



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:55 PM UTC

PDB ID : 6ARE / pdb_00006are
Title : Aspergillus fumigatus Cytosolic Thiolase in complex with two tetrahedral reaction intermediates and ammonium ions
Authors : Marshall, A.C.; Bond, C.S.; Bruning, J.B.
Deposited on : 2017-08-22
Resolution : 1.75 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

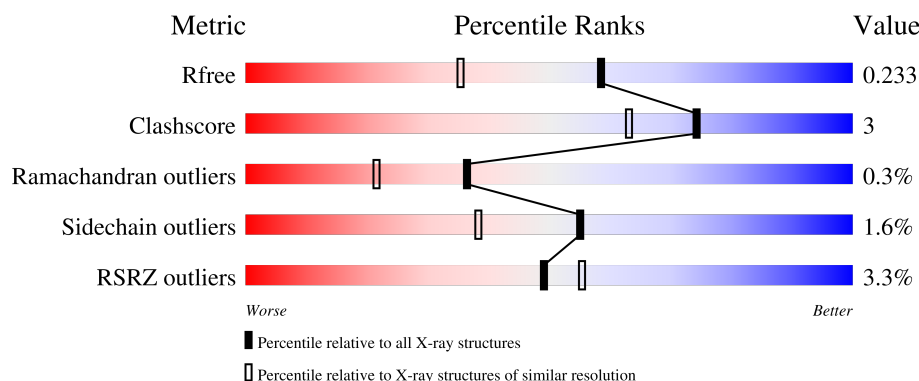
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

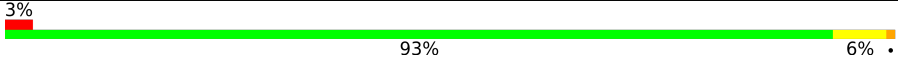
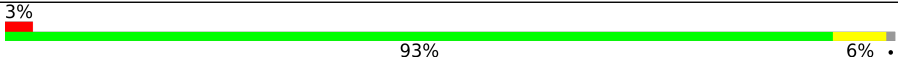
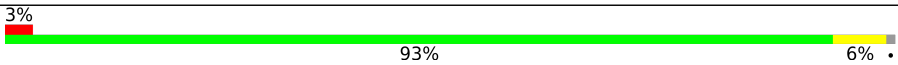
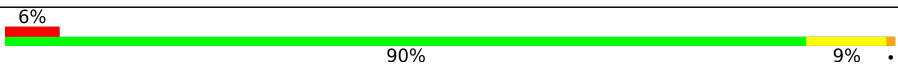
The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	399	
1	B	399	
2	C	399	
2	D	399	

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
4	CL	B	402	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13043 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, acetylated enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	6	0
			2888	1822	497	557	12			
1	B	397	Total	C	N	O	S	0	11	0
			2904	1830	498	564	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q4WCL5
B	0	GLY	-	expression tag	UNP Q4WCL5

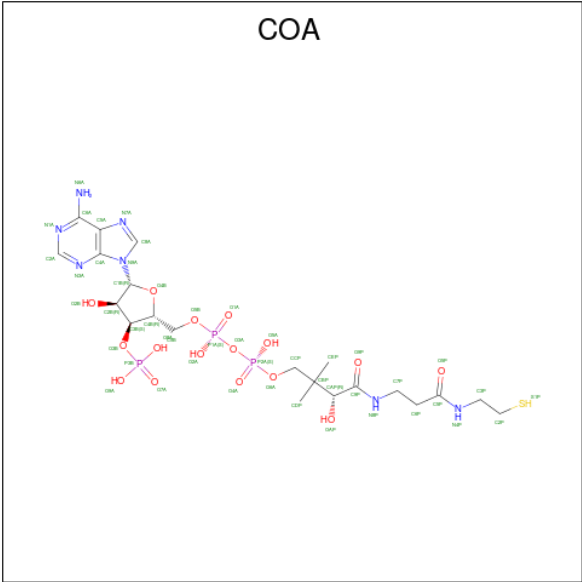
- Molecule 2 is a protein called Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	394	Total	C	N	O	S	0	3	0
			2836	1785	487	552	12			
2	D	398	Total	C	N	O	S	0	3	0
			2838	1787	490	549	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP Q4WCL5
D	0	GLY	-	expression tag	UNP Q4WCL5

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).

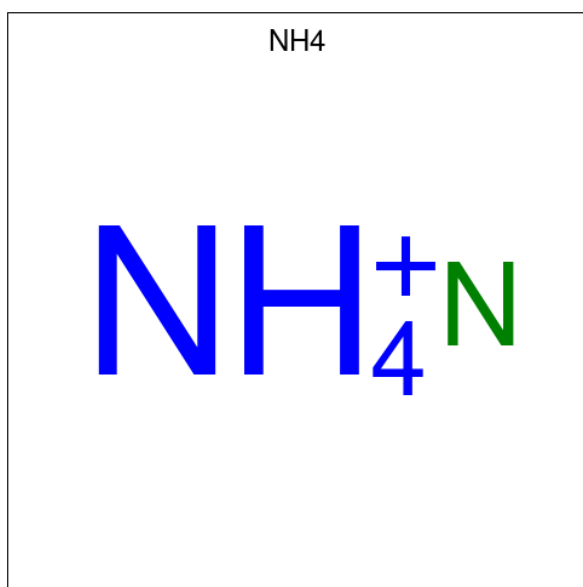


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	1
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	1
			48	21	7	16	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

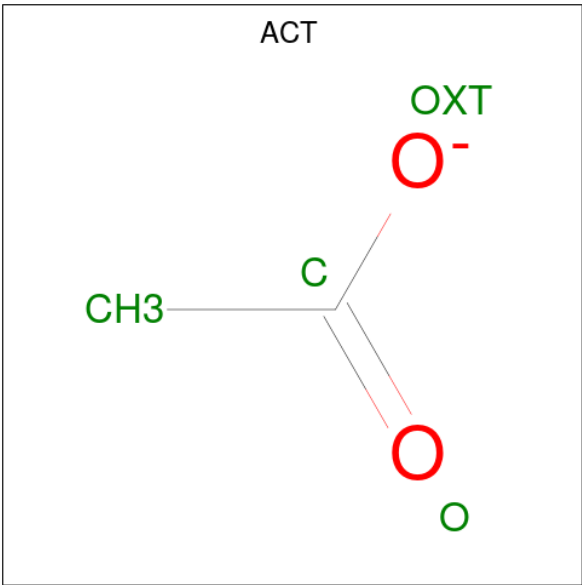
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



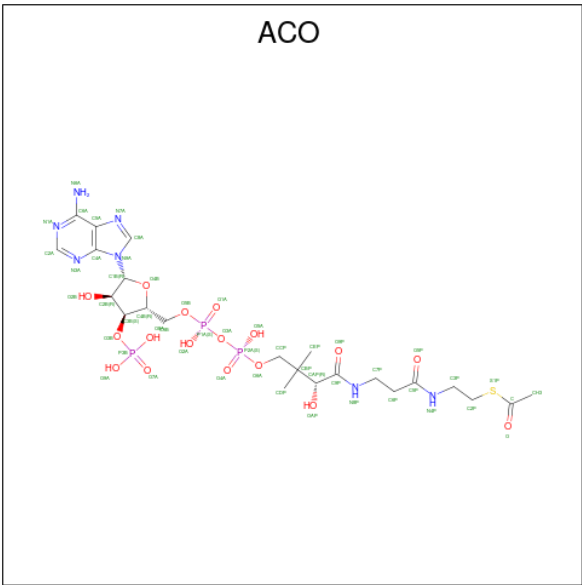
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N 1 1	0	0
5	A	1	Total N 1 1	0	0
5	B	1	Total N 1 1	0	0
5	B	1	Total N 1 1	0	0
5	B	1	Total N 1 1	0	0
5	C	1	Total N 1 1	0	0
5	C	1	Total N 1 1	0	0
5	C	1	Total N 1 1	0	0
5	D	1	Total N 1 1	0	0
5	D	1	Total N 1 1	0	0

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			3	2	1		
6	D	1	Total	C	O	0	0
			3	2	1		

- Molecule 7 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

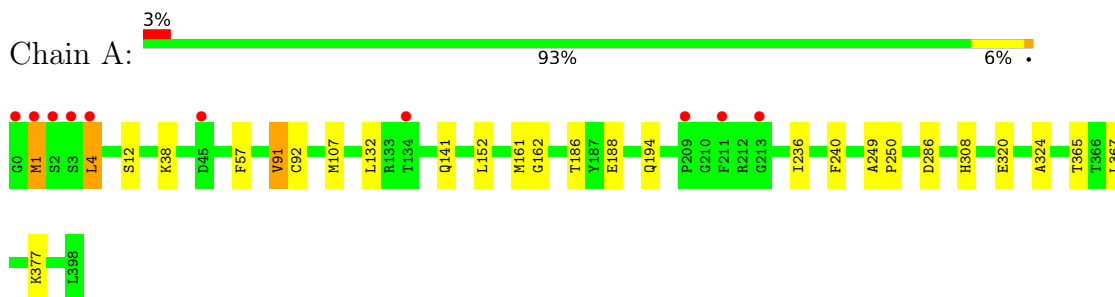
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	406	Total 407	O 407	0	1
8	B	462	Total 463	O 463	0	1
8	C	270	Total 270	O 270	0	0
8	D	222	Total 222	O 222	0	0

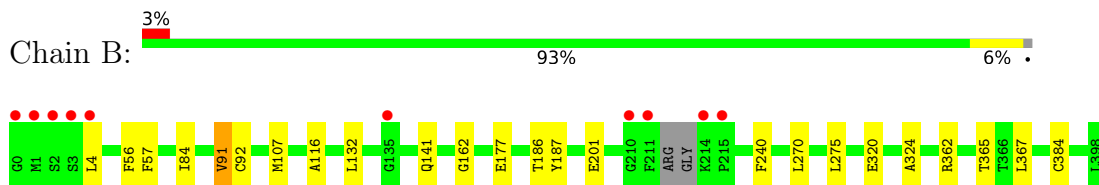
3 Residue-property plots

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.

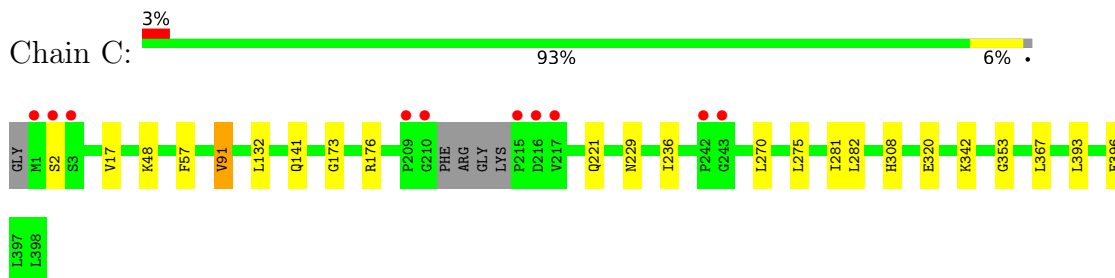
- Molecule 1: Acetyl-CoA acetyltransferase, acetylated enzyme



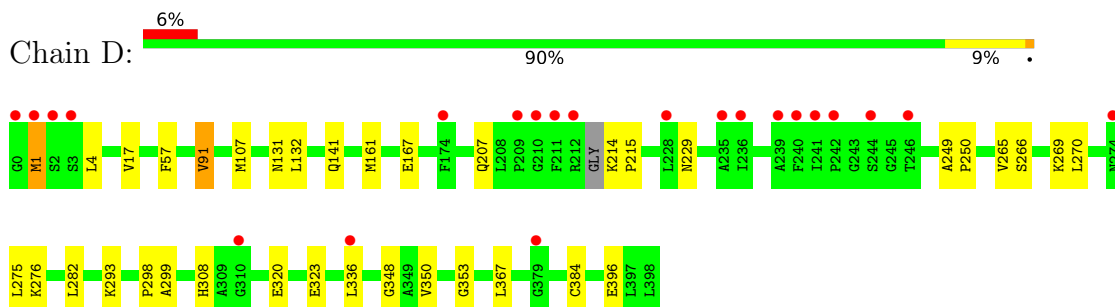
- Molecule 1: Acetyl-CoA acetyltransferase, acetylated enzyme



- Molecule 2: Acetyl-CoA acetyltransferase



- Molecule 2: Acetyl-CoA acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.36Å 106.59Å 110.84Å 90.00° 104.27° 90.00°	Depositor
Resolution (Å)	31.29 – 1.75 31.29 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (31.29-1.75) 99.6 (31.29-1.75)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.75Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.194 , 0.232 0.195 , 0.233	Depositor DCC
R_{free} test set	8014 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13043	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SCY, ACO, COA, NH4, ACT

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	0.33	0/2937	0.52	0/3982
1	B	0.34	0/2962	0.54	0/4016
2	C	0.24	0/2888	0.44	0/3920
2	D	0.24	0/2890	0.42	0/3927
All	All	0.29	0/11677	0.48	0/15845

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2888	0	2964	17	0
1	B	2904	0	2963	15	0
2	C	2836	0	2888	13	0
2	D	2838	0	2861	20	0
3	A	48	0	3	1	0
3	B	48	0	3	1	0
3	D	48	0	32	5	0
4	A	1	0	0	1	0
4	B	1	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	1	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
6	C	3	0	3	0	0
6	D	3	0	3	1	0
7	C	51	0	32	3	0
8	A	407	0	0	3	0
8	B	463	0	0	6	0
8	C	270	0	0	5	0
8	D	222	0	0	0	0
All	All	13043	0	11752	70	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 3.

All (70) 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:D:401:COA:O4B	3:D:401:COA:C1B	1.65	1.22
3:D:401:COA:S1P	6:D:402:ACT:C	2.33	1.15
7:C:406:ACO:C1B	7:C:406:ACO:O4B	1.65	1.13
4:A:402:CL:CL	8:B:798:HOH:O	2.28	0.87
8:C:670:HOH:O	4:D:403:CL:CL	2.48	0.69
1:B:270:LEU:HD12	1:B:275:LEU:HB2	1.80	0.64
2:D:167:GLU:OE1	2:D:293:LYS:NZ	2.28	0.60
2:D:320:GLU:HG3	2:D:367:LEU:HB2	1.81	0.60
2:D:265:VAL:HG13	2:D:269:LYS:HB3	1.84	0.60
2:D:270:LEU:HD12	2:D:275:LEU:HB2	1.83	0.59
1:B:384:CYS:SG	8:B:746[B]:HOH:O	2.57	0.58
1:A:1:MET:HG3	1:A:308:HIS:CE1	2.38	0.58
2:C:2:SER:HB3	2:C:308:HIS:NE2	2.20	0.56
1:A:324:ALA:HB1	3:A:401[B]:COA:H22	1.89	0.55
1:B:177[B]:GLU:HG3	8:B:562:HOH:O	2.06	0.55
1:A:4:LEU:HB3	1:A:107:MET:HE3	1.88	0.55
2:C:282:LEU:HD11	2:C:396[B]:GLU:HB2	1.89	0.54
1:B:4:LEU:HB3	1:B:107:MET:HE3	1.90	0.54
2:C:270:LEU:HD12	2:C:275:LEU:HB2	1.90	0.54
7:C:406:ACO:O	8:C:501:HOH:O	2.18	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD21	2:C:141:GLN:HG3	1.91	0.53
2:D:161:MET:HG3	3:D:401:COA:H21	1.92	0.52
2:C:176:ARG:NH1	8:C:503:HOH:O	2.37	0.51
1:B:141:GLN:HG3	2:D:132:LEU:HD21	1.92	0.51
1:A:141:GLN:HG3	2:C:132:LEU:HD21	1.94	0.49
1:A:188:GLU:OE1	8:A:501:HOH:O	2.20	0.49
2:D:323:GLU:CD	2:D:348:GLY:HA3	2.38	0.48
3:D:401:COA:H52A	3:D:401:COA:H8A	1.95	0.48
2:C:281:ILE:HG23	2:C:393:LEU:HD11	1.95	0.48
1:B:362:ARG:O	1:B:365[B]:THR:HG22	2.14	0.47
2:C:320:GLU:HG3	2:C:367:LEU:HB2	1.96	0.47
2:D:4:LEU:CB	2:D:107:MET:HE3	2.45	0.47
4:B:402:CL:CL	8:B:603:HOH:O	2.58	0.46
2:D:323:GLU:HB3	2:D:350:VAL:HG23	1.96	0.46
1:B:132:LEU:HD21	2:D:141:GLN:HG3	1.98	0.46
2:D:282:LEU:HD11	2:D:396:GLU:HB2	1.97	0.45
1:A:152:LEU:O	1:A:161:MET:HG2	2.17	0.45
1:A:286:ASP:HB2	1:B:84[A]:ILE:HD13	1.99	0.44
1:B:56:PHE:O	1:B:116:ALA:HA	2.16	0.44
1:B:320:GLU:HG3	1:B:367:LEU:HB2	1.99	0.44
2:C:229:ASN:HB3	7:C:406:ACO:H2A	1.99	0.44
2:D:214:LYS:HA	2:D:215:PRO:HD3	1.86	0.44
8:A:738:HOH:O	4:B:402:CL:CL	2.59	0.44
2:C:48:LYS:HE2	2:C:48:LYS:HB3	1.76	0.44
1:A:12:SER:HB2	1:A:365[B]:THR:HG22	2.00	0.44
1:A:320:GLU:HG3	1:A:367:LEU:HB2	1.99	0.44
1:A:162:GLY:HA3	1:A:240:PHE:CZ	2.53	0.43
2:D:17:VAL:HG11	2:D:353:GLY:HA3	2.00	0.43
1:B:162:GLY:HA3	1:B:240:PHE:CZ	2.55	0.42
2:D:229:ASN:HB3	3:D:401:COA:H2A	2.00	0.42
2:D:298:PRO:HD3	2:D:384:CYS:HB3	2.01	0.42
1:A:38[B]:LYS:HE2	8:A:817:HOH:O	2.20	0.42
2:C:17:VAL:HG11	2:C:353:GLY:HA3	2.02	0.42
2:C:342:LYS:NZ	8:C:505:HOH:O	2.38	0.41
2:D:249:ALA:HB3	2:D:250:PRO:HD3	2.02	0.41
2:D:1:MET:HG3	2:D:308:HIS:CE1	2.55	0.41
1:A:249:ALA:HB3	1:A:250:PRO:HD3	2.02	0.41
1:B:201:GLU:OE2	8:B:501:HOH:O	2.21	0.40
1:A:377:LYS:HA	1:A:377:LYS:HD3	1.83	0.40
2:D:299:ALA:HA	2:D:336:LEU:HD21	2.03	0.40
1:B:324:ALA:HB1	3:B:401[B]:COA:H22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:173:GLY:HA2	8:C:703:HOH:O	2.22	0.40
2:D:265:VAL:HG12	2:D:266:SER:O	2.21	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	401/399 (100%)	395 (98%)	5 (1%)	1 (0%)	43	27
1	B	402/399 (101%)	393 (98%)	8 (2%)	1 (0%)	43	27
2	C	393/399 (98%)	385 (98%)	7 (2%)	1 (0%)	36	21
2	D	397/399 (100%)	382 (96%)	14 (4%)	1 (0%)	36	21
All	All	1593/1596 (100%)	1555 (98%)	34 (2%)	4 (0%)	36	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	VAL
1	B	91	VAL
2	C	91	VAL
2	D	91	VAL

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	298/297 (100%)	291 (98%)	7 (2%)	44	24
1	B	301/297 (101%)	298 (99%)	3 (1%)	68	56
2	C	294/298 (99%)	290 (99%)	4 (1%)	59	44
2	D	287/298 (96%)	282 (98%)	5 (2%)	53	36
All	All	1180/1190 (99%)	1161 (98%)	19 (2%)	55	38

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	LEU
1	A	57	PHE
1	A	91	VAL
1	A	186	THR
1	A	194	GLN
1	A	236	ILE
1	B	57	PHE
1	B	91	VAL
1	B	186	THR
2	C	57	PHE
2	C	91	VAL
2	C	221	GLN
2	C	236	ILE
2	D	1	MET
2	D	57	PHE
2	D	91	VAL
2	D	207	GLN
2	D	276	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	110	ASN
1	A	289	GLN
1	A	322	ASN
1	B	59	ASN
1	B	104	GLN
1	B	124	ASN
2	C	59	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	104	GLN
2	C	110	ASN
2	C	221	GLN
2	D	110	ASN
2	D	158	GLN
2	D	227	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic and 10 are modelled with single atom - leaving 6 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
7	ACO	C	406	6	51,53,53	2.47	9 (17%)	73,79,79	1.75	11 (15%)
3	COA	D	401	-	47,50,50	2.58	10 (21%)	69,75,75	1.58	10 (14%)
6	ACT	C	401	2,7	1,2,3	4.82	1 (100%)	0,1,3	-	-
6	ACT	D	402	2	1,2,3	4.98	1 (100%)	0,1,3	-	-

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
7	ACO	C	406	6	-	16/51/67/67	0/3/3/3
3	COA	D	401	-	-	18/48/64/64	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	COA	O4B-C1B	10.03	1.65	1.42
7	C	406	ACO	O4B-C1B	9.97	1.65	1.42
7	C	406	ACO	C2B-C1B	-6.68	1.32	1.53
3	D	401	COA	C2B-C1B	-6.62	1.32	1.53
3	D	401	COA	O4B-C4B	-6.57	1.30	1.45
7	C	406	ACO	O4B-C4B	-6.39	1.30	1.45
3	D	401	COA	C9P-N8P	5.31	1.46	1.33
6	D	402	ACT	O-C	4.98	1.40	1.20
7	C	406	ACO	C5P-N4P	4.96	1.45	1.33
3	D	401	COA	C5P-N4P	4.95	1.45	1.33
6	C	401	ACT	O-C	4.82	1.40	1.20
7	C	406	ACO	P1A-O3A	4.03	1.63	1.59
7	C	406	ACO	C9P-N8P	4.01	1.43	1.33
7	C	406	ACO	C6A-N6A	3.52	1.43	1.34
3	D	401	COA	C6A-N6A	3.30	1.42	1.34
3	D	401	COA	O3B-C3B	-3.03	1.33	1.44
7	C	406	ACO	O3B-C3B	-2.86	1.34	1.44
3	D	401	COA	C8A-N7A	2.58	1.36	1.31
7	C	406	ACO	C2A-N3A	2.29	1.38	1.33
3	D	401	COA	C1B-N9A	-2.06	1.40	1.46
3	D	401	COA	C2A-N3A	2.02	1.37	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	406	ACO	N6A-C6A-N1A	-5.84	105.37	118.38
7	C	406	ACO	N3A-C2A-N1A	-5.45	120.33	128.58
3	D	401	COA	N3A-C2A-N1A	-5.40	120.41	128.58
7	C	406	ACO	C5A-C4A-N3A	-4.91	119.95	126.72
3	D	401	COA	C5A-C4A-N3A	-4.69	120.26	126.72
7	C	406	ACO	C5A-C6A-N6A	4.47	134.34	123.29
3	D	401	COA	N9A-C8A-N7A	-4.19	108.00	113.94
7	C	406	ACO	N9A-C8A-N7A	-3.97	108.30	113.94
7	C	406	ACO	C6P-C7P-N8P	-3.61	104.33	112.00
3	D	401	COA	C2A-N3A-C4A	3.32	119.95	111.83
7	C	406	ACO	C2A-N3A-C4A	3.32	119.94	111.83
3	D	401	COA	N6A-C6A-N1A	-3.24	111.15	118.38
7	C	406	ACO	N3A-C4A-N9A	3.01	132.28	127.17
3	D	401	COA	N3A-C4A-N9A	2.77	131.88	127.17
3	D	401	COA	C5A-N7A-C8A	2.72	107.72	103.45
7	C	406	ACO	C5A-N7A-C8A	2.70	107.69	103.45
3	D	401	COA	C4A-N9A-C1B	-2.32	121.20	126.63
3	D	401	COA	C4A-N9A-C8A	2.29	108.14	105.74
7	C	406	ACO	C2P-C3P-N4P	-2.27	107.68	112.41
7	C	406	ACO	C4A-N9A-C8A	2.06	107.91	105.74
3	D	401	COA	C4A-C5A-N7A	-2.01	108.28	110.58

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	COA	CCP-O6A-P2A-O3A
3	D	401	COA	CCP-O6A-P2A-O4A
3	D	401	COA	CCP-O6A-P2A-O5A
3	D	401	COA	CDP-CBP-CCP-O6A
3	D	401	COA	CEP-CBP-CCP-O6A
3	D	401	COA	CAP-CBP-CCP-O6A
3	D	401	COA	OAP-CAP-CBP-CCP
3	D	401	COA	C9P-CAP-CBP-CCP
3	D	401	COA	OAP-CAP-CBP-CDP
3	D	401	COA	C2P-C3P-N4P-C5P
3	D	401	COA	S1P-C2P-C3P-N4P
7	C	406	ACO	C5B-O5B-P1A-O1A
7	C	406	ACO	CDP-CBP-CCP-O6A
7	C	406	ACO	CEP-CBP-CCP-O6A
7	C	406	ACO	CAP-CBP-CCP-O6A
7	C	406	ACO	OAP-CAP-CBP-CCP
7	C	406	ACO	C9P-CAP-CBP-CCP

Continued on next page...

Continued from previous page...

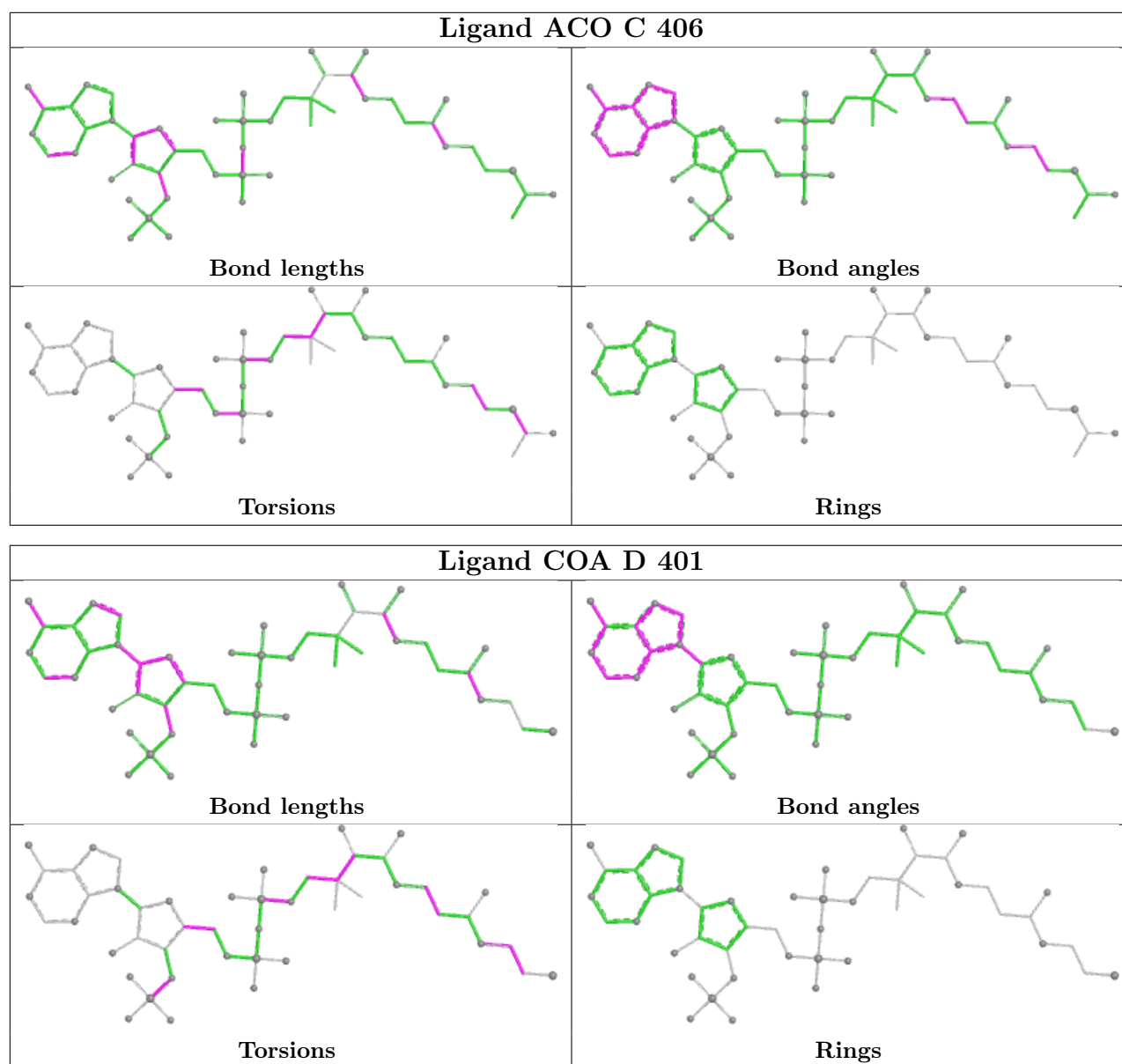
Mol	Chain	Res	Type	Atoms
7	C	406	ACO	OAP-CAP-CBP-CEP
7	C	406	ACO	S1P-C2P-C3P-N4P
7	C	406	ACO	O-C-S1P-C2P
7	C	406	ACO	CH3-C-S1P-C2P
7	C	406	ACO	O4B-C4B-C5B-O5B
7	C	406	ACO	C3B-C4B-C5B-O5B
3	D	401	COA	OAP-CAP-CBP-CEP
7	C	406	ACO	OAP-CAP-CBP-CDP
3	D	401	COA	C9P-CAP-CBP-CDP
7	C	406	ACO	C9P-CAP-CBP-CEP
7	C	406	ACO	CCP-O6A-P2A-O4A
3	D	401	COA	C5P-C6P-C7P-N8P
3	D	401	COA	C3B-O3B-P3B-O7A
3	D	401	COA	C9P-CAP-CBP-CEP
7	C	406	ACO	C9P-CAP-CBP-CDP
3	D	401	COA	O4B-C4B-C5B-O5B
3	D	401	COA	C3B-O3B-P3B-O9A

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	406	ACO	3	0
3	D	401	COA	5	0
6	D	402	ACT	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	398/399 (99%)	0.05	10 (2%) 58 64	4, 11, 26, 52	5 (1%)
1	B	396/399 (99%)	0.01	10 (2%) 58 64	4, 10, 26, 54	10 (2%)
2	C	394/399 (98%)	0.40	10 (2%) 58 64	7, 20, 38, 55	3 (0%)
2	D	398/399 (99%)	0.70	22 (5%) 30 35	11, 25, 44, 57	3 (0%)
All	All	1586/1596 (99%)	0.29	52 (3%) 49 55	4, 16, 38, 57	21 (1%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	PRO	5.3
1	A	4	LEU	5.3
1	B	211	PHE	4.9
1	A	2	SER	4.6
1	A	0	GLY	4.5
1	A	1	MET	4.5
1	A	213	GLY	4.2
1	B	1	MET	4.0
1	B	0	GLY	4.0
2	C	215	PRO	4.0
2	D	211	PHE	3.7
2	D	244	SER	3.6
2	D	1	MET	3.5
1	B	3	SER	3.3
2	C	1	MET	3.3
2	C	3	SER	3.2
2	D	2	SER	3.2
1	B	4	LEU	3.1
2	C	210	GLY	3.1
2	D	241	ILE	2.9
2	D	210	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	3	SER	2.8
1	B	214	LYS	2.8
2	C	2	SER	2.7
1	B	2	SER	2.7
2	D	274	ASN	2.7
2	D	310	GLY	2.6
2	D	235	ALA	2.6
2	C	243	GLY	2.5
2	D	239	ALA	2.5
1	B	135	GLY	2.5
2	D	0	GLY	2.4
2	D	209	PRO	2.4
2	C	209	PRO	2.4
2	D	246	THR	2.4
2	D	242	PRO	2.3
1	A	209	PRO	2.3
2	D	240	PHE	2.3
1	A	45	ASP	2.3
1	B	210	GLY	2.3
2	C	242	PRO	2.2
2	D	212	ARG	2.2
2	D	336	LEU	2.2
2	C	217	VAL	2.2
1	A	211	PHE	2.2
2	D	174	PHE	2.2
2	D	236	ILE	2.2
2	D	3	SER	2.2
1	A	134	THR	2.1
2	D	379	GLY	2.1
2	C	216	ASP	2.1
2	D	228	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SCY	B	92[A]	9/10	0.91	0.11	5,5,14,14	3
1	SCY	A	92[A]	9/10	0.93	0.10	5,6,12,14	3

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

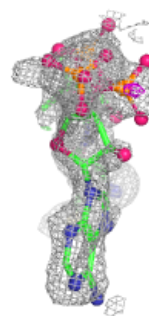
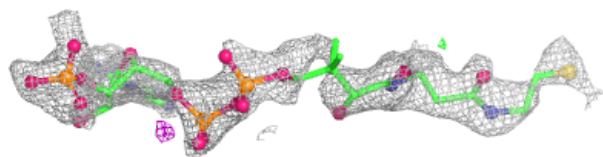
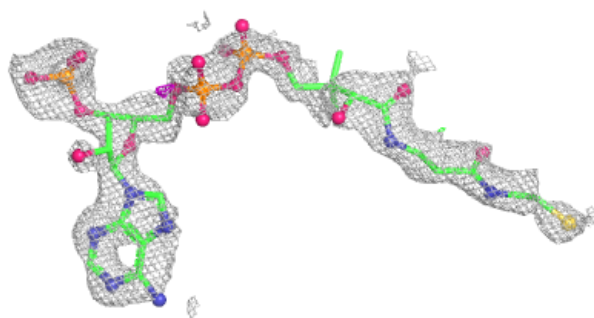
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NH4	C	405	1/1	0.70	0.20	38,38,38,38	0
3	COA	D	401	48/48	0.71	0.19	38,57,73,75	48
7	ACO	C	406	51/51	0.72	0.19	29,63,69,71	51
3	COA	B	401[B]	48/48	0.81	0.16	9,33,54,55	48
6	ACT	D	402	3/4	0.83	0.14	19,19,19,21	3
5	NH4	C	404	1/1	0.86	0.12	21,21,21,21	1
3	COA	A	401[B]	48/48	0.87	0.14	14,27,46,49	48
5	NH4	B	405	1/1	0.88	0.16	32,32,32,32	0
5	NH4	A	404	1/1	0.90	0.12	21,21,21,21	0
6	ACT	C	401	3/4	0.91	0.12	19,19,21,26	3
5	NH4	D	405	1/1	0.92	0.08	31,31,31,31	0
5	NH4	B	404	1/1	0.93	0.09	18,18,18,18	0
4	CL	B	402	1/1	0.95	0.04	6,6,6,6	1
4	CL	C	402	1/1	0.95	0.06	25,25,25,25	1
4	CL	D	403	1/1	0.95	0.06	23,23,23,23	1
5	NH4	C	403	1/1	0.96	0.05	14,14,14,14	0
5	NH4	D	404	1/1	0.96	0.06	17,17,17,17	0
4	CL	A	402	1/1	0.97	0.05	10,10,10,10	1
5	NH4	A	403	1/1	0.98	0.06	8,8,8,8	0
5	NH4	B	403	1/1	0.99	0.04	5,5,5,5	0

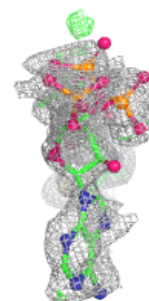
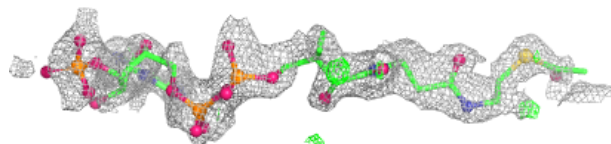
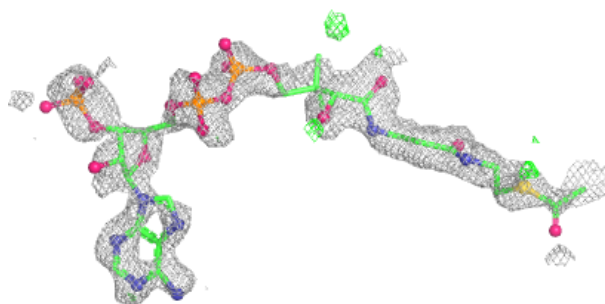
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA 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 ACO C 406:**

$2mF_o-DF_c$ (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.