



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2021 – 10:18 AM EDT

PDB ID : 7LCA
Title : Zoogloea ramigera biosynthetic thiolase Y218E/delH221 mutant
Authors : Marshall, A.C.; Bruning, J.B.
Deposited on : 2021-01-10
Resolution : 2.00 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

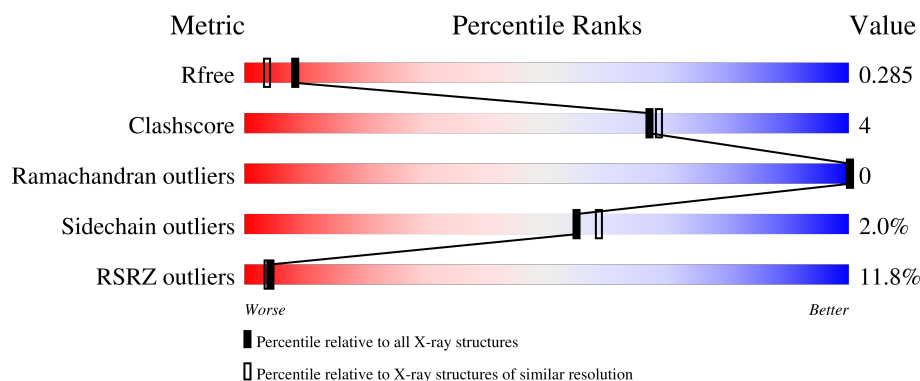
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	398	
1	B	398	
1	C	398	
1	D	398	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12023 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	389	Total	C	N	O	S	0	0	0
			2793	1734	499	539	21			
1	B	387	Total	C	N	O	S	0	1	0
			2782	1727	498	536	21			
1	C	387	Total	C	N	O	S	0	0	0
			2764	1721	490	532	21			
1	D	386	Total	C	N	O	S	0	0	0
			2712	1679	489	523	21			

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	218	GLU	TYR	engineered mutation	UNP P07097
A	?	-	HIS	deletion	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	218	GLU	TYR	engineered mutation	UNP P07097

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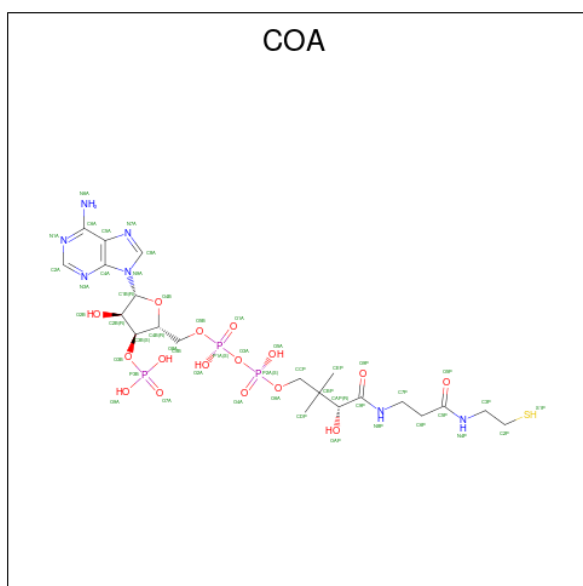
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	HIS	deletion	UNP P07097
C	-6	MET	-	initiating methionine	UNP P07097
C	-5	HIS	-	expression tag	UNP P07097
C	-4	HIS	-	expression tag	UNP P07097
C	-3	HIS	-	expression tag	UNP P07097
C	-2	HIS	-	expression tag	UNP P07097
C	-1	HIS	-	expression tag	UNP P07097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

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		

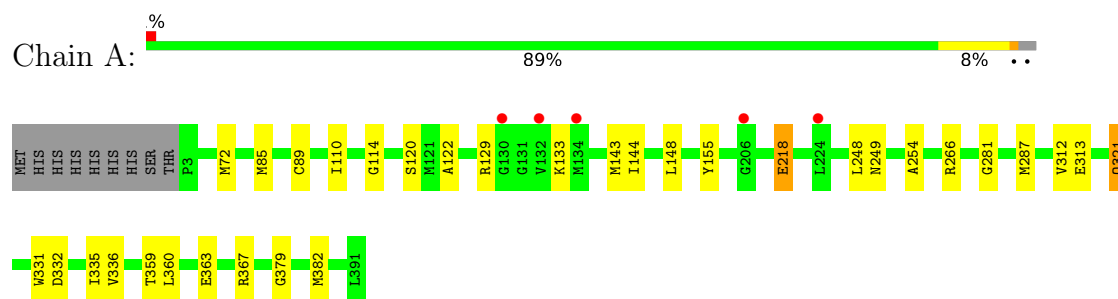
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	304	Total	O	0	0
			304	304		
5	B	302	Total	O	0	0
			302	302		
5	C	64	Total	O	0	0
			64	64		
5	D	73	Total	O	0	0
			73	73		

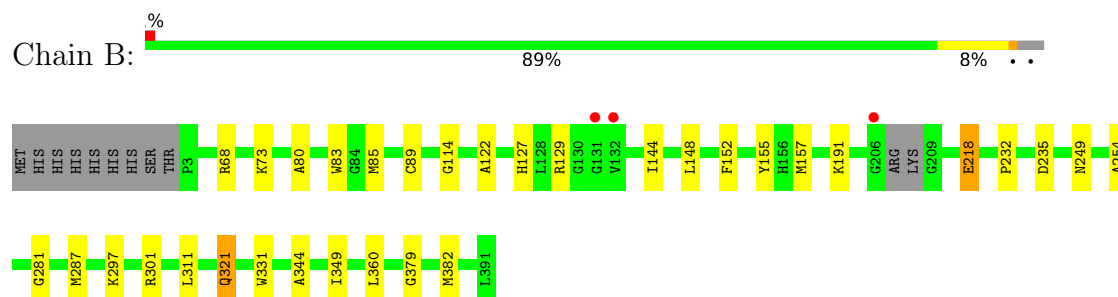
3 Residue-property plots [i](#)

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.

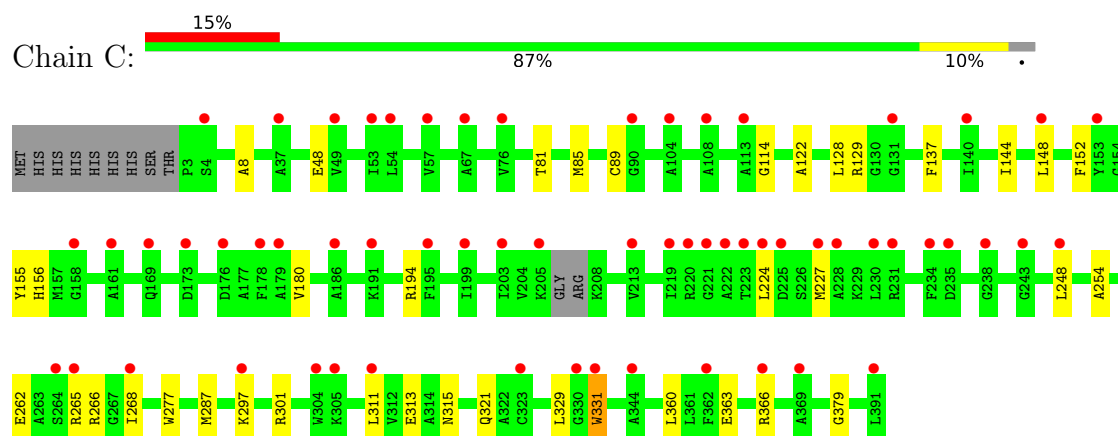
- Molecule 1: Acetyl-CoA acetyltransferase



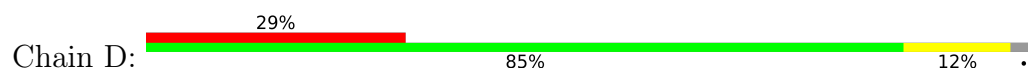
- Molecule 1: Acetyl-CoA acetyltransferase

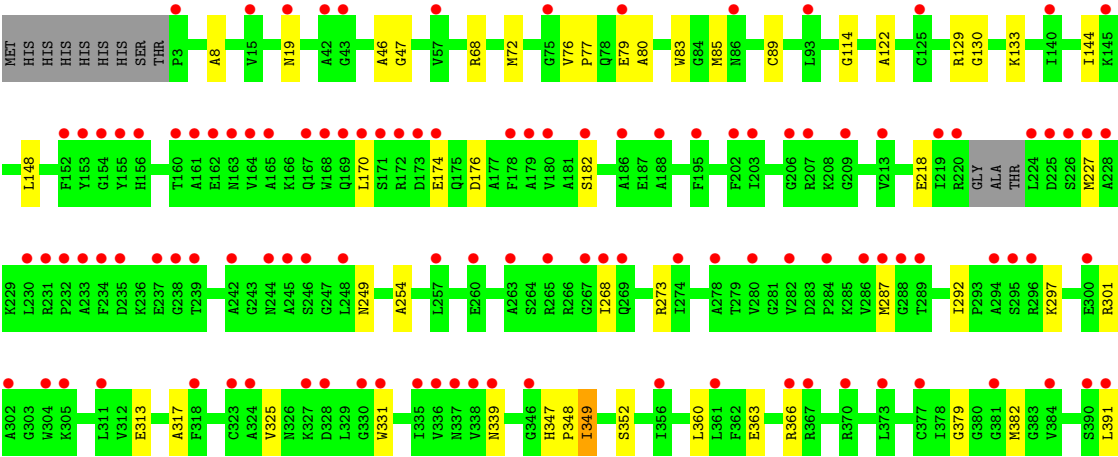


- Molecule 1: Acetyl-CoA acetyltransferase



- 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	84.45Å 79.34Å 149.14Å 90.00° 92.86° 90.00°	Depositor
Resolution (Å)	46.43 – 2.00 46.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.43-2.00) 86.2 (46.43-2.00)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.261 , 0.283 0.264 , 0.285	Depositor DCC
R_{free} test set	6575 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	1.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.138 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12023	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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, CL, 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	0/2823	0.45	0/3813
1	B	0.24	0/2814	0.44	0/3801
1	C	0.25	0/2793	0.44	0/3774
1	D	0.25	0/2736	0.45	0/3701
All	All	0.25	0/11166	0.44	0/15089

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	2793	0	2781	18	0
1	B	2782	0	2770	21	0
1	C	2764	0	2741	25	0
1	D	2712	0	2650	31	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	5	0	0	0	0
3	A	48	0	32	0	0
3	B	48	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	48	0	32	2	0
3	D	48	0	32	1	0
4	B	2	0	0	1	0
5	A	304	0	0	0	0
5	B	302	0	0	4	0
5	C	64	0	0	3	0
5	D	73	0	0	4	0
All	All	12023	0	11070	86	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:GLU:OE1	1:C:366:ARG:NH1	2.21	0.73
1:C:311:LEU:HD23	1:C:360:LEU:HD12	1.78	0.65
3:C:401:COA:H8A	3:C:401:COA:H52A	1.81	0.63
1:D:366:ARG:NH1	5:D:502:HOH:O	2.30	0.63
1:D:144:ILE:HD13	1:D:148:LEU:HD12	1.82	0.61
1:D:339:ASN:ND2	5:D:502:HOH:O	2.35	0.60
1:C:262:GLU:OE1	1:C:265:ARG:NH2	2.32	0.59
1:D:77:PRO:HB2	1:D:79:GLU:OE1	2.02	0.59
1:C:363:GLU:HA	1:C:366:ARG:HG2	1.83	0.59
1:A:129:ARG:HH21	1:B:122:ALA:HB3	1.67	0.58
1:C:315:ASN:ND2	5:C:504:HOH:O	2.35	0.57
1:C:122:ALA:HB3	1:D:129:ARG:HH21	1.70	0.57
1:B:89:SCY:OCD	1:B:379:GLY:N	2.31	0.57
1:D:130:GLY:O	1:D:133:LYS:NZ	2.38	0.56
1:D:297:LYS:HE3	1:D:301:ARG:NE	2.20	0.56
1:C:129:ARG:HH21	1:D:122:ALA:HB3	1.70	0.56
1:C:194:ARG:NH1	5:C:505:HOH:O	2.37	0.56
1:D:317:ALA:HB1	3:D:400:COA:H22	1.87	0.56
1:D:273:ARG:NH2	1:D:391:LEU:HD21	2.21	0.55
1:C:85:MET:HA	1:D:85:MET:HA	1.88	0.55
1:B:144:ILE:HD13	1:B:148:LEU:HD12	1.88	0.55
1:A:218:GLU:OE1	1:A:249:ASN:ND2	2.38	0.53
1:B:218:GLU:OE1	1:B:249:ASN:ND2	2.42	0.53
1:B:68:ARG:NH1	1:B:80:ALA:O	2.42	0.52
1:B:218:GLU:HB3	1:B:344:ALA:O	2.10	0.51
1:C:297:LYS:HE3	1:C:301:ARG:HE	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:SCY:OCD	1:A:379:GLY:N	2.37	0.51
1:A:85:MET:HA	1:B:85:MET:HA	1.92	0.51
1:D:47:GLY:HA2	1:D:77:PRO:HG3	1.92	0.51
1:C:144:ILE:HD13	1:C:148:LEU:HD12	1.94	0.50
1:D:182:SER:OG	5:D:501:HOH:O	2.20	0.49
1:A:144:ILE:HD13	1:A:148:LEU:HD12	1.94	0.49
1:C:152:PHE:CZ	1:D:72:MET:HG3	2.47	0.49
1:C:114:GLY:HA3	1:C:254:ALA:HA	1.94	0.49
1:A:313:GLU:HG3	1:A:360:LEU:HB2	1.95	0.48
1:B:148:LEU:O	1:B:157:MET:HG2	2.12	0.48
1:C:297:LYS:HE3	1:C:301:ARG:NE	2.28	0.48
1:A:312:VAL:HB	1:A:336:VAL:HG22	1.96	0.48
1:C:8:ALA:HB1	1:C:268:ILE:HG21	1.96	0.48
1:A:114:GLY:HA3	1:A:254:ALA:HA	1.96	0.48
1:A:72:MET:HG3	1:B:152:PHE:CZ	2.49	0.47
1:D:8:ALA:HB1	1:D:268:ILE:HG21	1.96	0.47
1:C:156:HIS:HE1	3:C:401:COA:H71	1.80	0.47
1:B:73:LYS:NZ	5:B:533:HOH:O	2.48	0.46
1:D:363:GLU:OE1	5:D:502:HOH:O	2.20	0.46
1:A:122:ALA:HB3	1:B:129:ARG:HH21	1.80	0.46
1:B:297:LYS:HE3	1:B:301:ARG:HE	1.81	0.46
1:A:133:LYS:NZ	1:D:19:ASN:HD22	2.14	0.46
1:C:277:TRP:O	1:C:301:ARG:NH1	2.48	0.45
1:D:46:ALA:HB1	1:D:76:VAL:HA	1.98	0.45
1:D:249:ASN:ND2	1:D:347:HIS:H	2.14	0.45
1:B:321:GLN:HE21	1:B:321:GLN:HB2	1.62	0.45
1:C:89:SCY:OCD	1:C:379:GLY:N	2.36	0.44
1:D:348:PRO:O	1:D:352:SER:N	2.50	0.44
1:A:120:SER:O	1:B:127:HIS:NE2	2.48	0.44
1:A:363:GLU:O	1:A:367:ARG:HG2	2.18	0.44
1:D:292:ILE:HG13	1:D:325:VAL:HG22	1.99	0.43
1:B:232:PRO:HB2	1:B:235:ASP:O	2.18	0.43
1:D:349:ILE:H	1:D:349:ILE:HG12	1.44	0.43
1:C:48:GLU:OE1	1:C:266:ARG:NH1	2.52	0.43
1:D:170:LEU:HD22	1:D:174:GLU:OE2	2.18	0.43
1:A:321:GLN:HE21	1:A:321:GLN:HB2	1.65	0.43
1:B:83:TRP:HZ3	1:B:85:MET:HB3	1.84	0.43
1:C:81:THR:HG22	1:D:382:MET:HG2	2.00	0.43
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.54	0.43
1:C:313:GLU:HG3	1:C:360:LEU:HB2	2.00	0.43
1:C:329:LEU:HD22	1:C:331:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLU:N	5:B:503:HOH:O	2.51	0.43
1:D:68:ARG:NH1	1:D:80:ALA:O	2.46	0.43
1:D:114:GLY:HA3	1:D:254:ALA:HA	2.01	0.42
1:D:176:ASP:HA	1:D:227:MET:HE3	2.01	0.42
1:B:114:GLY:HA3	1:B:254:ALA:HA	2.01	0.42
1:D:218:GLU:HG3	1:D:249:ASN:OD1	2.20	0.42
1:C:180:VAL:HG21	1:C:224:LEU:HD23	2.01	0.42
4:B:406:CL:CL	5:B:553:HOH:O	2.59	0.42
1:A:281:GLY:HA2	1:A:382:MET:HA	2.02	0.41
1:B:191:LYS:NZ	5:B:538:HOH:O	2.51	0.41
1:A:110:ILE:HD11	1:A:266:ARG:NH2	2.34	0.41
1:D:313:GLU:HG3	1:D:360:LEU:HB2	2.01	0.41
1:C:265:ARG:NH2	5:C:512:HOH:O	2.47	0.41
1:B:311:LEU:HD23	1:B:360:LEU:HD12	2.03	0.41
1:A:143:MET:SD	1:A:248:LEU:HD13	2.61	0.41
1:D:89:SCY:OCD	1:D:379:GLY:N	2.42	0.41
1:B:281:GLY:HA2	1:B:382:MET:HA	2.03	0.40
1:D:83:TRP:HZ3	1:D:85:MET:HB3	1.85	0.40
1:A:332:ASP:O	1:A:335:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	386/398 (97%)	376 (97%)	10 (3%)	0	100	100
1	B	383/398 (96%)	374 (98%)	9 (2%)	0	100	100
1	C	382/398 (96%)	374 (98%)	8 (2%)	0	100	100
1	D	381/398 (96%)	373 (98%)	8 (2%)	0	100	100
All	All	1532/1592 (96%)	1497 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	271/284 (95%)	265 (98%)	6 (2%)	52	55
1	B	270/284 (95%)	264 (98%)	6 (2%)	52	55
1	C	265/284 (93%)	259 (98%)	6 (2%)	50	53
1	D	252/284 (89%)	249 (99%)	3 (1%)	71	76
All	All	1058/1136 (93%)	1037 (98%)	21 (2%)	55	58

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	TYR
1	A	218	GLU
1	A	287	MET
1	A	321	GLN
1	A	331	TRP
1	A	359	THR
1	B	155	TYR
1	B	218	GLU
1	B	287	MET
1	B	321	GLN
1	B	331	TRP
1	B	349	ILE
1	C	155	TYR
1	C	227	MET
1	C	248	LEU
1	C	287	MET
1	C	321	GLN
1	C	331	TRP
1	D	287	MET
1	D	331	TRP
1	D	349	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	C	321	GLN
1	D	19	ASN

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	A	89	1	7,8,9	0.93	0	3,9,11	0.81	0
1	SCY	C	89	1	7,8,9	0.91	0	3,9,11	0.82	0
1	SCY	D	89	1	7,8,9	0.92	0	3,9,11	0.81	0
1	SCY	B	89	1	7,8,9	0.90	0	3,9,11	0.73	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	A	89	1	-	2/5/7/9	-
1	SCY	C	89	1	-	2/5/7/9	-
1	SCY	D	89	1	-	2/5/7/9	-
1	SCY	B	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
1	D	89	SCY	CE-CD-SG-CB

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z > 2$
2	SO4	A	401	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	401	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	COA	D	400	-	41,50,50	1.21	3 (7%)	52,75,75	1.51	9 (17%)
2	SO4	B	404	-	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	0.05	0
3	COA	A	403	-	41,50,50	1.19	2 (4%)	52,75,75	1.49	7 (13%)
2	SO4	C	402	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	402	-	4,4,4	0.15	0	6,6,6	0.05	0
3	COA	C	401	-	41,50,50	1.22	2 (4%)	52,75,75	1.44	8 (15%)
2	SO4	A	404	-	4,4,4	0.14	0	6,6,6	0.05	0
3	COA	B	403	-	41,50,50	1.20	2 (4%)	52,75,75	1.52	8 (15%)

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	D	400	-	-	14/44/64/64	0/3/3/3
3	COA	C	401	-	-	9/44/64/64	0/3/3/3
3	COA	A	403	-	-	8/44/64/64	0/3/3/3
3	COA	B	403	-	-	7/44/64/64	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	COA	O4B-C1B	4.25	1.47	1.41
3	B	403	COA	O4B-C1B	3.86	1.46	1.41
3	D	400	COA	O4B-C1B	3.81	1.46	1.41
3	A	403	COA	O4B-C1B	3.81	1.46	1.41
3	C	401	COA	C8A-N7A	-3.24	1.28	1.34
3	D	400	COA	C8A-N7A	-3.20	1.29	1.34
3	A	403	COA	C8A-N7A	-3.15	1.29	1.34
3	B	403	COA	C8A-N7A	-3.11	1.29	1.34
3	D	400	COA	P3B-O8A	2.01	1.62	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	COA	P2A-O3A-P1A	-5.46	114.09	132.83
3	C	401	COA	P2A-O3A-P1A	-5.45	114.12	132.83
3	D	400	COA	P2A-O3A-P1A	-5.20	114.97	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	COA	P2A-O3A-P1A	-4.97	115.77	132.83
3	B	403	COA	N3A-C2A-N1A	-3.34	123.46	128.68
3	C	401	COA	N3A-C2A-N1A	-3.30	123.52	128.68
3	D	400	COA	N3A-C2A-N1A	-3.29	123.53	128.68
3	A	403	COA	N3A-C2A-N1A	-3.29	123.54	128.68
3	A	403	COA	O4B-C1B-C2B	-3.04	102.49	106.93
3	D	400	COA	N6A-C6A-N1A	3.03	124.86	118.57
3	C	401	COA	N6A-C6A-N1A	3.02	124.84	118.57
3	B	403	COA	C7P-C6P-C5P	-2.94	107.46	112.36
3	B	403	COA	O4B-C1B-C2B	-2.93	102.64	106.93
3	A	403	COA	N6A-C6A-N1A	2.89	124.57	118.57
3	B	403	COA	N6A-C6A-N1A	2.85	124.48	118.57
3	D	400	COA	O4B-C1B-C2B	-2.50	103.27	106.93
3	D	400	COA	C5A-C6A-N6A	-2.48	116.59	120.35
3	C	401	COA	C5A-C6A-N6A	-2.47	116.60	120.35
3	D	400	COA	C1B-N9A-C4A	2.35	130.77	126.64
3	D	400	COA	CAP-C9P-N8P	2.32	121.20	116.58
3	A	403	COA	C5A-C6A-N6A	-2.24	116.94	120.35
3	A	403	COA	P1A-O5B-C5B	-2.17	108.95	121.68
3	C	401	COA	P1A-O5B-C5B	-2.17	108.95	121.68
3	C	401	COA	CAP-C9P-N8P	2.13	120.82	116.58
3	B	403	COA	O9P-C9P-N8P	-2.10	118.48	122.99
3	D	400	COA	O9P-C9P-N8P	-2.10	118.48	122.99
3	B	403	COA	C5A-C6A-N6A	-2.09	117.17	120.35
3	C	401	COA	C1B-N9A-C4A	2.09	130.31	126.64
3	A	403	COA	P2A-O6A-CCP	-2.08	109.54	121.56
3	C	401	COA	O9P-C9P-N8P	-2.03	118.63	122.99
3	B	403	COA	CAP-C9P-N8P	2.00	120.57	116.58
3	D	400	COA	C2B-C3B-C4B	-2.00	99.68	103.22

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	COA	CDP-CBP-CCP-O6A
3	A	403	COA	CAP-CBP-CCP-O6A
3	B	403	COA	CCP-O6A-P2A-O3A
3	B	403	COA	CCP-O6A-P2A-O5A
3	C	401	COA	CCP-O6A-P2A-O3A
3	C	401	COA	CCP-O6A-P2A-O4A
3	C	401	COA	CCP-O6A-P2A-O5A
3	D	400	COA	C5B-O5B-P1A-O1A

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Mol	Chain	Res	Type	Atoms
3	D	400	COA	C5B-O5B-P1A-O2A
3	D	400	COA	CAP-CBP-CCP-O6A
3	A	403	COA	C3B-C4B-C5B-O5B
3	A	403	COA	O4B-C4B-C5B-O5B
3	C	401	COA	O4B-C4B-C5B-O5B
3	D	400	COA	C4B-C3B-O3B-P3B
3	A	403	COA	CEP-CBP-CCP-O6A
3	D	400	COA	CDP-CBP-CCP-O6A
3	D	400	COA	CEP-CBP-CCP-O6A
3	C	401	COA	CDP-CBP-CCP-O6A
3	C	401	COA	CEP-CBP-CCP-O6A
3	A	403	COA	P1A-O3A-P2A-O4A
3	B	403	COA	C3B-O3B-P3B-O7A
3	A	403	COA	CCP-O6A-P2A-O3A
3	D	400	COA	C3B-O3B-P3B-O8A
3	C	401	COA	P2A-O3A-P1A-O1A
3	D	400	COA	C4B-C5B-O5B-P1A
3	B	403	COA	CCP-O6A-P2A-O4A
3	D	400	COA	C3B-C4B-C5B-O5B
3	C	401	COA	CAP-CBP-CCP-O6A
3	B	403	COA	P1A-O3A-P2A-O5A
3	D	400	COA	P1A-O3A-P2A-O5A
3	D	400	COA	O4B-C4B-C5B-O5B
3	D	400	COA	S1P-C2P-C3P-N4P
3	B	403	COA	C3B-O3B-P3B-O9A
3	D	400	COA	C5B-O5B-P1A-O3A
3	B	403	COA	P1A-O3A-P2A-O4A
3	C	401	COA	P2A-O3A-P1A-O2A
3	D	400	COA	P1A-O3A-P2A-O4A
3	A	403	COA	CCP-O6A-P2A-O4A

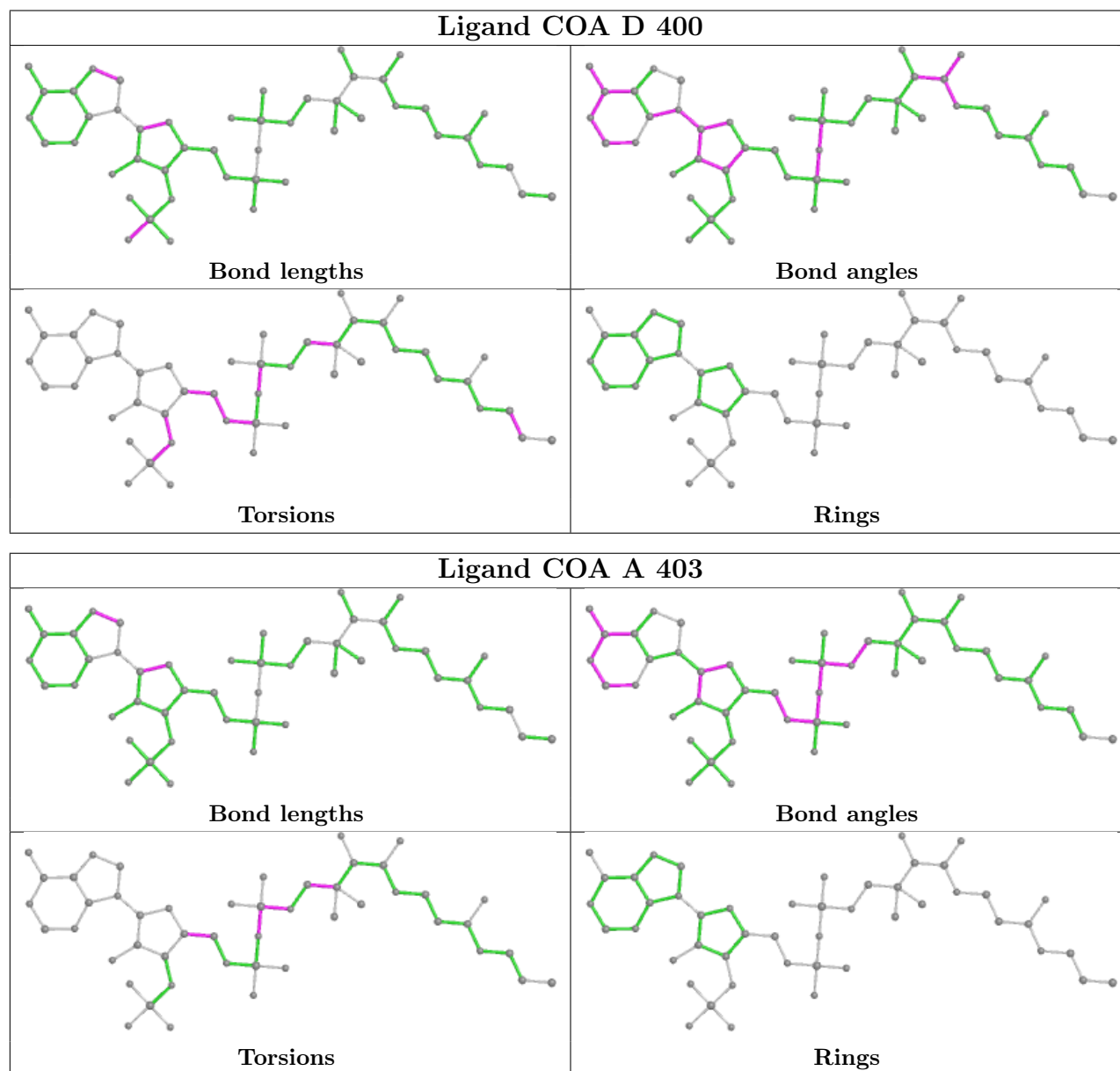
There are no ring outliers.

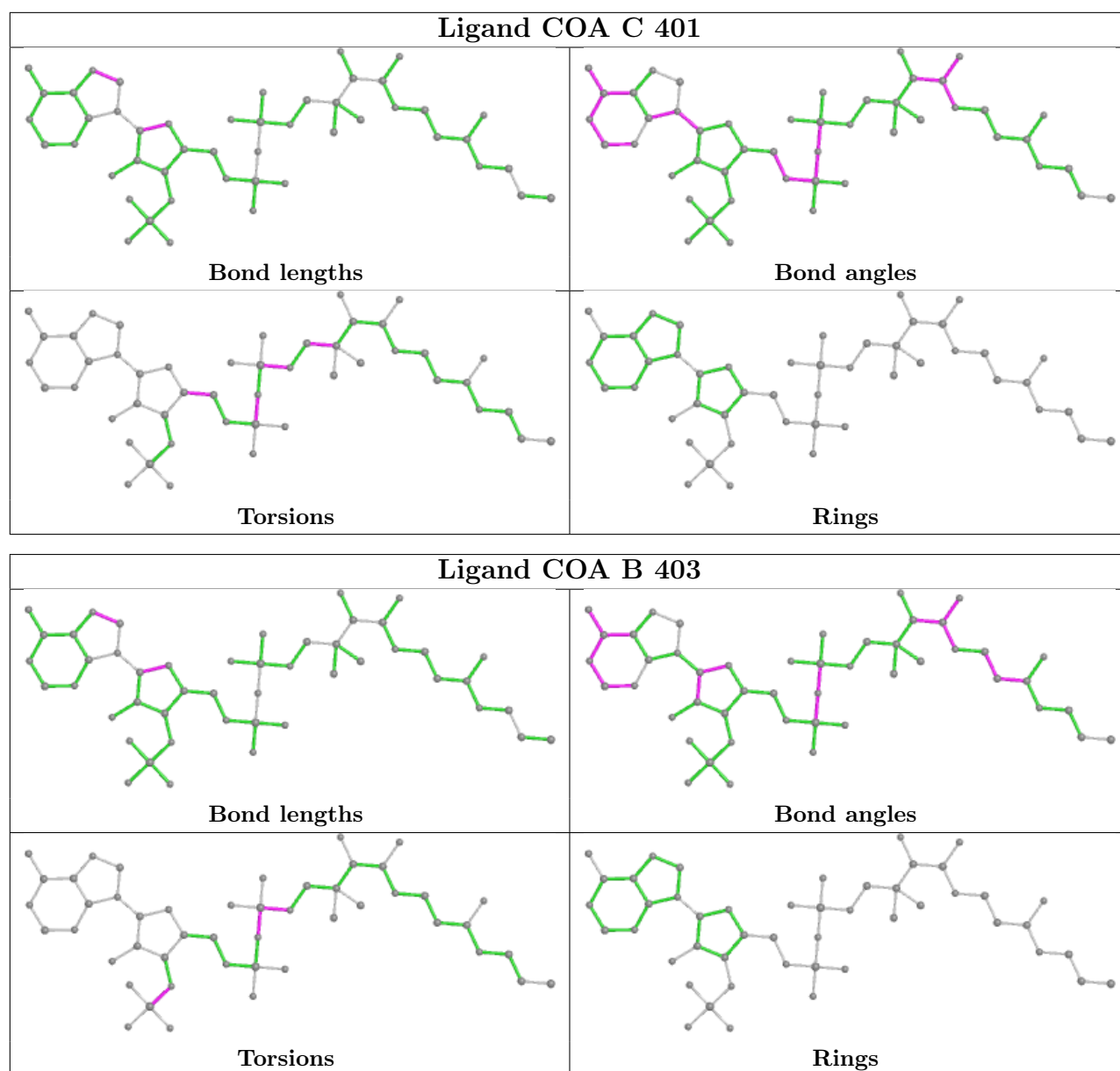
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	400	COA	1	0
3	C	401	COA	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	388/398 (97%)	0.03	5 (1%) 77 76	5, 15, 34, 44	0
1	B	386/398 (96%)	0.09	3 (0%) 86 85	7, 16, 36, 44	0
1	C	386/398 (96%)	1.07	61 (15%) 2 1	34, 45, 62, 74	0
1	D	385/398 (96%)	1.52	114 (29%) 0 0	37, 51, 81, 110	0
All	All	1545/1592 (97%)	0.68	183 (11%) 4 4	5, 37, 68, 110	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	225	ASP	9.7
1	D	239	THR	9.0
1	C	161	ALA	8.0
1	D	237	GLU	7.3
1	C	235	ASP	7.2
1	C	221	GLY	6.9
1	D	330	GLY	6.8
1	D	179	ALA	6.7
1	D	228	ALA	6.7
1	D	233	ALA	6.4
1	D	230	LEU	6.2
1	D	152	PHE	6.2
1	C	228	ALA	5.9
1	D	238	GLY	5.8
1	D	331	TRP	5.6
1	D	234	PHE	5.4
1	D	153	TYR	5.4
1	D	366	ARG	5.4
1	D	219	ILE	5.1
1	D	173	ASP	5.1
1	D	391	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	132	VAL	4.9
1	D	156	HIS	4.9
1	C	223	THR	4.7
1	C	213	VAL	4.7
1	D	178	PHE	4.6
1	D	171	SER	4.6
1	D	245	ALA	4.6
1	C	49	VAL	4.5
1	C	222	ALA	4.5
1	C	108	ALA	4.4
1	C	369	ALA	4.3
1	D	227	MET	4.3
1	D	206	GLY	4.2
1	D	381	GLY	4.1
1	D	161	ALA	4.1
1	C	53	ILE	4.0
1	D	287	MET	4.0
1	D	336	VAL	3.9
1	C	176	ASP	3.8
1	A	132	VAL	3.8
1	D	328	ASP	3.7
1	D	154	GLY	3.7
1	D	318	PHE	3.7
1	D	186	ALA	3.7
1	D	235	ASP	3.6
1	D	231	ARG	3.6
1	D	170	LEU	3.6
1	C	220	ARG	3.5
1	C	234	PHE	3.5
1	D	268	ILE	3.5
1	D	280	VAL	3.5
1	D	311	LEU	3.5
1	D	42	ALA	3.5
1	D	390	SER	3.5
1	B	131	GLY	3.5
1	D	267	GLY	3.4
1	D	75	GLY	3.4
1	D	226	SER	3.4
1	D	164	VAL	3.4
1	D	188	ALA	3.4
1	D	274	ILE	3.4
1	C	391	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	338	VAL	3.4
1	A	206	GLY	3.4
1	C	227	MET	3.3
1	D	169	GLN	3.3
1	C	323	CYS	3.3
1	C	230	LEU	3.3
1	C	219	ILE	3.2
1	D	384	VAL	3.2
1	C	57	VAL	3.2
1	C	67	ALA	3.2
1	C	113	ALA	3.2
1	D	305	LYS	3.1
1	D	224	LEU	3.1
1	B	206	GLY	3.1
1	D	324	ALA	3.1
1	D	246	SER	3.1
1	D	232	PRO	3.1
1	D	265	ARG	3.1
1	D	180	VAL	3.0
1	C	231	ARG	3.0
1	C	148	LEU	3.0
1	D	163	ASN	2.9
1	D	79	GLU	2.9
1	D	244	ASN	2.9
1	C	186	ALA	2.8
1	C	264	SER	2.8
1	C	243	GLY	2.8
1	C	311	LEU	2.8
1	D	167	GLN	2.8
1	D	165	ALA	2.7
1	D	242	ALA	2.7
1	D	335	ILE	2.7
1	D	304	TRP	2.7
1	C	54	LEU	2.7
1	D	19	ASN	2.7
1	C	104	ALA	2.7
1	C	362	PHE	2.7
1	D	288	GLY	2.7
1	C	330	GLY	2.7
1	D	160	THR	2.7
1	D	339	ASN	2.7
1	C	224	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	248	LEU	2.6
1	D	15	VAL	2.6
1	C	225	ASP	2.6
1	C	265	ARG	2.6
1	D	220	ARG	2.6
1	C	268	ILE	2.6
1	C	37	ALA	2.6
1	D	86	ASN	2.6
1	D	203	ILE	2.6
1	C	90	GLY	2.6
1	D	327	LYS	2.6
1	C	76	VAL	2.6
1	D	286	VAL	2.6
1	D	294	ALA	2.6
1	C	304	TRP	2.6
1	D	168	TRP	2.6
1	D	172	ARG	2.5
1	D	296	ARG	2.5
1	D	57	VAL	2.5
1	D	263	ALA	2.5
1	C	344	ALA	2.5
1	D	209	GLY	2.5
1	A	134	MET	2.5
1	C	179	ALA	2.5
1	D	213	VAL	2.5
1	C	158	GLY	2.5
1	D	282	VAL	2.5
1	A	130	GLY	2.4
1	C	178	PHE	2.4
1	C	195	PHE	2.4
1	C	153	TYR	2.4
1	D	370	ARG	2.4
1	D	295	SER	2.4
1	D	140	ILE	2.3
1	C	169	GLN	2.3
1	C	173	ASP	2.3
1	A	224	LEU	2.3
1	D	289	THR	2.3
1	D	195	PHE	2.3
1	D	377	CYS	2.3
1	D	269	GLN	2.3
1	D	300	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	191	LYS	2.2
1	C	203	ILE	2.2
1	D	174	GLU	2.2
1	C	199	ILE	2.2
1	D	337	ASN	2.2
1	D	356	ILE	2.2
1	D	93	LEU	2.2
1	C	4	SER	2.2
1	D	257	LEU	2.1
1	D	323	CYS	2.1
1	D	207	ARG	2.1
1	D	302	ALA	2.1
1	D	346	GLY	2.1
1	C	140	ILE	2.1
1	C	305	LYS	2.1
1	C	131	GLY	2.1
1	C	238	GLY	2.1
1	C	366	ARG	2.1
1	D	361	LEU	2.1
1	D	373	LEU	2.1
1	D	260	GLU	2.1
1	D	278	ALA	2.1
1	C	297	LYS	2.1
1	C	205	LYS	2.1
1	D	284	PRO	2.1
1	D	125	CYS	2.1
1	D	202	PHE	2.1
1	D	155	TYR	2.1
1	C	331	TRP	2.1
1	D	43	GLY	2.1
1	D	162	GLU	2.0
1	D	248	LEU	2.0
1	D	367	ARG	2.0
1	D	182	SER	2.0
1	D	3	PRO	2.0
1	D	145	LYS	2.0

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

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
1	SCY	C	89	9/10	0.78	0.19	40,42,45,45	0
1	SCY	A	89	9/10	0.86	0.17	13,13,30,31	0
1	SCY	B	89	9/10	0.92	0.16	14,14,24,25	0
1	SCY	D	89	9/10	0.93	0.10	45,47,48,50	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

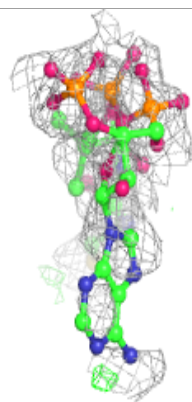
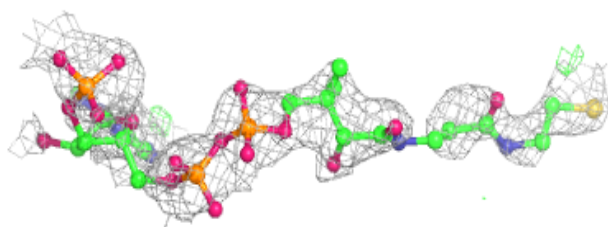
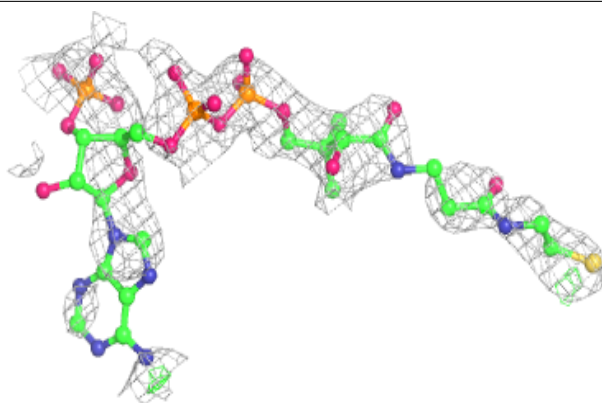
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	400	48/48	0.58	0.28	77,93,101,102	0
3	COA	C	401	48/48	0.77	0.21	40,74,83,83	48
3	COA	B	403	48/48	0.81	0.17	17,50,73,75	0
3	COA	A	403	48/48	0.86	0.15	14,48,61,63	48
2	SO4	B	401	5/5	0.90	0.18	93,93,93,93	0
2	SO4	A	401	5/5	0.91	0.17	69,70,72,72	0
2	SO4	A	404	5/5	0.92	0.14	63,65,67,68	0
2	SO4	A	402	5/5	0.93	0.17	14,25,29,30	0
2	SO4	C	402	5/5	0.93	0.10	79,79,79,80	0
2	SO4	B	404	5/5	0.95	0.16	71,72,72,72	0
2	SO4	B	402	5/5	0.97	0.11	39,40,42,42	0
4	CL	B	405	1/1	0.98	0.09	28,28,28,28	0
4	CL	B	406	1/1	0.99	0.09	26,26,26,26	0

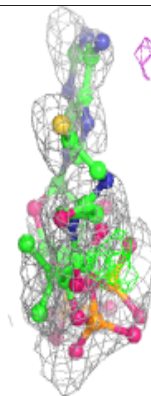
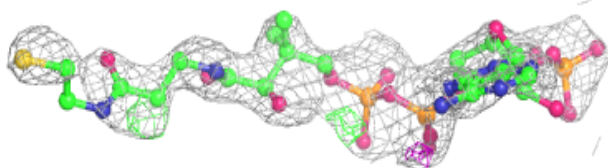
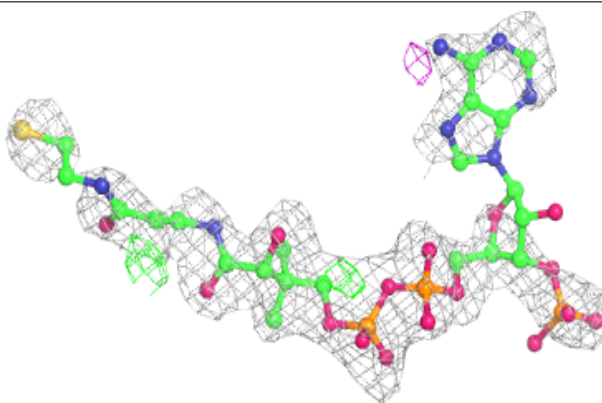
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA D 400:

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

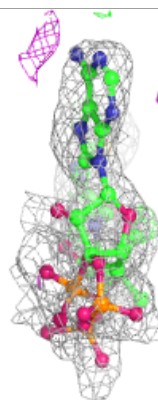
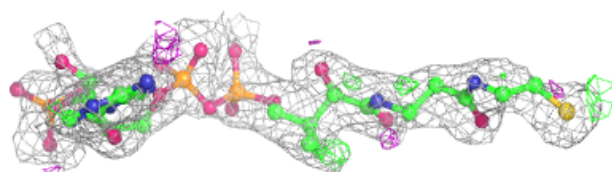
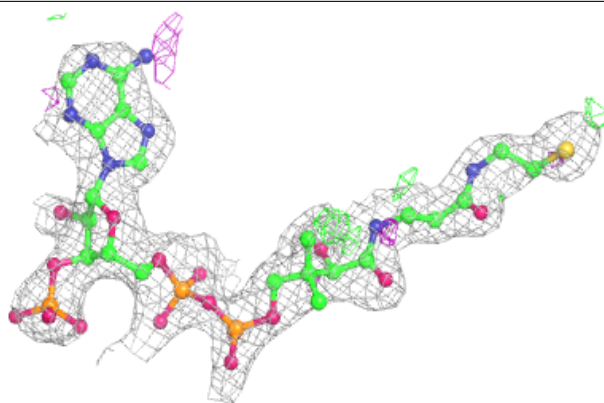
**Electron density around COA C 401:**

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

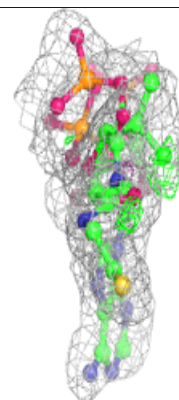
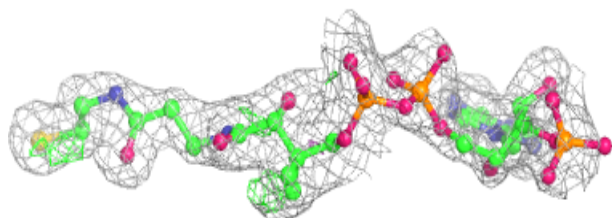
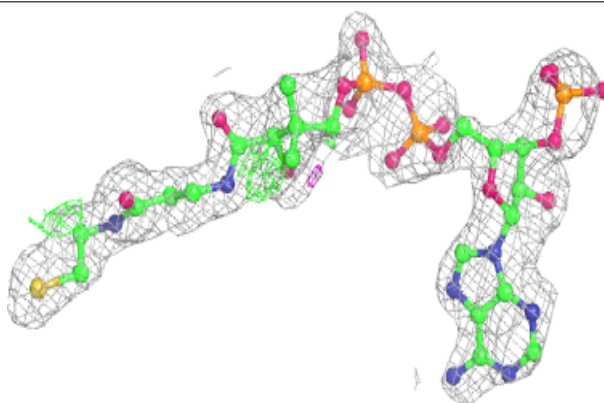


Electron density around COA B 403:

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

**Electron density around COA A 403:**

$2mF_o-DF_c$ (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.