



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2021 – 10:10 AM EDT

PDB ID : 7LDC
Title : Zoogloea ramigera biosynthetic thiolase Q183Y/Y218E mutant
Authors : Marshall, A.C.; Bruning, J.B.
Deposited on : 2021-01-13
Resolution : 2.50 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 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 : 2.23.1
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) : 2.23.1

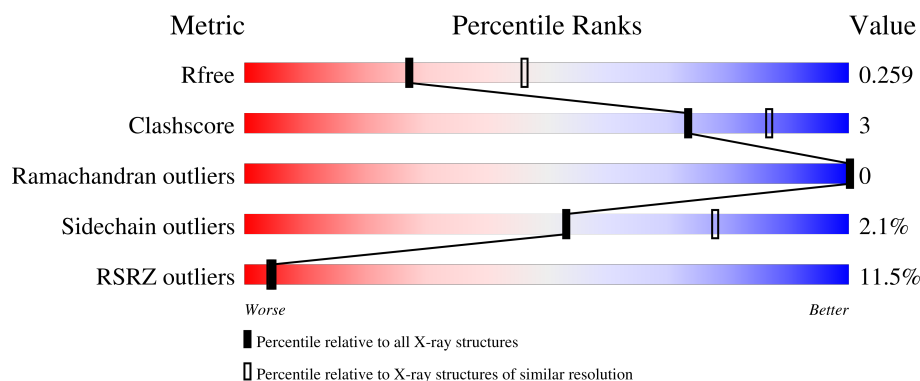
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	<div> <div>6%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
1	B	399	<div> <div>5%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	C	399	<div> <div>10%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	D	399	<div> <div>24%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11847 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			2786	1732	499	534	21			
1	B	387	Total	C	N	O	S	0	0	0
			2781	1729	497	534	21			
1	C	389	Total	C	N	O	S	0	0	0
			2789	1735	501	532	21			
1	D	387	Total	C	N	O	S	0	0	0
			2714	1684	488	522	20			

There are 44 discrepancies between the modelled and reference sequences:

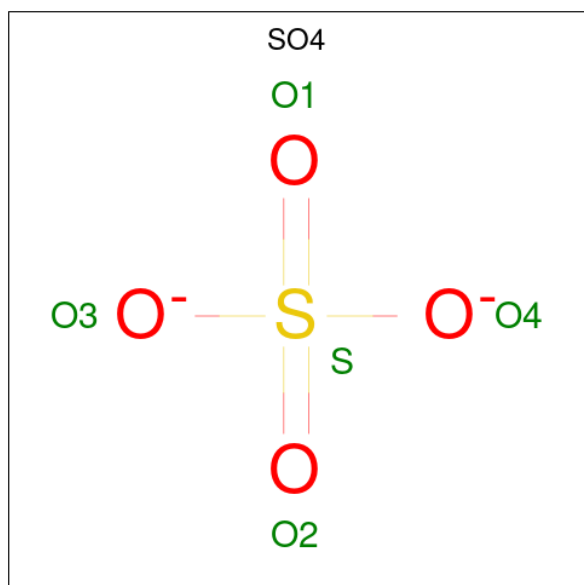
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P07097
A	-5	HIS	-	expression tag	UNP P07097
A	-4	HIS	-	expression tag	UNP P07097
A	-3	HIS	-	expression tag	UNP P07097
A	-2	HIS	-	expression tag	UNP P07097
A	-1	HIS	-	expression tag	UNP P07097
A	0	HIS	-	expression tag	UNP P07097
A	11	ALA	-	insertion	UNP P07097
A	129	ARG	ALA	conflict	UNP P07097
A	183	TYR	GLN	engineered mutation	UNP P07097
A	218	GLU	TYR	engineered mutation	UNP P07097
B	-6	MET	-	initiating methionine	UNP P07097
B	-5	HIS	-	expression tag	UNP P07097
B	-4	HIS	-	expression tag	UNP P07097
B	-3	HIS	-	expression tag	UNP P07097
B	-2	HIS	-	expression tag	UNP P07097
B	-1	HIS	-	expression tag	UNP P07097
B	0	HIS	-	expression tag	UNP P07097
B	11	ALA	-	insertion	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
B	183	TYR	GLN	engineered mutation	UNP P07097

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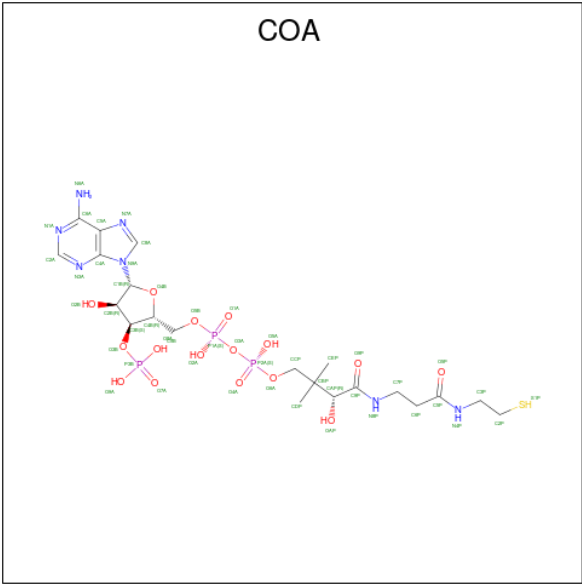
Chain	Residue	Modelled	Actual	Comment	Reference
B	218	GLU	TYR	engineered mutation	UNP P07097
C	-6	MET	-	initiating methionine	UNP P07097
C	-5	HIS	-	expression tag	UNP P07097
C	-4	HIS	-	expression tag	UNP P07097
C	-3	HIS	-	expression tag	UNP P07097
C	-2	HIS	-	expression tag	UNP P07097
C	-1	HIS	-	expression tag	UNP P07097
C	0	HIS	-	expression tag	UNP P07097
C	11	ALA	-	insertion	UNP P07097
C	129	ARG	ALA	conflict	UNP P07097
C	183	TYR	GLN	engineered mutation	UNP P07097
C	218	GLU	TYR	engineered mutation	UNP P07097
D	-6	MET	-	initiating methionine	UNP P07097
D	-5	HIS	-	expression tag	UNP P07097
D	-4	HIS	-	expression tag	UNP P07097
D	-3	HIS	-	expression tag	UNP P07097
D	-2	HIS	-	expression tag	UNP P07097
D	-1	HIS	-	expression tag	UNP P07097
D	0	HIS	-	expression tag	UNP P07097
D	11	ALA	-	insertion	UNP P07097
D	129	ARG	ALA	conflict	UNP P07097
D	183	TYR	GLN	engineered mutation	UNP P07097
D	218	GLU	TYR	engineered mutation	UNP P07097

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).



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

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

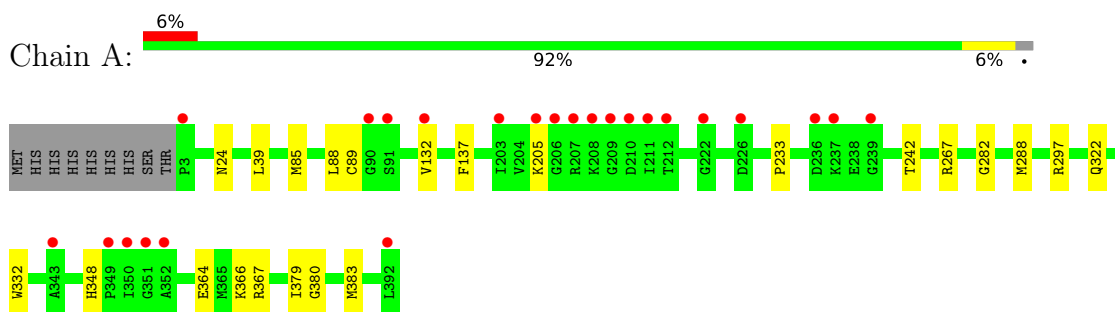
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	203	Total	O	0	0
			203	203		
4	B	179	Total	O	0	0
			179	179		
4	C	94	Total	O	0	0
			94	94		
4	D	59	Total	O	0	0
			59	59		

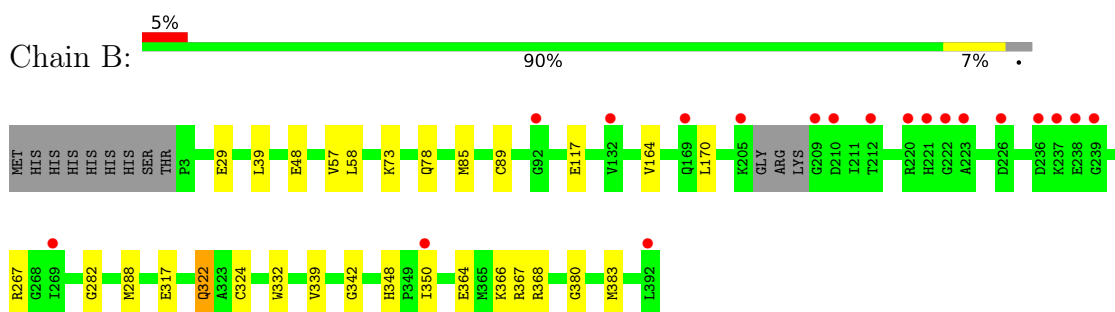
3 Residue-property plots [i](#)

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.

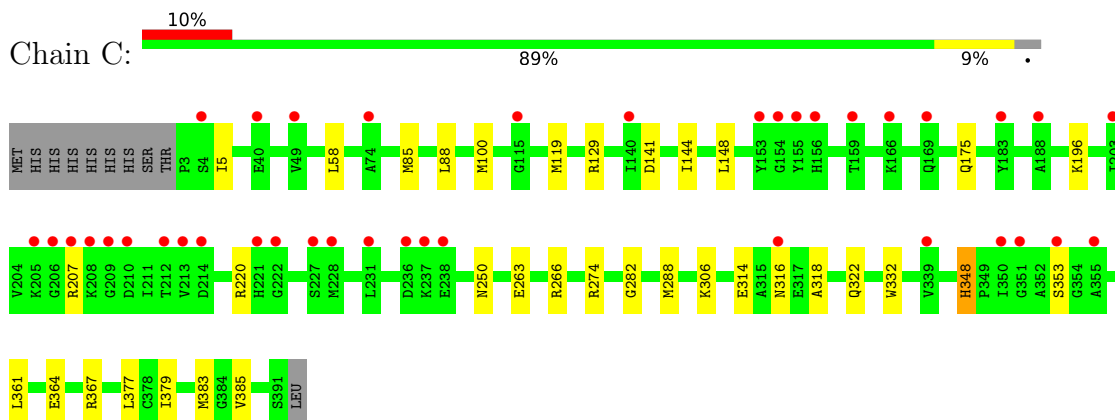
- Molecule 1: Acetyl-CoA acetyltransferase



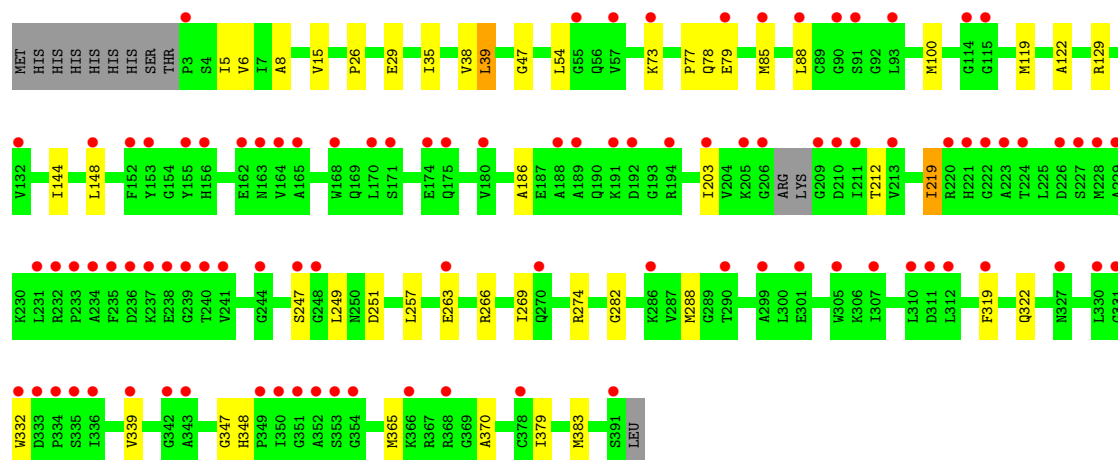
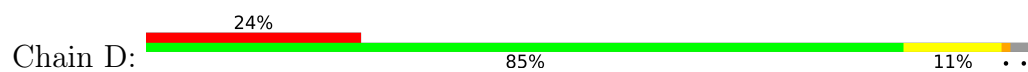
- Molecule 1: Acetyl-CoA acetyltransferase



- Molecule 1: Acetyl-CoA acetyltransferase



- Molecule 1: 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	83.72Å 79.55Å 151.54Å 90.00° 93.95° 90.00°	Depositor
Resolution (Å)	34.71 – 2.50 34.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.71-2.50) 99.9 (34.71-2.50)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.219 , 0.260 0.218 , 0.259	Depositor DCC
R_{free} test set	3451 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11847	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.93% 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: COA, SO4, SCY

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	0.25	0/2818	0.45	0/3810
1	B	0.25	0/2812	0.45	0/3800
1	C	0.25	0/2821	0.43	0/3812
1	D	0.25	0/2743	0.45	0/3715
All	All	0.25	0/11194	0.44	0/15137

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	2786	0	2750	13	0
1	B	2781	0	2759	14	0
1	C	2789	0	2759	23	0
1	D	2714	0	2618	28	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	48	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	32	0	0
3	C	48	0	32	1	0
3	D	48	0	32	0	0
4	A	203	0	0	4	0
4	B	179	0	0	2	0
4	C	94	0	0	5	0
4	D	59	0	0	1	0
All	All	11847	0	11014	74	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 (74) 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:D:29:GLU:HA	1:D:73:LYS:NZ	2.01	0.74
1:B:57:VAL:HG23	1:B:58:LEU:HG	1.72	0.70
1:C:88:LEU:HB2	1:C:379:ILE:HG23	1.75	0.68
1:B:364:GLU:OE1	1:B:367:ARG:NH1	2.31	0.63
1:C:316:ASN:HD22	1:C:377:LEU:HD23	1.63	0.63
1:B:366:LYS:NZ	4:B:506:HOH:O	2.31	0.62
1:D:29:GLU:HA	1:D:73:LYS:HZ2	1.64	0.61
1:A:85:MET:HA	1:B:85:MET:HA	1.83	0.60
1:D:203:ILE:HG12	1:D:212:THR:HG22	1.84	0.59
1:C:220:ARG:NH1	4:C:508:HOH:O	2.37	0.58
1:A:366:LYS:NZ	4:A:516:HOH:O	2.36	0.57
1:D:144:ILE:HD13	1:D:148:LEU:HD12	1.86	0.57
1:A:89:SCY:OCD	1:A:380:GLY:N	2.34	0.56
1:C:85:MET:HA	1:D:85:MET:HA	1.87	0.55
1:D:282:GLY:HA2	1:D:383:MET:HA	1.88	0.55
1:A:24:ASN:ND2	4:A:511:HOH:O	2.33	0.55
1:D:77:PRO:HB2	1:D:79:GLU:OE1	2.07	0.55
1:D:29:GLU:HA	1:D:73:LYS:HZ1	1.69	0.54
1:D:5:ILE:HG13	1:D:100:MET:HG2	1.89	0.54
1:B:29:GLU:HG2	1:B:73:LYS:NZ	2.22	0.54
1:D:8:ALA:HB3	1:D:257:LEU:HD12	1.90	0.54
1:C:318:ALA:HB1	3:C:401:COA:H22	1.89	0.54
1:A:282:GLY:HA2	1:A:383:MET:HA	1.91	0.52
1:C:282:GLY:HA2	1:C:383:MET:HA	1.92	0.52
1:C:144:ILE:HD13	1:C:148:LEU:HD12	1.91	0.51
1:B:282:GLY:HA2	1:B:383:MET:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:GLU:HG3	1:C:361:LEU:HB2	1.93	0.51
1:A:364:GLU:HA	1:A:367:ARG:HG2	1.93	0.50
1:C:196:LYS:NZ	4:C:512:HOH:O	2.43	0.50
1:C:175:GLN:NE2	4:C:514:HOH:O	2.44	0.50
1:D:38:VAL:HG23	1:D:39:LEU:HD13	1.94	0.50
1:D:186:ALA:HB1	1:D:219:ILE:HD11	1.94	0.49
1:C:364:GLU:OE1	1:C:367:ARG:NH1	2.46	0.48
1:B:339:VAL:HG11	1:B:368:ARG:NH2	2.28	0.48
1:C:58:LEU:HD12	1:C:119:MET:HG2	1.96	0.47
1:C:316:ASN:ND2	1:C:377:LEU:HD23	2.28	0.47
1:C:379:ILE:HD11	1:C:385:VAL:HG12	1.96	0.47
1:C:306:LYS:NZ	4:C:516:HOH:O	2.48	0.46
1:A:267:ARG:NH1	4:A:530:HOH:O	2.48	0.46
1:B:89:SCY:OCD	1:B:380:GLY:N	2.35	0.46
1:A:364:GLU:OE1	1:A:367:ARG:NH1	2.37	0.46
1:D:78:GLN:NE2	4:D:502:HOH:O	2.39	0.46
1:D:47:GLY:HA2	1:D:77:PRO:HG3	1.97	0.46
1:D:15:VAL:HG11	1:D:347:GLY:HA3	1.98	0.45
1:D:263:GLU:OE2	1:D:266:ARG:NH1	2.49	0.45
1:C:306:LYS:HA	1:C:306:LYS:HD2	1.80	0.45
1:A:233:PRO:HA	1:A:242:THR:HG22	1.97	0.45
1:C:141:ASP:OD1	1:D:129:ARG:NH2	2.38	0.45
1:C:348:HIS:ND1	1:C:353:SER:OG	2.51	0.44
1:D:88:LEU:HB2	1:D:379:ILE:HG23	2.00	0.44
1:A:297:ARG:NE	4:A:527:HOH:O	2.47	0.44
1:D:6:VAL:HA	1:D:274:ARG:HA	2.00	0.44
1:B:57:VAL:HG22	1:B:117:GLU:OE1	2.19	0.43
1:A:132:VAL:HG21	1:A:137:PHE:CD1	2.54	0.42
1:D:8:ALA:HB1	1:D:269:ILE:HG21	2.00	0.42
1:C:274:ARG:NE	4:C:518:HOH:O	2.52	0.42
1:D:119:MET:HE2	1:D:249:LEU:HB3	2.01	0.42
1:A:88:LEU:HB2	1:A:379:ILE:HG23	2.01	0.42
1:D:26:PRO:HD2	1:D:29:GLU:CD	2.40	0.42
1:D:247:SER:HB2	1:D:348:HIS:HB2	2.01	0.42
1:D:319:PHE:O	1:D:322:GLN:HG3	2.20	0.42
1:D:35:ILE:HD11	1:D:54:LEU:HD11	2.02	0.42
1:D:365:MET:HG2	1:D:370:ALA:HB3	2.02	0.41
1:B:78:GLN:HG2	4:B:508:HOH:O	2.21	0.41
1:B:317:GLU:CD	1:B:342:GLY:HA3	2.40	0.41
1:A:364:GLU:OE1	1:A:367:ARG:HD2	2.20	0.41
1:B:48:GLU:OE1	1:B:267:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:HG13	1:C:100:MET:HG2	2.03	0.41
1:B:170:LEU:HD13	1:B:324:CYS:HB2	2.03	0.41
1:C:129:ARG:HH21	1:D:122:ALA:HB3	1.86	0.41
1:B:164:VAL:HG11	1:B:322:GLN:HA	2.01	0.41
1:C:119:MET:CE	1:C:250:ASN:H	2.33	0.41
1:C:263:GLU:OE1	1:C:266:ARG:NH2	2.37	0.40
1:D:119:MET:N	1:D:251:ASP:OD1	2.54	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	387/399 (97%)	379 (98%)	8 (2%)	0	100	100
1	B	382/399 (96%)	376 (98%)	6 (2%)	0	100	100
1	C	386/399 (97%)	379 (98%)	7 (2%)	0	100	100
1	D	382/399 (96%)	375 (98%)	7 (2%)	0	100	100
All	All	1537/1596 (96%)	1509 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	266/285 (93%)	260 (98%)	6 (2%)	50	76
1	B	269/285 (94%)	263 (98%)	6 (2%)	52	77
1	C	265/285 (93%)	260 (98%)	5 (2%)	57	80
1	D	248/285 (87%)	243 (98%)	5 (2%)	55	79
All	All	1048/1140 (92%)	1026 (98%)	22 (2%)	53	78

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	205	LYS
1	A	288	MET
1	A	322	GLN
1	A	332	TRP
1	A	348	HIS
1	B	39	LEU
1	B	288	MET
1	B	322	GLN
1	B	332	TRP
1	B	348	HIS
1	B	350	ILE
1	C	207	ARG
1	C	288	MET
1	C	322	GLN
1	C	332	TRP
1	C	348	HIS
1	D	39	LEU
1	D	219	ILE
1	D	288	MET
1	D	332	TRP
1	D	339	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	SCY	C	89	1	7,8,9	0.89	0	3,9,11	0.80	0
1	SCY	B	89	1	7,8,9	0.90	0	3,9,11	0.81	0
1	SCY	A	89	1	7,8,9	0.94	0	3,9,11	0.80	0
1	SCY	D	89	1	7,8,9	0.93	0	3,9,11	0.83	0

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	SCY	C	89	1	-	2/5/7/9	-
1	SCY	B	89	1	-	2/5/7/9	-
1	SCY	A	89	1	-	2/5/7/9	-
1	SCY	D	89	1	-	2/5/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	89	SCY	OCD-CD-SG-CB
1	B	89	SCY	OCD-CD-SG-CB
1	C	89	SCY	OCD-CD-SG-CB
1	D	89	SCY	OCD-CD-SG-CB
1	A	89	SCY	CE-CD-SG-CB
1	B	89	SCY	CE-CD-SG-CB
1	C	89	SCY	CE-CD-SG-CB

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Mol	Chain	Res	Type	Atoms
1	D	89	SCY	CE-CD-SG-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	89	SCY	1	0
1	A	89	SCY	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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$
3	COA	C	401	-	41,50,50	1.24	5 (12%)	52,75,75	1.49	8 (15%)
3	COA	D	401	-	41,50,50	1.24	5 (12%)	52,75,75	1.49	9 (17%)
2	SO4	A	401	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	403	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	402	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	D	403	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	403	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	402	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	402	-	4,4,4	0.15	0	6,6,6	0.05	0
3	COA	A	404	-	41,50,50	1.23	5 (12%)	52,75,75	1.49	8 (15%)
2	SO4	B	401	-	4,4,4	0.14	0	6,6,6	0.05	0
3	COA	B	404	-	41,50,50	1.22	5 (12%)	52,75,75	1.47	7 (13%)

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
3	COA	C	401	-	-	12/44/64/64	0/3/3/3
3	COA	D	401	-	-	20/44/64/64	0/3/3/3
3	COA	A	404	-	-	9/44/64/64	0/3/3/3
3	COA	B	404	-	-	9/44/64/64	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	COA	O4B-C1B	3.99	1.46	1.41
3	D	401	COA	O4B-C1B	3.85	1.46	1.41
3	A	404	COA	O4B-C1B	3.82	1.46	1.41
3	B	404	COA	O4B-C1B	3.57	1.46	1.41
3	C	401	COA	C8A-N7A	-2.99	1.29	1.34
3	A	404	COA	C8A-N7A	-2.98	1.29	1.34
3	B	404	COA	C8A-N7A	-2.96	1.29	1.34
3	D	401	COA	C8A-N7A	-2.96	1.29	1.34
3	B	404	COA	C2B-C1B	2.54	1.57	1.53
3	D	401	COA	C2B-C1B	2.44	1.57	1.53
3	A	404	COA	C2B-C1B	2.39	1.57	1.53
3	C	401	COA	C2B-C1B	2.36	1.57	1.53
3	C	401	COA	P3B-O8A	2.23	1.63	1.54
3	D	401	COA	P3B-O9A	2.14	1.63	1.54
3	B	404	COA	P3B-O8A	2.14	1.63	1.54
3	D	401	COA	P3B-O8A	2.13	1.63	1.54
3	C	401	COA	P3B-O9A	2.12	1.63	1.54
3	B	404	COA	P3B-O9A	2.12	1.63	1.54
3	A	404	COA	P3B-O8A	2.11	1.63	1.54
3	A	404	COA	P3B-O9A	2.08	1.62	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	COA	P2A-O3A-P1A	-5.79	112.96	132.83
3	A	404	COA	P2A-O3A-P1A	-5.74	113.13	132.83
3	B	404	COA	P2A-O3A-P1A	-5.49	113.98	132.83
3	D	401	COA	P2A-O3A-P1A	-5.16	115.11	132.83
3	C	401	COA	N3A-C2A-N1A	-3.63	123.01	128.68
3	D	401	COA	N3A-C2A-N1A	-3.62	123.03	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	COA	N3A-C2A-N1A	-3.57	123.10	128.68
3	A	404	COA	N3A-C2A-N1A	-3.56	123.12	128.68
3	B	404	COA	O4B-C1B-C2B	-2.98	102.57	106.93
3	C	401	COA	N6A-C6A-N1A	2.93	124.65	118.57
3	D	401	COA	N6A-C6A-N1A	2.86	124.52	118.57
3	B	404	COA	N6A-C6A-N1A	2.73	124.24	118.57
3	A	404	COA	N6A-C6A-N1A	2.64	124.05	118.57
3	D	401	COA	O4B-C1B-C2B	-2.64	103.07	106.93
3	A	404	COA	O4B-C1B-C2B	-2.58	103.16	106.93
3	B	404	COA	CAP-C9P-N8P	2.38	121.32	116.58
3	C	401	COA	C5A-C6A-N6A	-2.37	116.75	120.35
3	C	401	COA	P1A-O5B-C5B	-2.32	108.10	121.68
3	B	404	COA	P2A-O6A-CCP	-2.31	108.22	121.56
3	A	404	COA	CAP-C9P-N8P	2.28	121.11	116.58
3	A	404	COA	C6P-C5P-N4P	2.23	120.17	116.42
3	C	401	COA	O4B-C1B-C2B	-2.23	103.67	106.93
3	C	401	COA	C2B-C3B-C4B	-2.22	99.29	103.22
3	D	401	COA	C5A-C6A-N6A	-2.19	117.03	120.35
3	A	404	COA	P1A-O5B-C5B	-2.16	109.03	121.68
3	C	401	COA	C6P-C5P-N4P	2.14	120.03	116.42
3	D	401	COA	C6P-C5P-N4P	2.13	120.00	116.42
3	A	404	COA	P2A-O6A-CCP	-2.10	109.48	121.56
3	D	401	COA	CAP-C9P-N8P	2.09	120.75	116.58
3	D	401	COA	P2A-O6A-CCP	-2.06	109.67	121.56
3	D	401	COA	P1A-O5B-C5B	-2.05	109.66	121.68
3	B	404	COA	P1A-O5B-C5B	-2.03	109.79	121.68

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	COA	CCP-O6A-P2A-O3A
3	A	404	COA	CCP-O6A-P2A-O5A
3	A	404	COA	S1P-C2P-C3P-N4P
3	B	404	COA	C5B-O5B-P1A-O3A
3	B	404	COA	CCP-O6A-P2A-O4A
3	B	404	COA	CCP-O6A-P2A-O5A
3	B	404	COA	CAP-CBP-CCP-O6A
3	C	401	COA	C4B-C3B-O3B-P3B
3	C	401	COA	CCP-O6A-P2A-O3A
3	C	401	COA	CCP-O6A-P2A-O4A
3	C	401	COA	CCP-O6A-P2A-O5A

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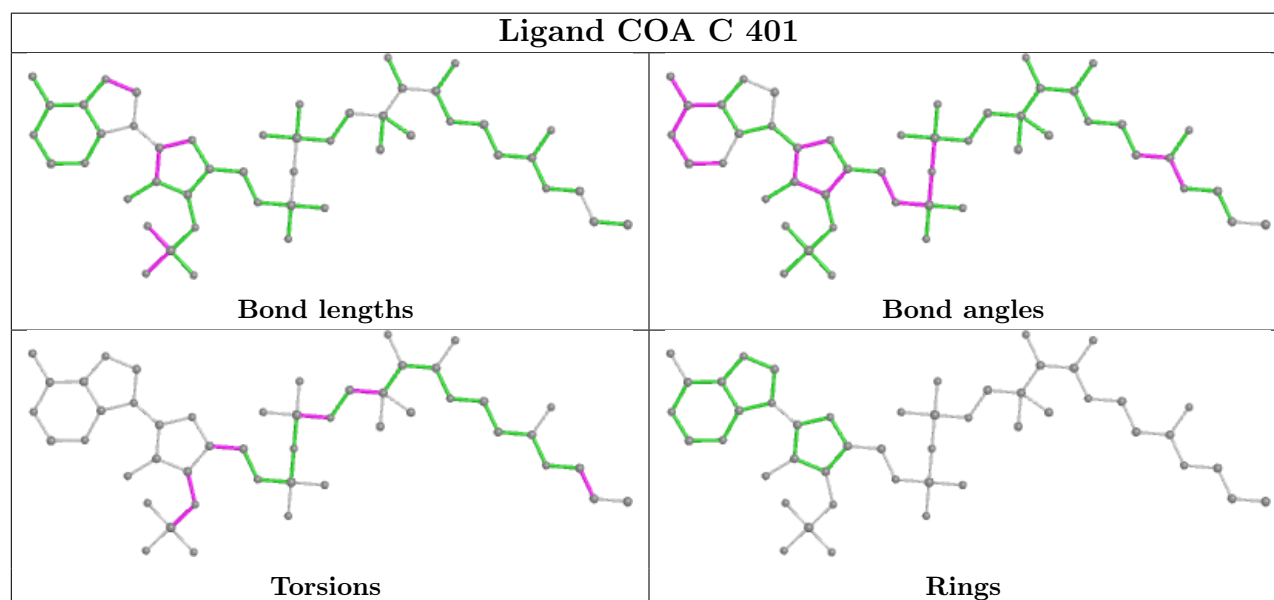
Mol	Chain	Res	Type	Atoms
3	C	401	COA	CDP-CBP-CCP-O6A
3	C	401	COA	CAP-CBP-CCP-O6A
3	C	401	COA	S1P-C2P-C3P-N4P
3	D	401	COA	CCP-O6A-P2A-O4A
3	D	401	COA	CCP-O6A-P2A-O5A
3	D	401	COA	CAP-CBP-CCP-O6A
3	D	401	COA	OAP-CAP-CBP-CCP
3	D	401	COA	C9P-CAP-CBP-CCP
3	D	401	COA	OAP-CAP-CBP-CDP
3	D	401	COA	C9P-CAP-CBP-CDP
3	D	401	COA	OAP-CAP-CBP-CEP
3	D	401	COA	C9P-CAP-CBP-CEP
3	D	401	COA	S1P-C2P-C3P-N4P
3	A	404	COA	O4B-C4B-C5B-O5B
3	D	401	COA	C4B-C3B-O3B-P3B
3	B	404	COA	CDP-CBP-CCP-O6A
3	B	404	COA	CEP-CBP-CCP-O6A
3	C	401	COA	CEP-CBP-CCP-O6A
3	D	401	COA	CDP-CBP-CCP-O6A
3	D	401	COA	CEP-CBP-CCP-O6A
3	D	401	COA	C2B-C3B-O3B-P3B
3	C	401	COA	O4B-C4B-C5B-O5B
3	D	401	COA	P2A-O3A-P1A-O1A
3	A	404	COA	C3B-C4B-C5B-O5B
3	D	401	COA	CCP-O6A-P2A-O3A
3	D	401	COA	O4B-C4B-C5B-O5B
3	A	404	COA	CCP-O6A-P2A-O4A
3	B	404	COA	C5B-O5B-P1A-O2A
3	A	404	COA	P2A-O3A-P1A-O2A
3	C	401	COA	C2B-C3B-O3B-P3B
3	C	401	COA	C3B-O3B-P3B-O7A
3	B	404	COA	CCP-O6A-P2A-O3A
3	C	401	COA	C3B-O3B-P3B-O8A
3	D	401	COA	C3B-O3B-P3B-O9A
3	A	404	COA	P2A-O3A-P1A-O1A
3	D	401	COA	CBP-CCP-O6A-P2A
3	A	404	COA	C5B-O5B-P1A-O1A
3	B	404	COA	C5B-O5B-P1A-O1A
3	D	401	COA	C5B-O5B-P1A-O1A

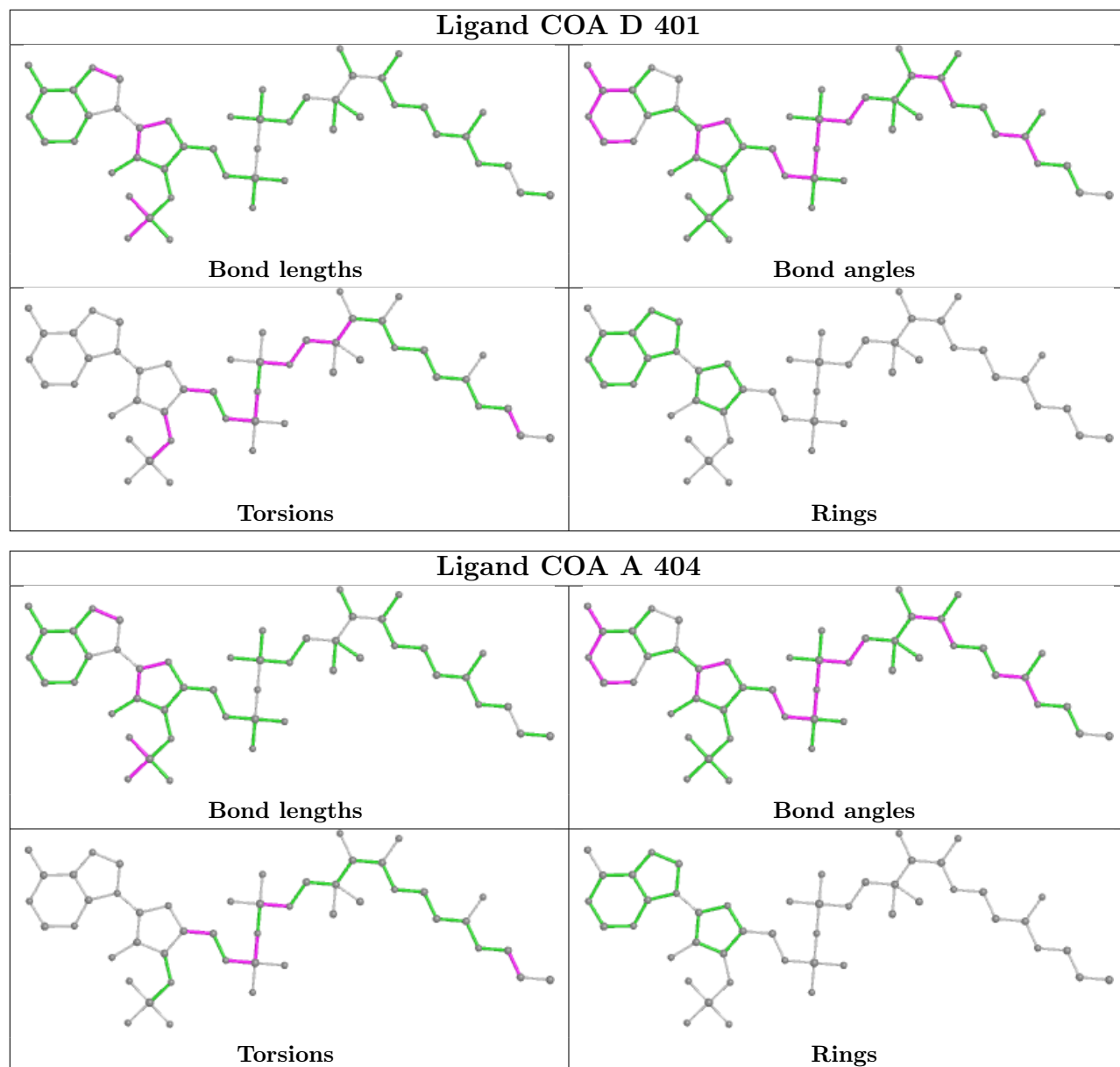
There are no ring outliers.

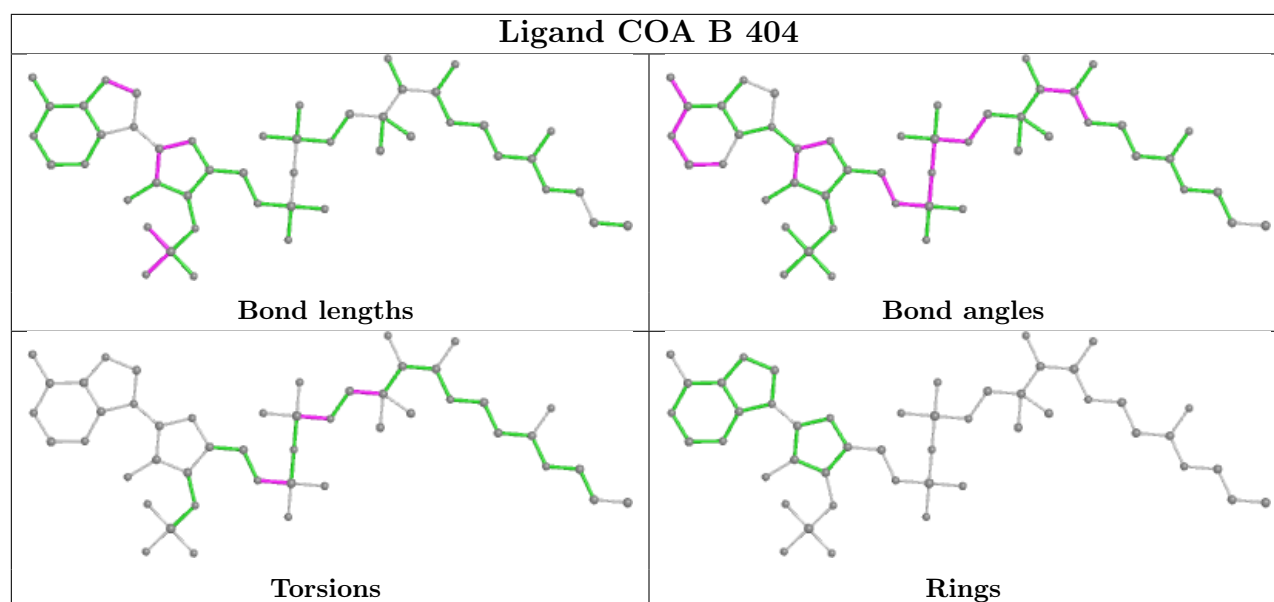
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	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 [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	389/399 (97%)	0.43	24 (6%) 20 21	18, 32, 56, 89	0
1	B	386/399 (96%)	0.38	19 (4%) 29 31	15, 33, 58, 78	0
1	C	388/399 (97%)	0.65	39 (10%) 7 6	29, 50, 80, 100	0
1	D	386/399 (96%)	1.33	96 (24%) 0 0	29, 57, 97, 127	0
All	All	1549/1596 (97%)	0.70	178 (11%) 4 4	15, 43, 80, 127	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	ASP	8.1
1	D	228	MET	7.3
1	D	229	ALA	6.8
1	D	170	LEU	6.6
1	D	227	SER	5.7
1	C	222	GLY	5.6
1	D	239	GLY	5.5
1	D	236	ASP	5.3
1	D	331	GLY	5.2
1	D	168	TRP	5.2
1	D	352	ALA	5.1
1	D	221	HIS	5.0
1	D	353	SER	5.0
1	B	132	VAL	4.8
1	C	209	GLY	4.8
1	D	234	ALA	4.8
1	D	237	LYS	4.8
1	B	210	ASP	4.8
1	A	206	GLY	4.7
1	A	236	ASP	4.7
1	D	164	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	236	ASP	4.4
1	D	3	PRO	4.4
1	B	237	LYS	4.4
1	A	210	ASP	4.4
1	D	244	GLY	4.3
1	D	238	GLU	4.3
1	A	207	ARG	4.2
1	D	153	TYR	4.2
1	D	332	TRP	4.2
1	D	175	GLN	4.2
1	C	221	HIS	4.2
1	D	210	ASP	4.2
1	C	207	ARG	4.2
1	D	334	PRO	4.1
1	D	224	THR	4.1
1	D	241	VAL	4.1
1	D	233	PRO	4.0
1	D	240	THR	4.0
1	D	165	ALA	4.0
1	D	205	LYS	4.0
1	D	350	ILE	3.9
1	D	319	PHE	3.8
1	B	220	ARG	3.8
1	B	236	ASP	3.8
1	C	205	LYS	3.8
1	D	286	LYS	3.7
1	B	226	ASP	3.7
1	D	231	LEU	3.7
1	B	221	HIS	3.7
1	D	180	VAL	3.6
1	C	210	ASP	3.6
1	C	206	GLY	3.6
1	D	171	SER	3.5
1	D	152	PHE	3.5
1	B	222	GLY	3.5
1	B	209	GLY	3.4
1	A	343	ALA	3.4
1	C	237	LYS	3.4
1	D	163	ASN	3.4
1	D	213	VAL	3.4
1	D	310	LEU	3.3
1	D	335	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	301	GLU	3.3
1	A	222	GLY	3.3
1	A	392	LEU	3.3
1	B	238	GLU	3.3
1	C	208	LYS	3.3
1	D	305	TRP	3.3
1	D	232	ARG	3.2
1	B	212	THR	3.2
1	C	231	LEU	3.2
1	A	237	LYS	3.1
1	C	228	MET	3.1
1	D	391	SER	3.1
1	A	239	GLY	3.0
1	D	333	ASP	3.0
1	D	57	VAL	3.0
1	C	227	SER	3.0
1	D	189	ALA	2.9
1	D	330	LEU	2.9
1	D	223	ALA	2.9
1	C	214	ASP	2.9
1	D	155	TYR	2.9
1	D	368	ARG	2.9
1	B	350	ILE	2.9
1	D	349	PRO	2.9
1	C	153	TYR	2.9
1	D	378	CYS	2.8
1	D	203	ILE	2.8
1	D	220	ARG	2.8
1	D	354	GLY	2.8
1	A	208	LYS	2.8
1	D	247	SER	2.8
1	D	156	HIS	2.8
1	C	169	GLN	2.8
1	D	270	GLN	2.7
1	A	226	ASP	2.7
1	A	205	LYS	2.7
1	D	90	GLY	2.7
1	D	55	GLY	2.7
1	D	366	LYS	2.7
1	A	350	ILE	2.7
1	C	203	ILE	2.7
1	A	90	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	166	LYS	2.7
1	C	353	SER	2.7
1	D	209	GLY	2.6
1	D	351	GLY	2.6
1	D	311	ASP	2.6
1	D	88	LEU	2.6
1	D	211	ILE	2.6
1	D	115	GLY	2.6
1	A	91	SER	2.5
1	B	205	LYS	2.5
1	C	355	ALA	2.5
1	D	235	PHE	2.5
1	D	91	SER	2.5
1	D	299	ALA	2.5
1	D	192	ASP	2.4
1	C	159	THR	2.4
1	C	212	THR	2.4
1	D	290	THR	2.4
1	D	206	GLY	2.4
1	C	140	ILE	2.4
1	C	351	GLY	2.4
1	C	154	GLY	2.4
1	A	352	ALA	2.4
1	D	312	LEU	2.4
1	A	132	VAL	2.4
1	C	156	HIS	2.4
1	A	3	PRO	2.3
1	C	155	TYR	2.3
1	D	79	GLU	2.3
1	A	211	ILE	2.3
1	A	209	GLY	2.3
1	B	392	LEU	2.3
1	D	114	GLY	2.3
1	D	342	GLY	2.3
1	C	74	ALA	2.3
1	D	343	ALA	2.3
1	C	183	TYR	2.3
1	D	263	GLU	2.3
1	A	349	PRO	2.2
1	D	191	LYS	2.2
1	C	213	VAL	2.2
1	C	40	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	238	GLU	2.2
1	B	223	ALA	2.2
1	C	350	ILE	2.2
1	D	307	ILE	2.2
1	D	194	ARG	2.2
1	C	115	GLY	2.2
1	D	93	LEU	2.2
1	A	351	GLY	2.2
1	B	92	GLY	2.2
1	D	162	GLU	2.2
1	D	336	ILE	2.2
1	D	339	VAL	2.2
1	A	203	ILE	2.2
1	A	212	THR	2.2
1	C	316	ASN	2.2
1	B	239	GLY	2.2
1	D	248	GLY	2.2
1	C	49	VAL	2.1
1	C	188	ALA	2.1
1	D	222	GLY	2.1
1	B	269	ILE	2.1
1	D	85	MET	2.1
1	D	73	LYS	2.1
1	C	339	VAL	2.1
1	D	188	ALA	2.1
1	D	148	LEU	2.1
1	D	132	VAL	2.1
1	D	174	GLU	2.1
1	C	4	SER	2.0
1	D	327	ASN	2.0
1	B	169	GLN	2.0

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	C	89	9/10	0.87	0.24	41,55,59,63	0
1	SCY	D	89	9/10	0.89	0.31	46,53,71,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SCY	A	89	9/10	0.90	0.25	23,44,57,63	0
1	SCY	B	89	9/10	0.91	0.19	24,32,62,64	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

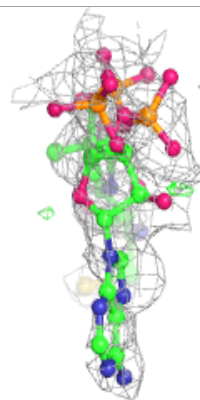
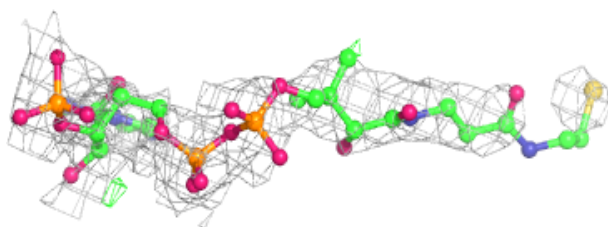
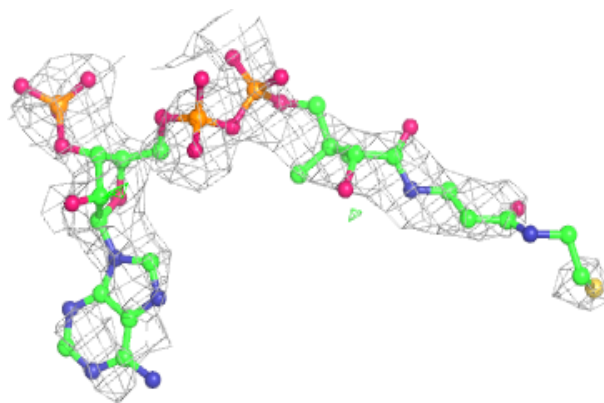
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	COA	D	401	48/48	0.63	0.33	71,105,115,116	48
2	SO4	C	402	5/5	0.76	0.26	89,90,92,93	0
3	COA	C	401	48/48	0.77	0.24	49,72,97,100	48
3	COA	A	404	48/48	0.82	0.22	34,47,66,70	48
3	COA	B	404	48/48	0.84	0.20	17,46,82,85	48
2	SO4	C	403	5/5	0.88	0.20	96,96,98,99	0
2	SO4	A	401	5/5	0.90	0.24	69,76,77,78	0
2	SO4	A	402	5/5	0.90	0.16	61,65,67,72	0
2	SO4	A	403	5/5	0.91	0.23	75,77,78,79	0
2	SO4	B	403	5/5	0.91	0.30	74,76,76,78	0
2	SO4	D	403	5/5	0.93	0.29	85,85,87,89	0
2	SO4	D	402	5/5	0.96	0.21	93,94,94,94	0
2	SO4	B	401	5/5	0.96	0.10	81,81,82,84	0
2	SO4	B	402	5/5	0.97	0.21	60,63,64,67	0

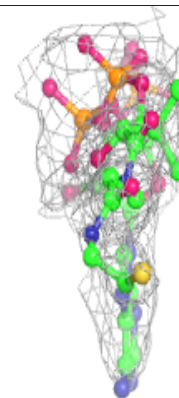
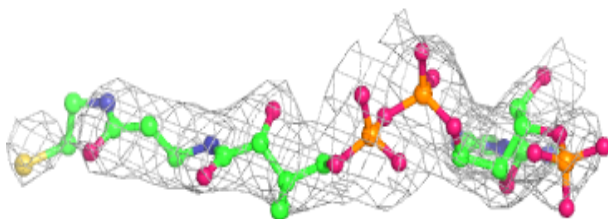
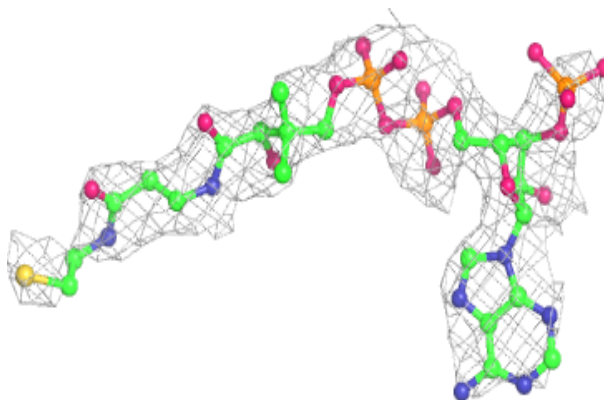
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

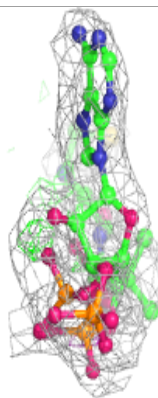
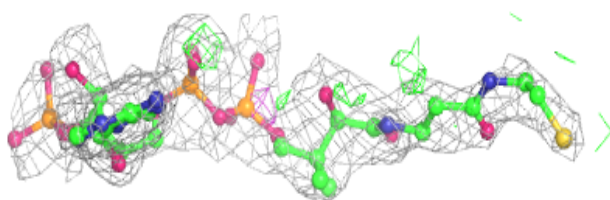
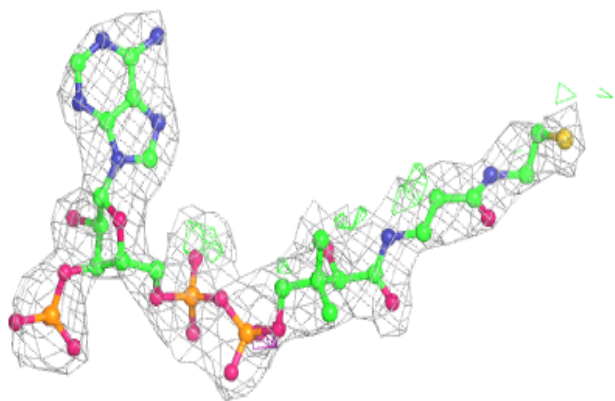
**Electron density around COA C 401:**

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

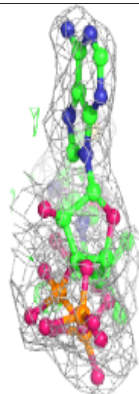
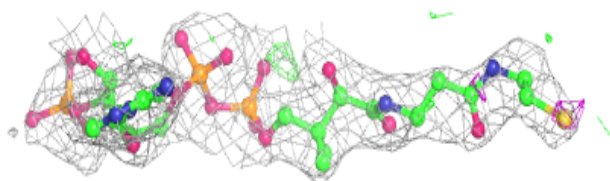
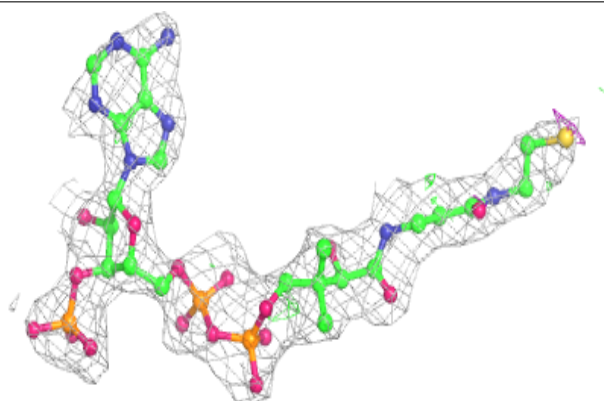


Electron density around COA A 404:

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

**Electron density around COA B 404:**

$2mF_o-DF_c$ (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.