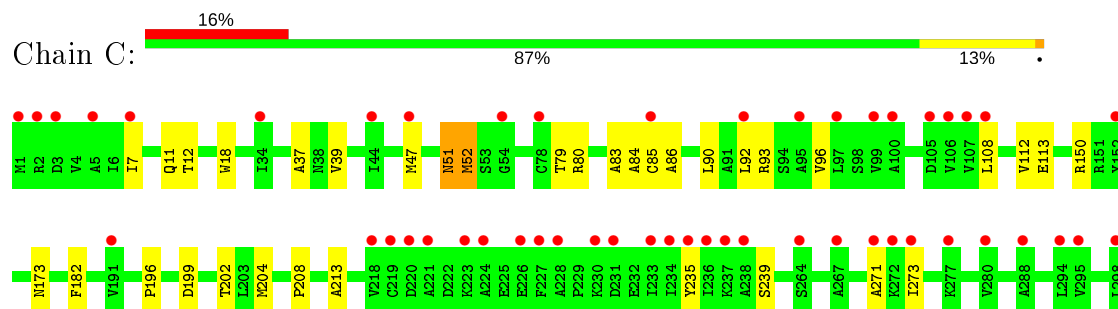
- Molecule 1: acetoacetyl-CoA thiolase



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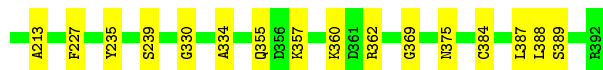
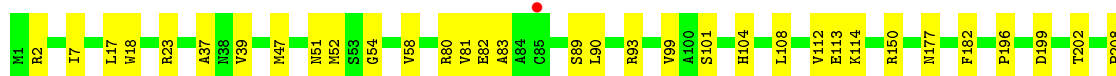
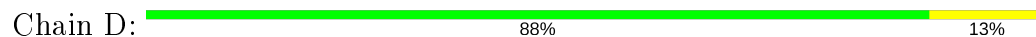
- Molecule 1: acetoacetyl-CoA thiolase



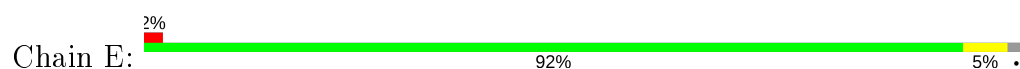




- Molecule 1: acetoacetyl-CoA thiolase



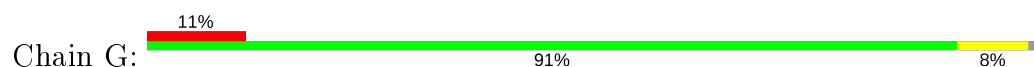
- Molecule 2: Pfam DUF35



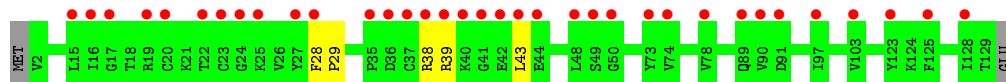
- Molecule 2: Pfam DUF35



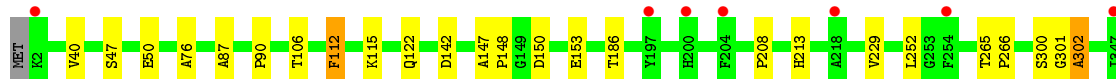
- Molecule 2: Pfam DUF35



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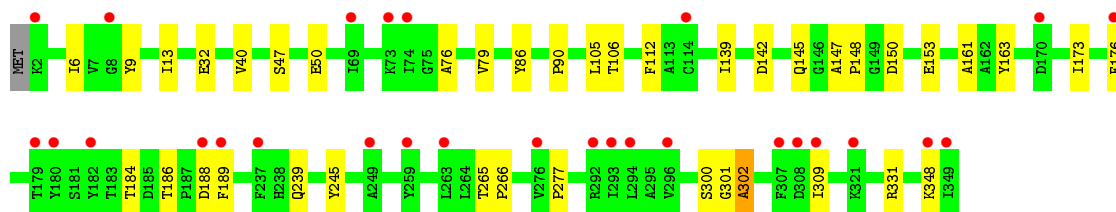
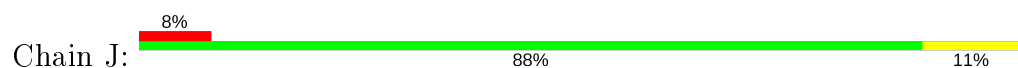


- Molecule 3: HydroxyMethylGlutaryl-CoA synthase

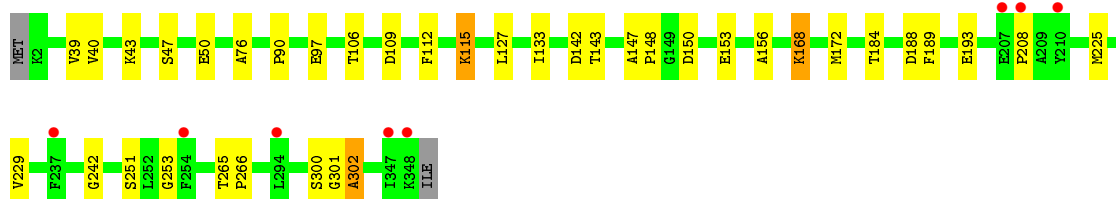
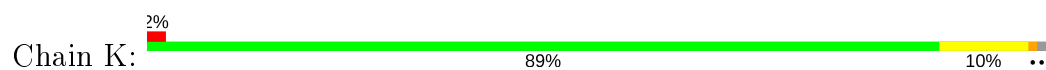




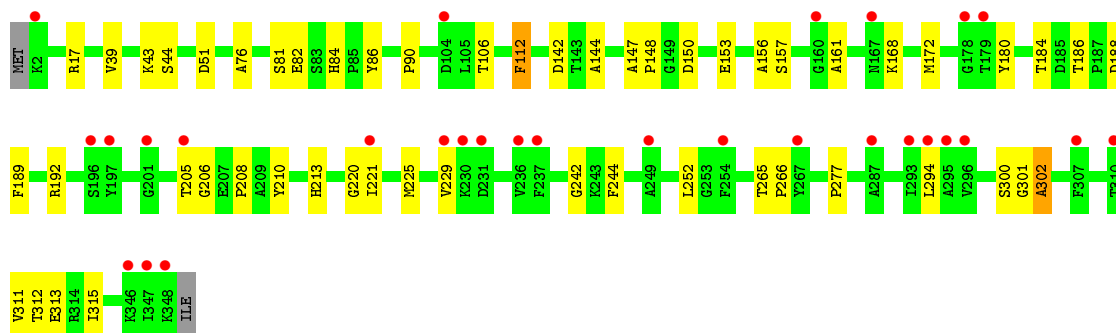
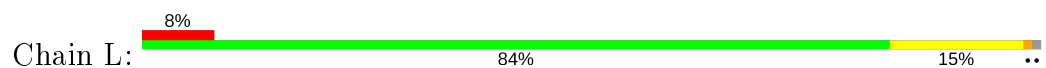
• Molecule 3: HydroxyMethylGlutaryl-CoA synthase



• Molecule 3: HydroxyMethylGlutaryl-CoA synthase



• Molecule 3: HydroxyMethylGlutaryl-CoA synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.60Å 145.18Å 230.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.95 49.29 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.29-2.95) 99.3 (49.29-2.95)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.182 , 0.230 0.188 , 0.234	Depositor DCC
$R_{free}$ test set	3807 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.7	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 73.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	52823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: COA, NA, ZN, K, CL

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	0.21	0/2976	0.33	0/4028
1	B	0.29	0/2980	0.37	0/4032
1	C	0.22	0/2980	0.34	0/4032
1	D	0.28	0/2980	0.35	0/4032
2	E	0.23	0/1044	0.35	0/1407
2	F	0.27	0/1060	0.40	0/1429
2	G	0.29	0/1051	0.37	0/1417
2	H	0.21	0/1051	0.35	0/1417
3	I	0.27	0/2676	0.36	0/3623
3	J	0.21	0/2688	0.34	0/3638
3	K	0.27	0/2680	0.37	0/3627
3	L	0.23	0/2680	0.34	0/3627
All	All	0.25	0/26846	0.35	0/36309

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	2
1	D	0	3
2	G	0	1
3	J	0	2
3	K	0	2
3	L	0	1
All	All	0	18

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ARG	Sidechain
1	A	154	TYR	Sidechain
1	A	162	GLU	Sidechain
1	B	14	PHE	Sidechain
1	B	211	ASP	Mainchain

## 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	2927	2873	2873	48	0
1	B	2931	2884	2884	29	0
1	C	2931	2883	2884	31	0
1	D	2931	2884	2884	27	0
2	E	1021	1045	1044	8	0
2	F	1037	1058	1058	4	0
2	G	1028	1053	1052	3	0
2	H	1028	1052	1052	1	0
3	I	2620	2599	2599	18	0
3	J	2632	2621	2621	25	0
3	K	2624	2610	2610	28	0
3	L	2624	2610	2610	40	0
4	A	40	21	21	5	0
4	B	40	21	21	1	0
4	C	40	21	21	2	0
4	D	40	21	21	0	0
5	B	2	0	0	0	0
5	I	1	0	0	0	0
5	L	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	E	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	1	0	0	2	0
7	G	1	0	0	0	0
8	K	1	0	0	0	0
9	A	1	0	0	0	0
9	B	7	0	0	0	0
9	C	6	0	0	0	0
9	D	9	0	0	1	0
9	E	2	0	0	0	0
9	F	4	0	0	0	0
9	G	6	0	0	0	0
9	H	2	0	0	0	0
9	I	11	0	0	0	0
9	J	3	0	0	0	0
9	K	3	0	0	0	0
9	L	7	0	0	0	0
All	All	26567	26256	26255	243	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 5.

The worst 5 of 243 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)
3:K:184:THR:O	3:K:302:ALA:HB3	1.60	0.99
1:A:52:MET:HG3	1:A:84:ALA:HA	1.52	0.91
1:D:17:LEU:O	1:D:114:LYS:NZ	2.11	0.83
3:K:184:THR:O	3:K:302:ALA:CB	2.26	0.83
1:A:49:ILE:O	1:A:80:ARG:HA	1.86	0.75

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	390/392 (100%)	379 (97%)	10 (3%)	1 (0%)	41	73
1	B	390/392 (100%)	380 (97%)	10 (3%)	0	100	100
1	C	390/392 (100%)	377 (97%)	12 (3%)	1 (0%)	41	73
1	D	390/392 (100%)	379 (97%)	11 (3%)	0	100	100
2	E	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
2	F	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
2	G	126/130 (97%)	123 (98%)	3 (2%)	0	100	100
2	H	126/130 (97%)	124 (98%)	1 (1%)	1 (1%)	19	53
3	I	345/349 (99%)	334 (97%)	9 (3%)	2 (1%)	25	60
3	J	346/349 (99%)	334 (96%)	11 (3%)	1 (0%)	41	73
3	K	345/349 (99%)	334 (97%)	10 (3%)	1 (0%)	41	73
3	L	345/349 (99%)	334 (97%)	8 (2%)	3 (1%)	17	51
All	All	3445/3484 (99%)	3344 (97%)	91 (3%)	10 (0%)	41	73

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
3	J	302	ALA
3	K	302	ALA
3	L	302	ALA
3	L	206	GLY

### 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	301/303 (99%)	295 (98%)	6 (2%)	55	80
1	B	302/303 (100%)	299 (99%)	3 (1%)	76	90
1	C	302/303 (100%)	298 (99%)	4 (1%)	69	87
1	D	302/303 (100%)	299 (99%)	3 (1%)	76	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	112/115 (97%)	112 (100%)	0	100	100
2	F	114/115 (99%)	113 (99%)	1 (1%)	78	91
2	G	113/115 (98%)	109 (96%)	4 (4%)	36	68
2	H	113/115 (98%)	111 (98%)	2 (2%)	59	82
3	I	264/267 (99%)	262 (99%)	2 (1%)	81	92
3	J	266/267 (100%)	264 (99%)	2 (1%)	81	92
3	K	265/267 (99%)	260 (98%)	5 (2%)	57	81
3	L	265/267 (99%)	264 (100%)	1 (0%)	91	96
All	All	2719/2740 (99%)	2686 (99%)	33 (1%)	71	88

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	362	ARG
2	G	39	ARG
3	K	225	MET
1	D	375	ASN
2	F	124	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	51	ASN
1	D	51	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 monosaccharides in this entry.



## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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
4	COA	D	401	-	35,42,50	0.55	0	45,66,75	0.73	1 (2%)
4	COA	A	401	-	35,42,50	0.57	0	45,66,75	0.80	2 (4%)
4	COA	C	401	-	35,42,50	0.56	0	45,66,75	0.78	2 (4%)
4	COA	B	401	-	35,42,50	0.63	0	45,66,75	0.70	1 (2%)

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
4	COA	D	401	-	-	11/33/54/64	0/3/3/3
4	COA	A	401	-	-	14/33/54/64	0/3/3/3
4	COA	C	401	-	-	15/33/54/64	0/3/3/3
4	COA	B	401	-	-	18/33/54/64	0/3/3/3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	COA	C5A-C6A-N6A	2.47	124.11	120.35
4	A	401	COA	CEP-CBP-CCP	2.37	112.09	108.23
4	C	401	COA	CEP-CBP-CCP	2.34	112.05	108.23
4	C	401	COA	C5A-C6A-N6A	2.31	123.86	120.35
4	D	401	COA	C5A-C6A-N6A	2.26	123.78	120.35

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

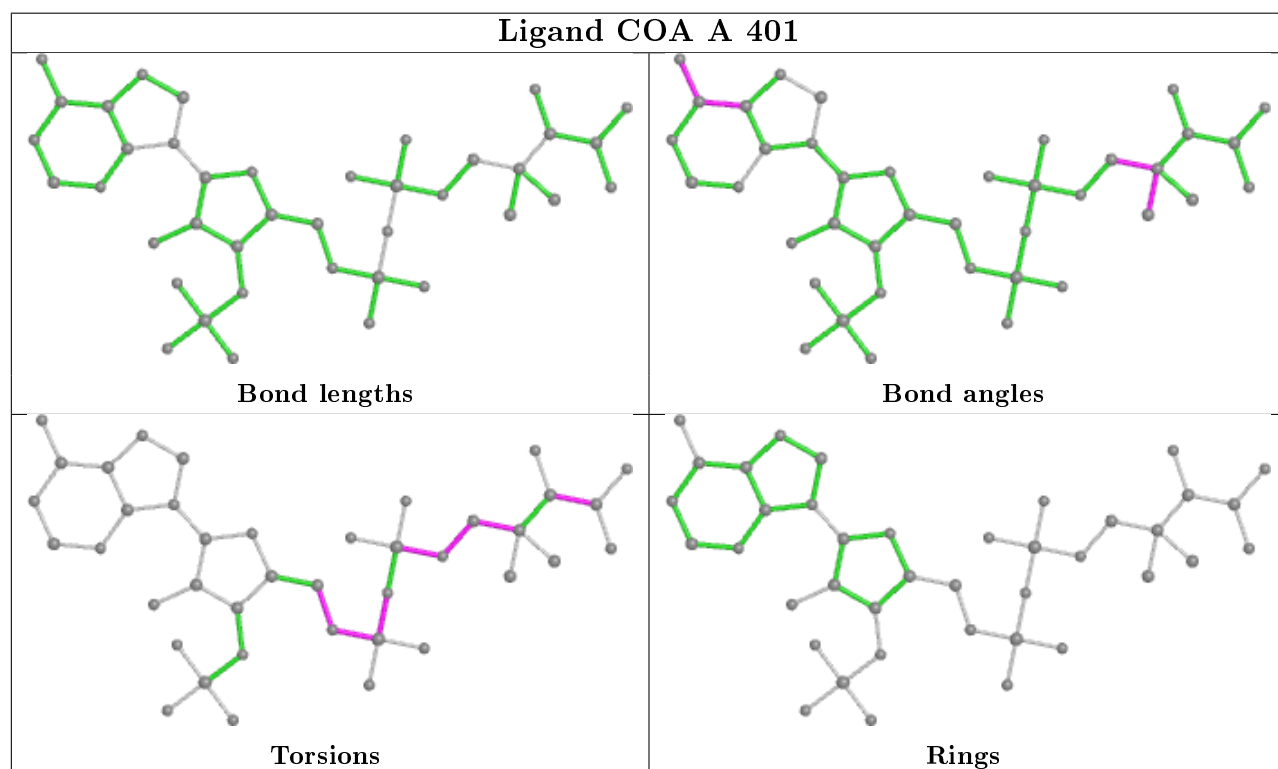
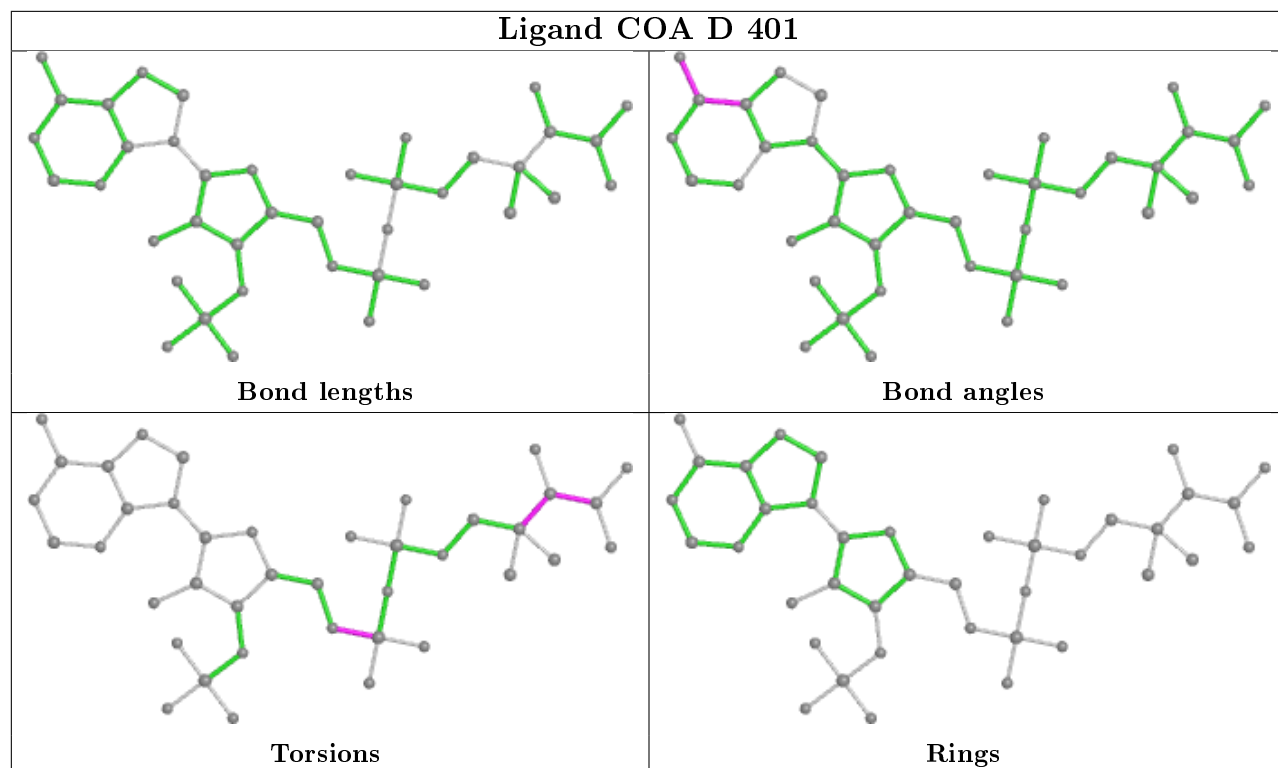
Mol	Chain	Res	Type	Atoms
4	A	401	COA	C5B-O5B-P1A-O2A
4	A	401	COA	C5B-O5B-P1A-O3A
4	A	401	COA	CCP-O6A-P2A-O3A
4	A	401	COA	CCP-O6A-P2A-O4A
4	A	401	COA	CBP-CCP-O6A-P2A

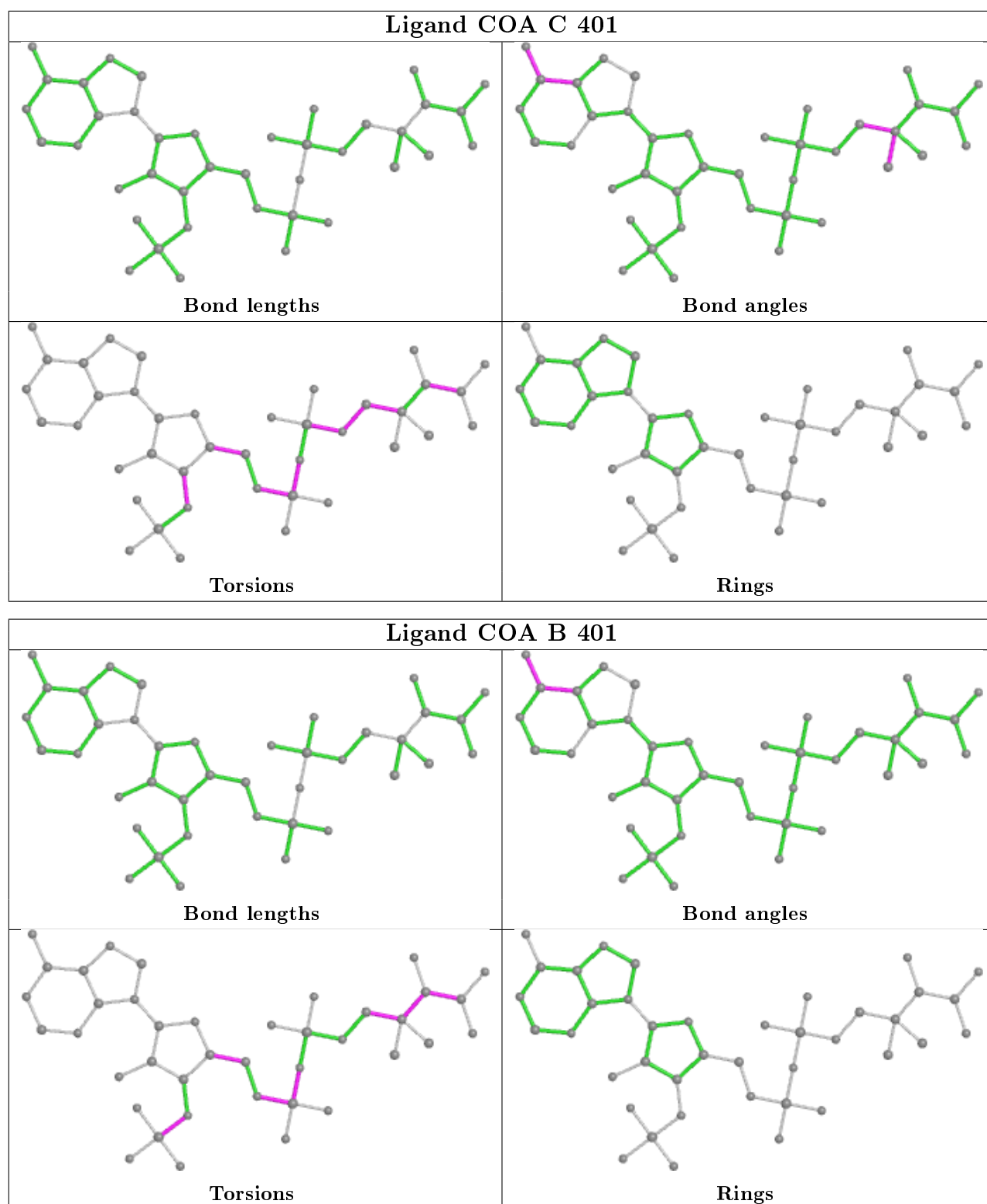
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	COA	5	0
4	C	401	COA	2	0
4	B	401	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 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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	392/392 (100%)	0.81	53 (13%) <b>3</b> <b>1</b>	68, 134, 173, 199	0
1	B	392/392 (100%)	0.18	7 (1%) 68 51	56, 78, 114, 147	0
1	C	392/392 (100%)	0.79	62 (15%) <b>2</b> <b>1</b>	89, 120, 162, 193	0
1	D	392/392 (100%)	0.04	1 (0%) 94 87	53, 79, 112, 158	0
2	E	127/130 (97%)	0.30	3 (2%) 59 42	72, 107, 180, 216	0
2	F	129/130 (99%)	0.24	4 (3%) 49 32	61, 91, 173, 219	0
2	G	128/130 (98%)	0.42	14 (10%) <b>5</b> <b>3</b>	57, 88, 167, 209	0
2	H	128/130 (98%)	1.17	35 (27%) <b>0</b> <b>0</b>	93, 127, 194, 227	0
3	I	347/349 (99%)	0.15	8 (2%) 60 43	59, 80, 117, 149	0
3	J	348/349 (99%)	0.44	28 (8%) <b>12</b> <b>7</b>	77, 118, 154, 180	0
3	K	347/349 (99%)	0.16	8 (2%) 60 43	56, 82, 119, 154	0
3	L	347/349 (99%)	0.55	29 (8%) <b>11</b> <b>6</b>	76, 112, 152, 184	0
All	All	3469/3484 (99%)	0.42	252 (7%) <b>15</b> <b>8</b>	53, 101, 160, 227	0

The worst 5 of 252 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	ALA	7.1
3	L	197	TYR	6.8
3	L	347	ILE	6.6
1	C	312	GLU	6.5
1	C	227	PHE	6.5

### 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

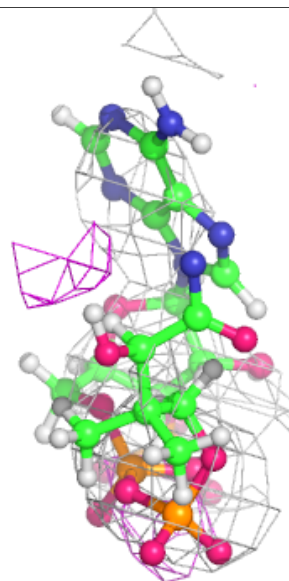
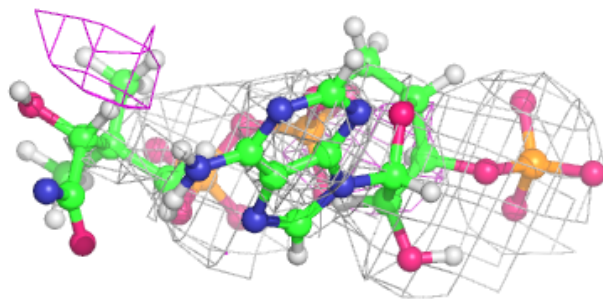
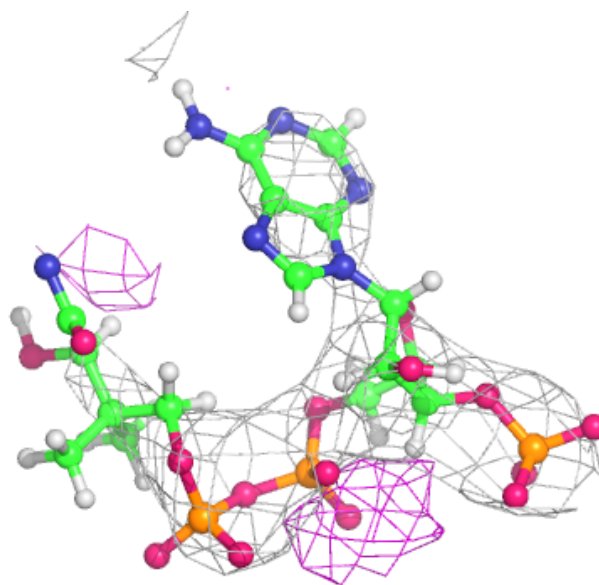
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	COA	A	401	40/48	0.74	0.37	216,228,237,241	0
4	COA	D	401	40/48	0.74	0.31	138,167,184,185	0
6	ZN	E	201	1/1	0.75	0.08	159,159,159,159	1
4	COA	B	401	40/48	0.77	0.30	154,181,203,209	0
5	K	B	403	1/1	0.78	0.11	134,134,134,134	0
4	COA	C	401	40/48	0.81	0.22	129,161,185,189	0
5	K	B	402	1/1	0.87	0.54	124,124,124,124	0
6	ZN	G	201	1/1	0.88	0.14	122,122,122,122	1
7	CL	F	202	1/1	0.89	0.57	63,63,63,63	1
6	ZN	F	201	1/1	0.91	0.08	174,174,174,174	1
7	CL	G	202	1/1	0.93	0.23	69,69,69,69	1
6	ZN	H	201	1/1	0.93	0.37	115,115,115,115	1
7	CL	E	202	1/1	0.93	0.32	104,104,104,104	0
5	K	L	401	1/1	0.94	0.49	147,147,147,147	0
5	K	I	401	1/1	0.96	0.28	99,99,99,99	0
8	NA	K	401	1/1	0.96	0.19	63,63,63,63	0

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

**Electron density around COA A 401:**

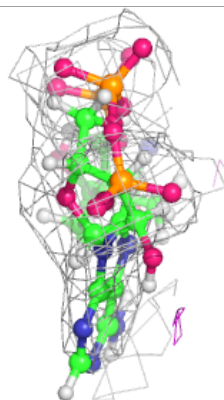
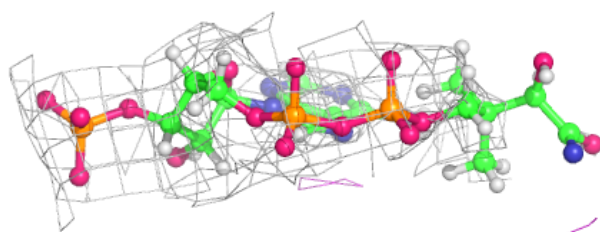
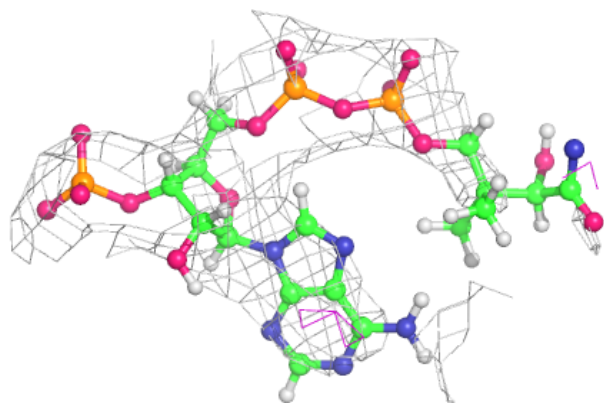
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



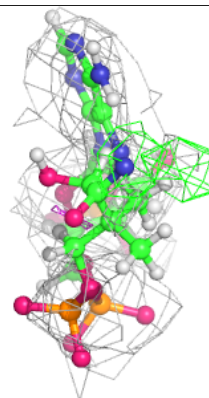
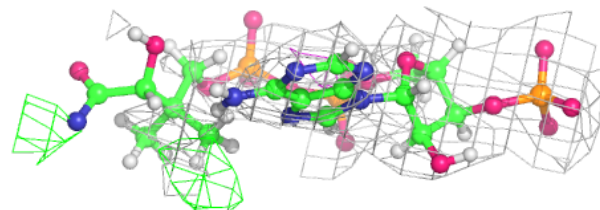
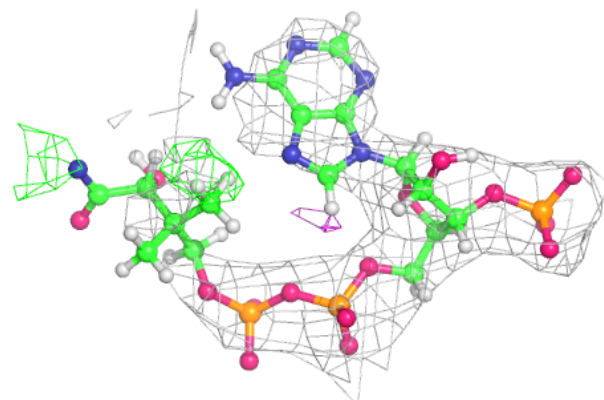


**Electron density around COA D 401:**

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

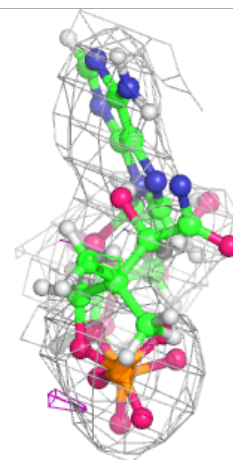
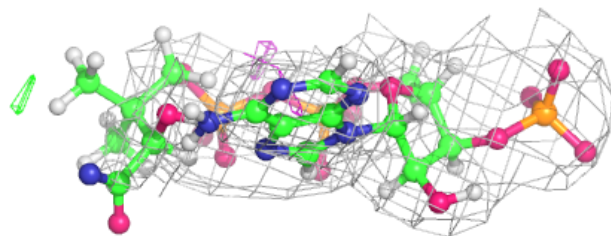
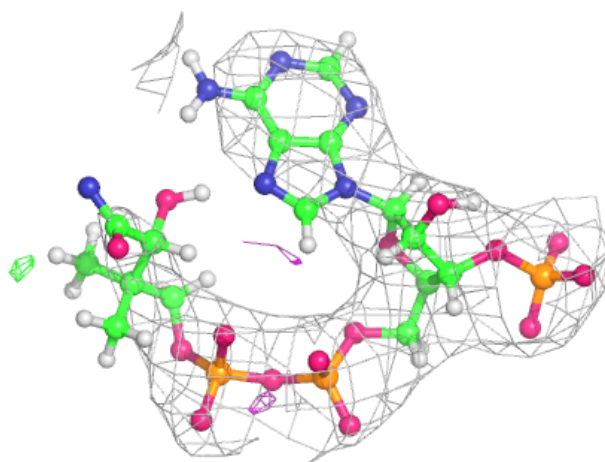
**Electron density around COA B 401:**

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



**Electron density around COA C 401:**

$2mF_o-DF_c$  (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.