



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2021 – 10:09 AM EDT

PDB ID : 7LBZ
Title : Zoogloea ramigera biosynthetic thiolase Y218E mutant
Authors : Marshall, A.C.; Bruning, J.B.
Deposited on : 2021-01-09
Resolution : 2.60 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

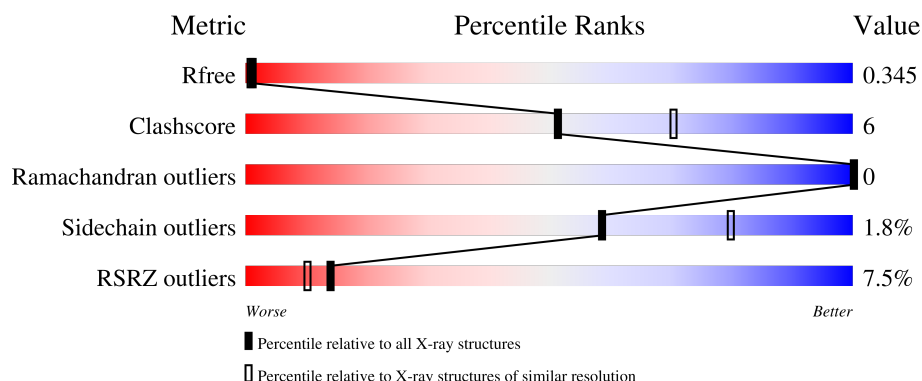
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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>3%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	B	399	<div> <div>4%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	C	399	<div> <div>5%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	D	399	<div> <div>18%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11762 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	388	Total	C	N	O	S	0	0	0
			2787	1731	502	533	21			
1	B	390	Total	C	N	O	S	0	0	0
			2808	1741	506	540	21			
1	C	390	Total	C	N	O	S	0	0	0
			2793	1732	504	536	21			
1	D	390	Total	C	N	O	S	0	0	0
			2765	1716	500	529	20			

There are 40 discrepancies between the modelled and reference sequences:

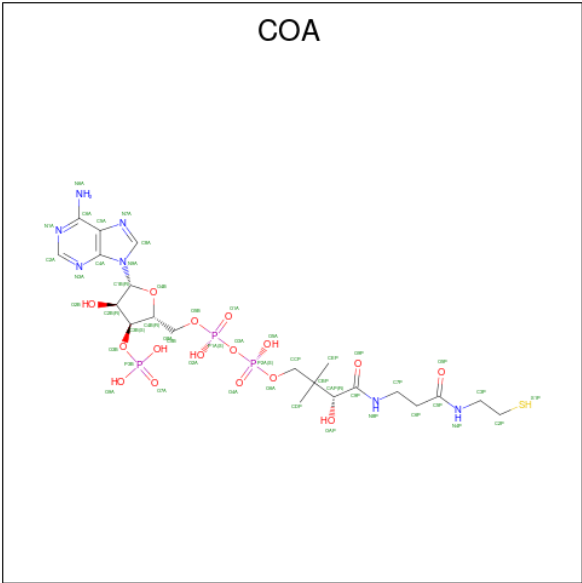
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P07097
A	-5	HIS	-	expression tag	UNP P07097
A	-4	HIS	-	expression tag	UNP P07097
A	-3	HIS	-	expression tag	UNP P07097
A	-2	HIS	-	expression tag	UNP P07097
A	-1	HIS	-	expression tag	UNP P07097
A	0	HIS	-	expression tag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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

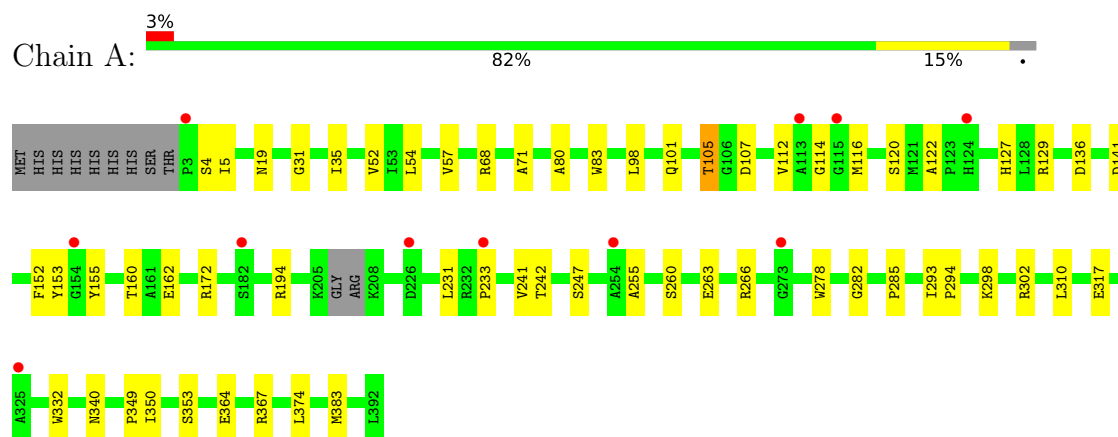
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	170	Total	O	0	0
			170	170		
4	C	44	Total	O	0	0
			44	44		
4	D	32	Total	O	0	0
			32	32		

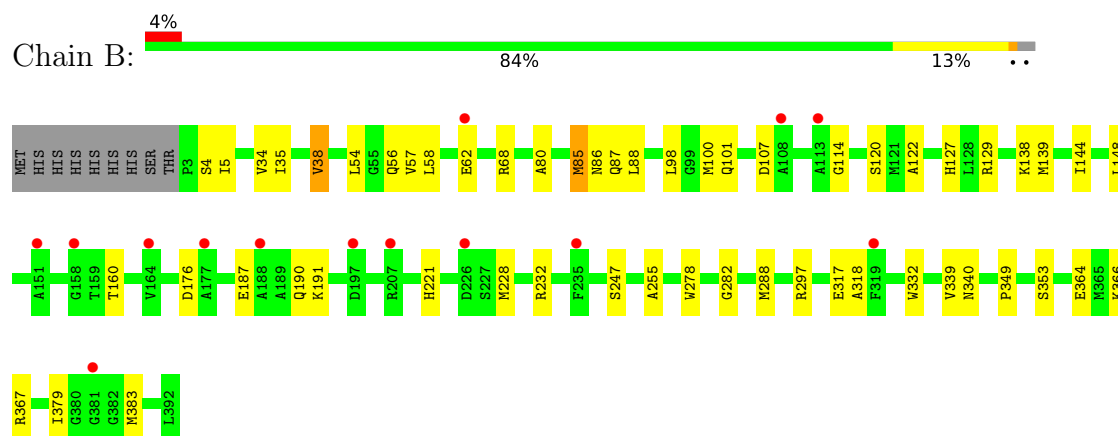
3 Residue-property plots [i](#)

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.

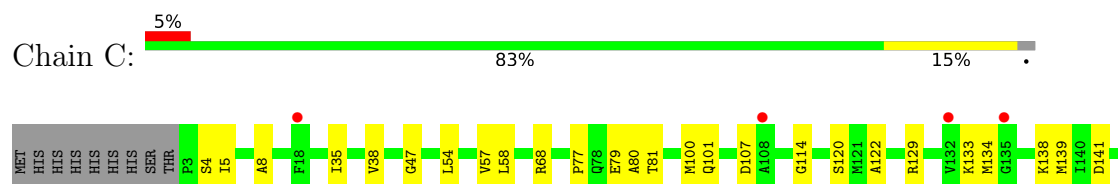
- Molecule 1: Acetyl-CoA acetyltransferase

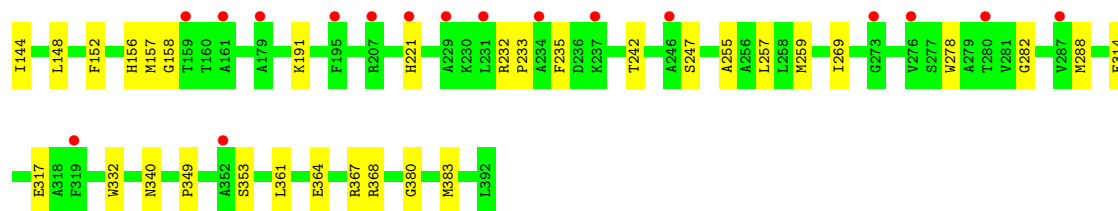


- Molecule 1: Acetyl-CoA acetyltransferase

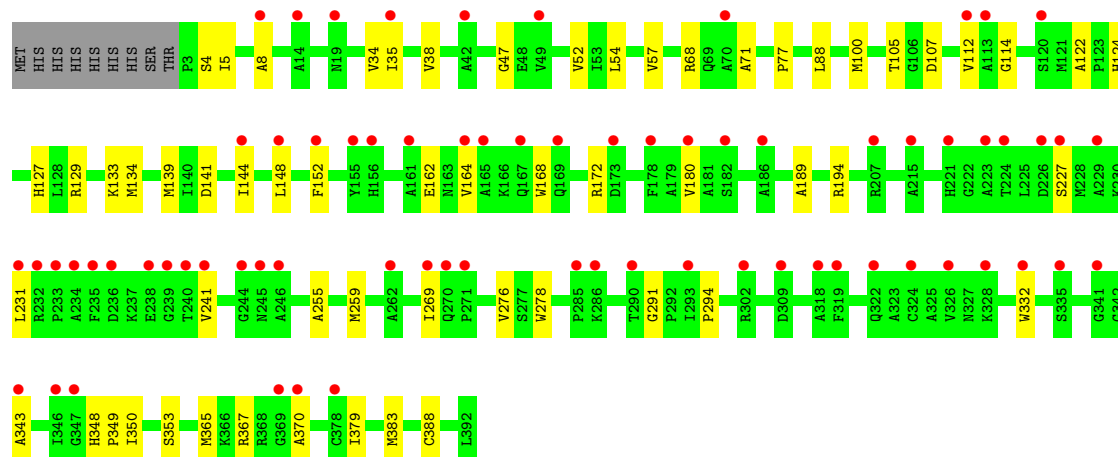
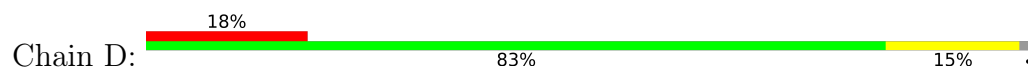


- Molecule 1: Acetyl-CoA acetyltransferase





● 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	84.34Å 79.70Å 149.76Å 90.00° 92.90° 90.00°	Depositor
Resolution (Å)	46.57 – 2.60 46.57 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.57-2.60) 86.4 (46.57-2.60)	Depositor EDS
R_{merge}	0.55	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.306 , 0.320 0.323 , 0.345	Depositor DCC
R_{free} test set	3138 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	1.960	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
Reported twinning fraction	0.160 for h,-k,-l	Depositor
Outliers	2 of 61364 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	11762	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: SO4, SCY, COA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/2817	0.44	0/3804
1	B	0.24	0/2839	0.43	0/3833
1	C	0.24	0/2824	0.42	0/3816
1	D	0.25	0/2794	0.44	0/3777
All	All	0.24	0/11274	0.43	0/15230

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	2787	0	2777	40	0
1	B	2808	0	2797	36	0
1	C	2793	0	2769	37	0
1	D	2765	0	2728	41	0
2	A	48	0	32	1	0
2	B	48	0	32	1	0
2	C	48	0	32	1	0
2	D	48	0	32	0	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	5	0	0	0	0
4	A	161	0	0	0	0
4	B	170	0	0	4	0
4	C	44	0	0	0	0
4	D	32	0	0	0	0
All	All	11762	0	11199	127	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 6.

All (127) 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:B:138:LYS:HE2	1:C:138:LYS:HE2	1.67	0.77
1:B:57:VAL:HG23	1:B:58:LEU:HG	1.72	0.72
1:C:35:ILE:HD11	1:C:54:LEU:HD11	1.71	0.71
1:D:52:VAL:HG12	1:D:112:VAL:HB	1.74	0.69
1:A:52:VAL:HG12	1:A:112:VAL:HB	1.72	0.69
1:C:57:VAL:HG23	1:C:58:LEU:HG	1.73	0.69
1:D:124:HIS:HB3	1:D:139:MET:HG3	1.77	0.67
1:A:282:GLY:HA2	1:A:383:MET:HA	1.79	0.64
1:B:129:ARG:NH1	1:D:133:LYS:O	2.30	0.64
1:D:35:ILE:HD11	1:D:54:LEU:HD11	1.80	0.63
1:A:129:ARG:HH21	1:B:122:ALA:HB3	1.64	0.63
1:C:129:ARG:HH21	1:D:122:ALA:HB3	1.63	0.63
1:B:68:ARG:NH1	1:B:80:ALA:O	2.29	0.62
1:C:364:GLU:OE1	1:C:367:ARG:NH1	2.31	0.62
1:C:156:HIS:HE1	2:C:401:COA:H71	1.65	0.61
1:D:343:ALA:HB1	1:D:348:HIS:HB2	1.82	0.61
1:A:105:THR:HG21	1:B:101:GLN:HG2	1.82	0.61
1:D:88:LEU:HB2	1:D:379:ILE:HG23	1.82	0.60
1:C:120:SER:O	1:D:127:HIS:NE2	2.31	0.60
1:A:114:GLY:HA3	1:A:255:ALA:HA	1.84	0.60
1:B:282:GLY:HA2	1:B:383:MET:HA	1.85	0.59
1:B:297:ARG:NH1	4:B:519:HOH:O	2.35	0.59
1:A:172:ARG:NH2	1:A:231:LEU:O	2.36	0.58
1:D:144:ILE:HA	1:D:148:LEU:HB2	1.84	0.58
1:A:247:SER:OG	1:A:317:GLU:O	2.22	0.57
1:A:340:ASN:ND2	1:A:364:GLU:OE2	2.31	0.57
1:B:340:ASN:ND2	1:B:364:GLU:OE1	2.36	0.57
1:C:144:ILE:HD13	1:C:148:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:SER:O	1:B:127:HIS:NE2	2.39	0.55
1:B:114:GLY:HA3	1:B:255:ALA:HA	1.88	0.55
1:C:340:ASN:ND2	1:C:364:GLU:OE1	2.37	0.55
1:C:191:LYS:HE2	1:C:221:HIS:CE1	2.42	0.54
1:D:4:SER:O	1:D:5:ILE:HG13	2.08	0.54
1:B:144:ILE:HA	1:B:148:LEU:HB2	1.90	0.54
1:A:35:ILE:HD11	1:A:54:LEU:HD11	1.91	0.53
1:C:114:GLY:HA3	1:C:255:ALA:HA	1.90	0.53
1:A:101:GLN:O	1:A:105:THR:HG23	2.08	0.53
1:D:52:VAL:HG21	1:D:71:ALA:HB2	1.89	0.53
1:A:122:ALA:HB3	1:B:129:ARG:HH21	1.74	0.52
1:A:136:ASP:OD1	1:D:141:ASP:N	2.33	0.52
1:B:190:GLN:HB3	4:B:504:HOH:O	2.09	0.52
1:D:189:ALA:HB1	1:D:194:ARG:HB2	1.91	0.52
1:C:4:SER:O	1:C:5:ILE:HG13	2.08	0.52
1:D:114:GLY:HA3	1:D:255:ALA:HA	1.91	0.52
1:D:365:MET:O	1:D:370:ALA:N	2.35	0.52
1:B:4:SER:O	1:B:5:ILE:HG13	2.09	0.51
1:A:19:ASN:ND2	1:D:133:LYS:HG3	2.25	0.51
1:A:52:VAL:HG21	1:A:71:ALA:HB2	1.93	0.51
1:C:77:PRO:HB2	1:C:79:GLU:OE1	2.11	0.51
1:D:34:VAL:O	1:D:38:VAL:HG13	2.10	0.51
1:C:107:ASP:OD2	1:D:278:TRP:NE1	2.43	0.51
1:C:157:MET:HE1	1:C:380:GLY:HA2	1.93	0.51
1:A:107:ASP:OD2	1:B:278:TRP:NE1	2.42	0.50
1:D:172:ARG:NH2	1:D:231:LEU:O	2.44	0.50
1:C:81:THR:HG22	1:D:383:MET:HG2	1.92	0.50
1:B:318:ALA:HB1	2:B:402:COA:H21	1.94	0.50
1:A:278:TRP:NE1	1:B:107:ASP:OD2	2.44	0.49
1:C:5:ILE:HD13	1:C:100:MET:HG2	1.94	0.49
1:D:349:PRO:O	1:D:353:SER:N	2.45	0.49
1:A:263:GLU:OE2	1:A:266:ARG:NH2	2.21	0.49
1:C:38:VAL:HG12	1:C:257:LEU:HB2	1.95	0.49
1:C:101:GLN:HG2	1:D:105:THR:HG21	1.93	0.49
1:D:47:GLY:HA2	1:D:77:PRO:HG3	1.94	0.48
1:B:34:VAL:O	1:B:38:VAL:HG23	2.13	0.48
1:A:31:GLY:HA3	1:A:116:MET:HE2	1.95	0.48
1:C:68:ARG:NH1	1:C:80:ALA:O	2.37	0.48
1:C:68:ARG:HG3	1:D:152:PHE:HZ	1.79	0.48
1:A:5:ILE:HD13	1:A:260:SER:HA	1.95	0.48
1:B:144:ILE:HD11	1:C:134:MET:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:VAL:O	1:D:168:TRP:HB2	2.13	0.48
1:A:293:ILE:HB	1:A:294:PRO:HD3	1.95	0.48
1:C:278:TRP:NE1	1:D:107:ASP:OD2	2.46	0.48
1:A:298:LYS:HE3	1:A:302:ARG:HE	1.78	0.48
1:A:194:ARG:HB3	1:A:367:ARG:NH1	2.29	0.48
1:D:5:ILE:HD13	1:D:100:MET:HG2	1.96	0.47
1:C:8:ALA:HB1	1:C:269:ILE:HG21	1.96	0.47
1:D:227:SER:O	1:D:231:LEU:HG	2.15	0.47
1:B:86:ASN:ND2	4:B:532:HOH:O	2.48	0.47
1:B:88:LEU:HB2	1:B:379:ILE:HG23	1.97	0.46
1:B:191:LYS:HE2	1:B:221:HIS:CE1	2.50	0.46
1:A:68:ARG:NH1	1:A:80:ALA:O	2.37	0.46
1:A:233:PRO:HA	1:A:242:THR:HG22	1.98	0.46
1:B:349:PRO:O	1:B:353:SER:N	2.47	0.45
1:C:47:GLY:HA2	1:C:77:PRO:HG3	1.99	0.45
1:B:187:GLU:HA	4:B:504:HOH:O	2.15	0.45
1:A:4:SER:OG	1:A:5:ILE:N	2.46	0.45
1:C:148:LEU:HB3	1:C:156:HIS:NE2	2.32	0.45
1:C:349:PRO:O	1:C:353:SER:N	2.47	0.45
1:D:35:ILE:HA	1:D:38:VAL:HG22	1.99	0.45
1:B:5:ILE:HD13	1:B:100:MET:HG2	1.99	0.44
1:C:152:PHE:HZ	1:D:68:ARG:HG3	1.81	0.44
1:C:247:SER:OG	1:C:317:GLU:O	2.36	0.43
1:B:35:ILE:HD11	1:B:54:LEU:HD11	2.00	0.43
1:C:364:GLU:O	1:C:368:ARG:HG2	2.19	0.43
1:D:162:GLU:OE2	1:D:241:VAL:HG22	2.19	0.43
1:A:83:TRP:HH2	1:A:98:LEU:HD13	1.83	0.43
1:A:141:ASP:OD1	1:B:129:ARG:NH2	2.50	0.43
1:A:54:LEU:HD13	1:A:116:MET:HE3	2.01	0.42
1:A:162:GLU:OE1	1:A:241:VAL:HG22	2.19	0.42
1:A:129:ARG:NH1	1:C:133:LYS:O	2.51	0.42
1:C:282:GLY:HA2	1:C:383:MET:HA	2.01	0.42
1:A:152:PHE:HZ	1:B:68:ARG:HG3	1.84	0.42
1:A:153:TYR:HE2	1:A:285:PRO:HB2	1.84	0.42
1:A:349:PRO:O	1:A:353:SER:N	2.50	0.42
1:C:233:PRO:HA	1:C:242:THR:HG22	2.01	0.42
1:D:57:VAL:HG21	1:D:350:ILE:HG22	2.02	0.42
1:D:194:ARG:HB3	1:D:367:ARG:HH12	1.84	0.42
1:A:155:TYR:HE1	1:A:160:THR:HG22	1.85	0.42
1:C:158:GLY:HA3	1:C:235:PHE:CE2	2.55	0.42
1:A:310:LEU:HD11	1:A:374:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ALA:HB3	1:D:129:ARG:HH21	1.84	0.42
1:C:314:GLU:HG3	1:C:361:LEU:HB2	2.02	0.42
1:A:83:TRP:HB3	1:B:87:GLN:HG3	2.02	0.41
1:B:56:GLN:NE2	1:B:62:GLU:OE1	2.45	0.41
1:C:141:ASP:OD1	1:D:129:ARG:NH2	2.41	0.41
1:A:136:ASP:HB3	1:D:139:MET:O	2.20	0.41
1:B:247:SER:OG	1:B:317:GLU:O	2.38	0.41
1:A:57:VAL:HG21	1:A:350:ILE:HG22	2.03	0.41
2:A:801:COA:H143	1:D:134:MET:HE1	2.02	0.41
1:D:8:ALA:HB1	1:D:269:ILE:HG21	2.03	0.41
1:D:276:VAL:HG12	1:D:388:CYS:HB2	2.02	0.41
1:B:364:GLU:OE1	1:B:367:ARG:NH1	2.54	0.41
1:D:291:GLY:O	1:D:294:PRO:HD2	2.21	0.40
1:B:176:ASP:HA	1:B:228:MET:HE2	2.03	0.40
1:A:127:HIS:NE2	1:B:120:SER:O	2.44	0.40
1:B:85:MET:CE	1:B:98:LEU:HD12	2.52	0.40
1:D:276:VAL:CG1	1:D:388:CYS:HB2	2.52	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	383/399 (96%)	371 (97%)	12 (3%)	0	100	100
1	B	387/399 (97%)	376 (97%)	11 (3%)	0	100	100
1	C	387/399 (97%)	376 (97%)	11 (3%)	0	100	100
1	D	387/399 (97%)	374 (97%)	13 (3%)	0	100	100
All	All	1544/1596 (97%)	1497 (97%)	47 (3%)	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	270/285 (95%)	268 (99%)	2 (1%)	84	94
1	B	273/285 (96%)	264 (97%)	9 (3%)	38	64
1	C	269/285 (94%)	264 (98%)	5 (2%)	57	79
1	D	260/285 (91%)	257 (99%)	3 (1%)	71	87
All	All	1072/1140 (94%)	1053 (98%)	19 (2%)	59	80

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

Mol	Chain	Res	Type
1	A	105	THR
1	A	332	TRP
1	B	38	VAL
1	B	85	MET
1	B	139	MET
1	B	160	THR
1	B	232	ARG
1	B	288	MET
1	B	332	TRP
1	B	339	VAL
1	B	366	LYS
1	C	139	MET
1	C	232	ARG
1	C	259	MET
1	C	288	MET
1	C	332	TRP
1	D	180	VAL
1	D	259	MET
1	D	332	TRP

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

Mol	Chain	Res	Type
1	C	190	GLN
1	C	221	HIS
1	C	322	GLN

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	0.91	0	3,9,11	0.83	0
1	SCY	B	89	1	7,8,9	0.92	0	3,9,11	0.84	0
1	SCY	A	89	1	7,8,9	0.93	0	3,9,11	0.85	0
1	SCY	D	89	1	7,8,9	0.91	0	3,9,11	0.84	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
1	D	89	SCY	CE-CD-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	COA	B	402	-	41,50,50	1.20	3 (7%)	52,75,75	1.47	10 (19%)
2	COA	D	401	-	41,50,50	1.27	3 (7%)	52,75,75	1.43	6 (11%)
2	COA	A	801	-	41,50,50	1.21	3 (7%)	52,75,75	1.44	9 (17%)
3	SO4	B	401	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	D	402	-	4,4,4	0.14	0	6,6,6	0.05	0
2	COA	C	401	-	41,50,50	1.23	3 (7%)	52,75,75	1.42	6 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	B	402	-	-	10/44/64/64	0/3/3/3
2	COA	C	401	-	-	17/44/64/64	0/3/3/3
2	COA	A	801	-	-	7/44/64/64	0/3/3/3
2	COA	D	401	-	-	21/44/64/64	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	COA	O4B-C1B	4.31	1.47	1.41
2	C	401	COA	O4B-C1B	4.19	1.46	1.41
2	B	402	COA	O4B-C1B	3.75	1.46	1.41
2	A	801	COA	O4B-C1B	3.63	1.46	1.41
2	D	401	COA	C8A-N7A	-3.16	1.29	1.34
2	C	401	COA	C8A-N7A	-3.10	1.29	1.34
2	A	801	COA	C8A-N7A	-2.99	1.29	1.34
2	B	402	COA	C8A-N7A	-2.97	1.29	1.34
2	C	401	COA	P3B-O8A	2.06	1.62	1.54
2	B	402	COA	P3B-O8A	2.05	1.62	1.54
2	D	401	COA	P3B-O8A	2.02	1.62	1.54
2	A	801	COA	P3B-O8A	2.02	1.62	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	COA	P2A-O3A-P1A	-5.25	114.83	132.83
2	A	801	COA	P2A-O3A-P1A	-5.18	115.04	132.83
2	D	401	COA	P2A-O3A-P1A	-5.13	115.22	132.83
2	C	401	COA	P2A-O3A-P1A	-4.97	115.76	132.83
2	B	402	COA	N3A-C2A-N1A	-3.33	123.48	128.68
2	C	401	COA	N3A-C2A-N1A	-3.32	123.49	128.68
2	A	801	COA	N3A-C2A-N1A	-3.30	123.51	128.68
2	D	401	COA	N3A-C2A-N1A	-3.28	123.55	128.68
2	C	401	COA	O4B-C1B-C2B	-2.78	102.87	106.93
2	D	401	COA	N6A-C6A-N1A	2.76	124.31	118.57
2	B	402	COA	O4B-C1B-C2B	-2.74	102.92	106.93
2	B	402	COA	N6A-C6A-N1A	2.66	124.10	118.57
2	A	801	COA	N6A-C6A-N1A	2.65	124.07	118.57
2	C	401	COA	N6A-C6A-N1A	2.63	124.03	118.57
2	D	401	COA	C1B-N9A-C4A	2.51	131.04	126.64
2	D	401	COA	CAP-C9P-N8P	2.50	121.56	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	COA	CAP-C9P-N8P	2.47	121.50	116.58
2	A	801	COA	C6P-C5P-N4P	2.43	120.52	116.42
2	B	402	COA	C6P-C5P-N4P	2.38	120.43	116.42
2	C	401	COA	C6P-C5P-N4P	2.35	120.38	116.42
2	C	401	COA	C1B-N9A-C4A	2.21	130.53	126.64
2	D	401	COA	C5A-C6A-N6A	-2.20	117.01	120.35
2	B	402	COA	O9P-C9P-N8P	-2.20	118.28	122.99
2	A	801	COA	P1A-O5B-C5B	-2.14	109.11	121.68
2	A	801	COA	O4B-C1B-C2B	-2.13	103.82	106.93
2	A	801	COA	O5P-C5P-N4P	-2.08	119.08	123.01
2	B	402	COA	P1A-O5B-C5B	-2.07	109.55	121.68
2	A	801	COA	O9P-C9P-N8P	-2.06	118.56	122.99
2	B	402	COA	C3P-N4P-C5P	-2.02	119.08	122.84
2	B	402	COA	C5A-C6A-N6A	-2.01	117.30	120.35
2	A	801	COA	C5A-C6A-N6A	-2.01	117.30	120.35

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	COA	C5B-O5B-P1A-O3A
2	A	801	COA	S1P-C2P-C3P-N4P
2	B	402	COA	C5B-O5B-P1A-O3A
2	B	402	COA	CCP-O6A-P2A-O4A
2	B	402	COA	CDP-CBP-CCP-O6A
2	B	402	COA	CAP-CBP-CCP-O6A
2	B	402	COA	S1P-C2P-C3P-N4P
2	C	401	COA	C5B-O5B-P1A-O1A
2	C	401	COA	C5B-O5B-P1A-O3A
2	C	401	COA	CDP-CBP-CCP-O6A
2	C	401	COA	CEP-CBP-CCP-O6A
2	C	401	COA	CAP-CBP-CCP-O6A
2	D	401	COA	C4B-C3B-O3B-P3B
2	D	401	COA	C3B-C4B-C5B-O5B
2	D	401	COA	C5B-O5B-P1A-O1A
2	D	401	COA	C5B-O5B-P1A-O2A
2	D	401	COA	C5B-O5B-P1A-O3A
2	D	401	COA	C9P-CAP-CBP-CCP
2	D	401	COA	C9P-CAP-CBP-CEP
2	D	401	COA	N8P-C9P-CAP-OAP
2	D	401	COA	S1P-C2P-C3P-N4P
2	C	401	COA	O4B-C4B-C5B-O5B

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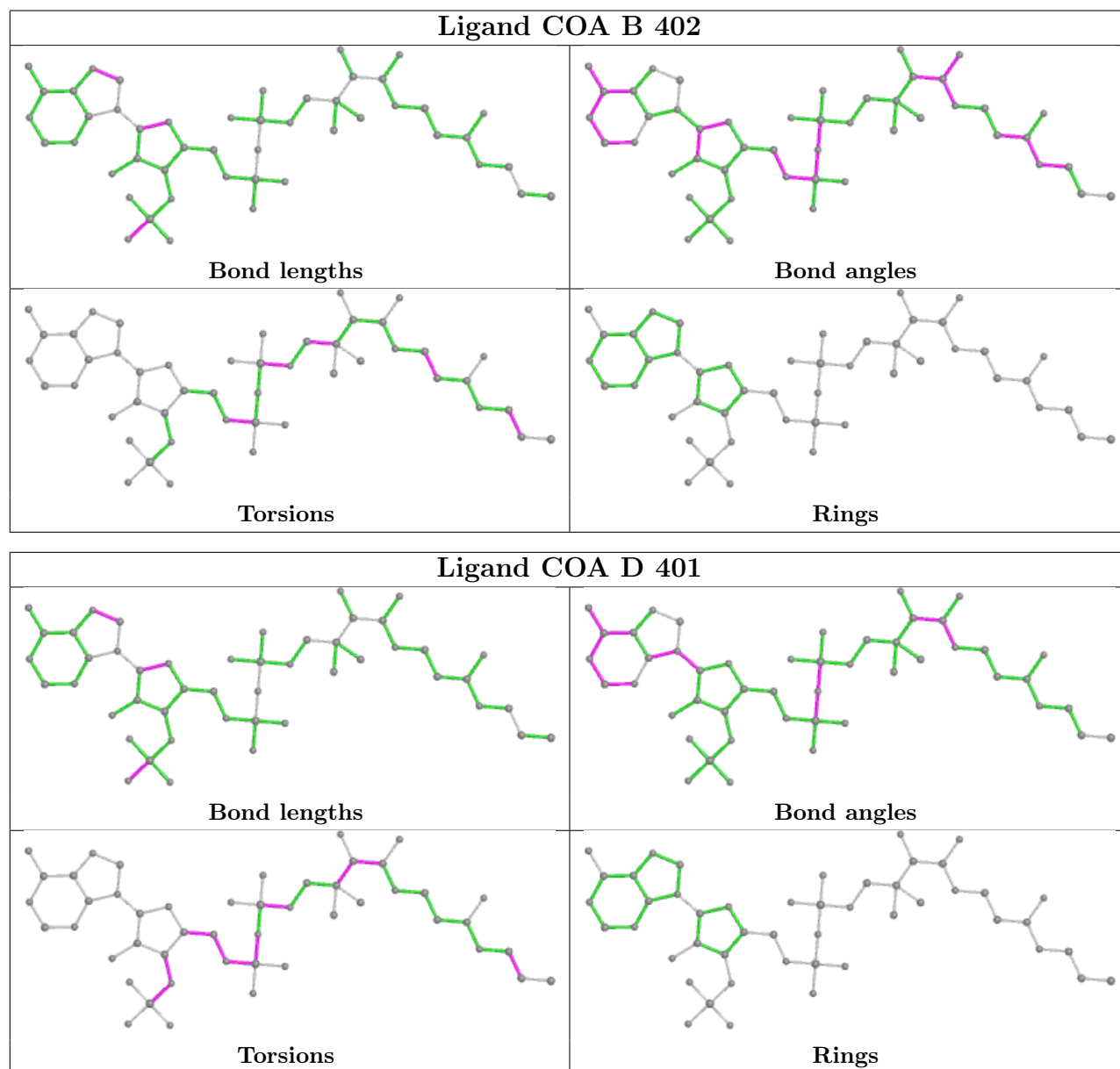
Mol	Chain	Res	Type	Atoms
2	D	401	COA	O4B-C4B-C5B-O5B
2	B	402	COA	CEP-CBP-CCP-O6A
2	A	801	COA	O9P-C9P-CAP-OAP
2	C	401	COA	O9P-C9P-CAP-OAP
2	D	401	COA	O9P-C9P-CAP-OAP
2	D	401	COA	OAP-CAP-CBP-CEP
2	C	401	COA	C3B-C4B-C5B-O5B
2	D	401	COA	O9P-C9P-CAP-CBP
2	D	401	COA	N8P-C9P-CAP-CBP
2	C	401	COA	S1P-C2P-C3P-N4P
2	D	401	COA	P2A-O3A-P1A-O5B
2	A	801	COA	N8P-C9P-CAP-OAP
2	C	401	COA	N8P-C9P-CAP-OAP
2	B	402	COA	C5P-C6P-C7P-N8P
2	B	402	COA	CCP-O6A-P2A-O3A
2	D	401	COA	C3B-O3B-P3B-O8A
2	A	801	COA	C5B-O5B-P1A-O2A
2	B	402	COA	C5B-O5B-P1A-O2A
2	C	401	COA	C5B-O5B-P1A-O2A
2	D	401	COA	OAP-CAP-CBP-CCP
2	C	401	COA	C2B-C3B-O3B-P3B
2	D	401	COA	OAP-CAP-CBP-CDP
2	C	401	COA	C4B-C3B-O3B-P3B
2	D	401	COA	C4B-C5B-O5B-P1A
2	C	401	COA	C3B-O3B-P3B-O7A
2	C	401	COA	C9P-CAP-CBP-CEP
2	D	401	COA	C9P-CAP-CBP-CDP
2	C	401	COA	C3B-O3B-P3B-O8A
2	C	401	COA	C3B-O3B-P3B-O9A
2	D	401	COA	CCP-O6A-P2A-O3A
2	A	801	COA	C5B-O5B-P1A-O1A
2	A	801	COA	CCP-O6A-P2A-O4A
2	B	402	COA	C5B-O5B-P1A-O1A

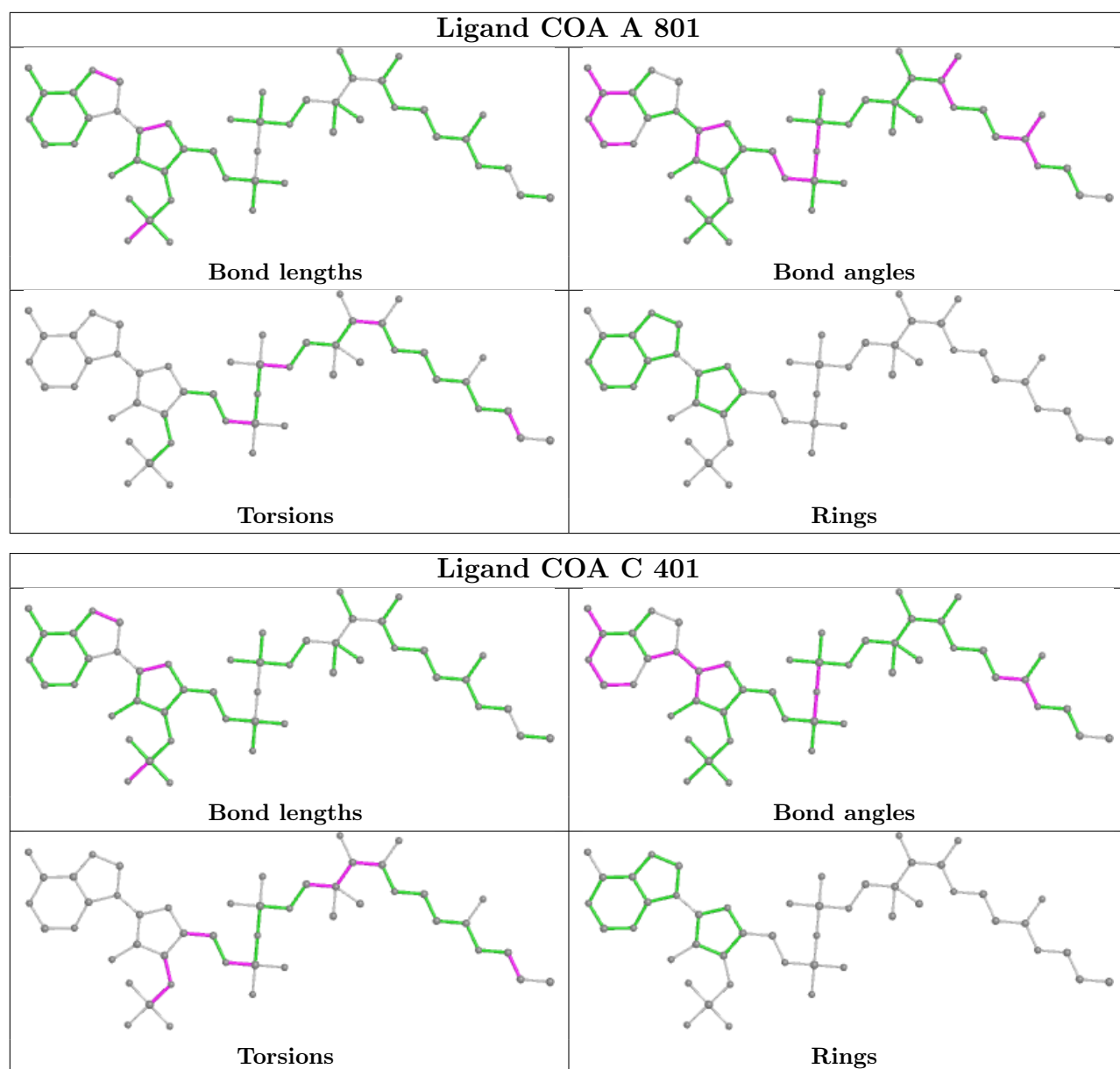
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	COA	1	0
2	A	801	COA	1	0
2	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	387/399 (96%)	0.59	11 (2%)	53	46	3, 31, 38, 42	0
1	B	389/399 (97%)	0.63	14 (3%)	42	35	10, 31, 40, 43	0
1	C	389/399 (97%)	0.68	21 (5%)	25	20	30, 39, 56, 60	0
1	D	389/399 (97%)	1.11	71 (18%)	1	0	45, 56, 64, 92	0
All	All	1554/1596 (97%)	0.75	117 (7%)	14	10	3, 36, 60, 92	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	ASP	5.9
1	D	370	ALA	5.8
1	D	246	ALA	5.4
1	C	161	ALA	5.3
1	D	173	ASP	5.1
1	D	232	ARG	5.0
1	D	221	HIS	4.6
1	A	273	GLY	4.5
1	D	229	ALA	4.3
1	C	229	ALA	4.2
1	D	235	PHE	4.1
1	D	156	HIS	4.0
1	C	246	ALA	4.0
1	D	234	ALA	4.0
1	D	236	ASP	3.9
1	D	269	ILE	3.9
1	D	224	THR	3.7
1	D	223	ALA	3.7
1	D	161	ALA	3.7
1	D	238	GLU	3.7
1	D	169	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	227	SER	3.7
1	D	180	VAL	3.6
1	D	318	ALA	3.6
1	D	285	PRO	3.6
1	D	231	LEU	3.6
1	C	276	VAL	3.6
1	A	154	GLY	3.6
1	D	240	THR	3.6
1	D	178	PHE	3.4
1	D	271	PRO	3.4
1	D	165	ALA	3.3
1	D	167	GLN	3.3
1	D	186	ALA	3.2
1	C	207	ARG	3.2
1	D	319	PHE	3.1
1	D	326	VAL	3.1
1	C	135	GLY	3.1
1	A	254	ALA	3.0
1	B	235	PHE	3.0
1	D	239	GLY	3.0
1	C	234	ALA	3.0
1	D	244	GLY	3.0
1	D	182	SER	2.9
1	C	319	PHE	2.9
1	D	347	GLY	2.9
1	D	14	ALA	2.9
1	C	231	LEU	2.9
1	B	207	ARG	2.9
1	D	42	ALA	2.8
1	B	381	GLY	2.8
1	C	195	PHE	2.8
1	D	245	ASN	2.8
1	D	49	VAL	2.7
1	C	237	LYS	2.7
1	D	324	CYS	2.7
1	B	158	GLY	2.7
1	D	233	PRO	2.7
1	D	148	LEU	2.7
1	D	290	THR	2.7
1	D	341	GLY	2.6
1	D	328	LYS	2.6
1	D	346	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	286	LYS	2.6
1	A	124	HIS	2.5
1	D	152	PHE	2.5
1	D	262	ALA	2.5
1	C	287	VAL	2.5
1	D	155	TYR	2.5
1	A	233	PRO	2.5
1	D	309	ASP	2.5
1	B	62	GLU	2.5
1	C	108	ALA	2.5
1	D	343	ALA	2.4
1	A	3	PRO	2.4
1	D	113	ALA	2.4
1	D	241	VAL	2.4
1	C	273	GLY	2.4
1	D	369	GLY	2.4
1	B	113	ALA	2.4
1	D	378	CYS	2.4
1	D	8	ALA	2.4
1	B	164	VAL	2.4
1	D	293	ILE	2.3
1	A	115	GLY	2.3
1	C	18	PHE	2.3
1	C	280	THR	2.3
1	D	35	ILE	2.3
1	D	207	ARG	2.3
1	B	319	PHE	2.3
1	D	332	TRP	2.3
1	B	108	ALA	2.3
1	D	215	ALA	2.2
1	A	325	ALA	2.2
1	B	226	ASP	2.2
1	D	144	ILE	2.2
1	C	179	ALA	2.2
1	C	221	HIS	2.2
1	A	226	ASP	2.2
1	B	177	ALA	2.2
1	C	132	VAL	2.1
1	D	270	GLN	2.1
1	D	302	ARG	2.1
1	B	151	ALA	2.1
1	D	70	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	197	ASP	2.1
1	B	188	ALA	2.1
1	D	164	VAL	2.1
1	D	322	GLN	2.1
1	C	352	ALA	2.1
1	D	120	SER	2.1
1	A	113	ALA	2.1
1	D	335	SER	2.1
1	D	112	VAL	2.0
1	A	182	SER	2.0
1	C	159	THR	2.0
1	D	19	ASN	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	D	89	9/10	0.72	0.32	45,45,45,45	0
1	SCY	A	89	9/10	0.81	0.24	33,33,33,34	0
1	SCY	C	89	9/10	0.83	0.23	35,35,36,36	0
1	SCY	B	89	9/10	0.88	0.24	33,34,35,35	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.

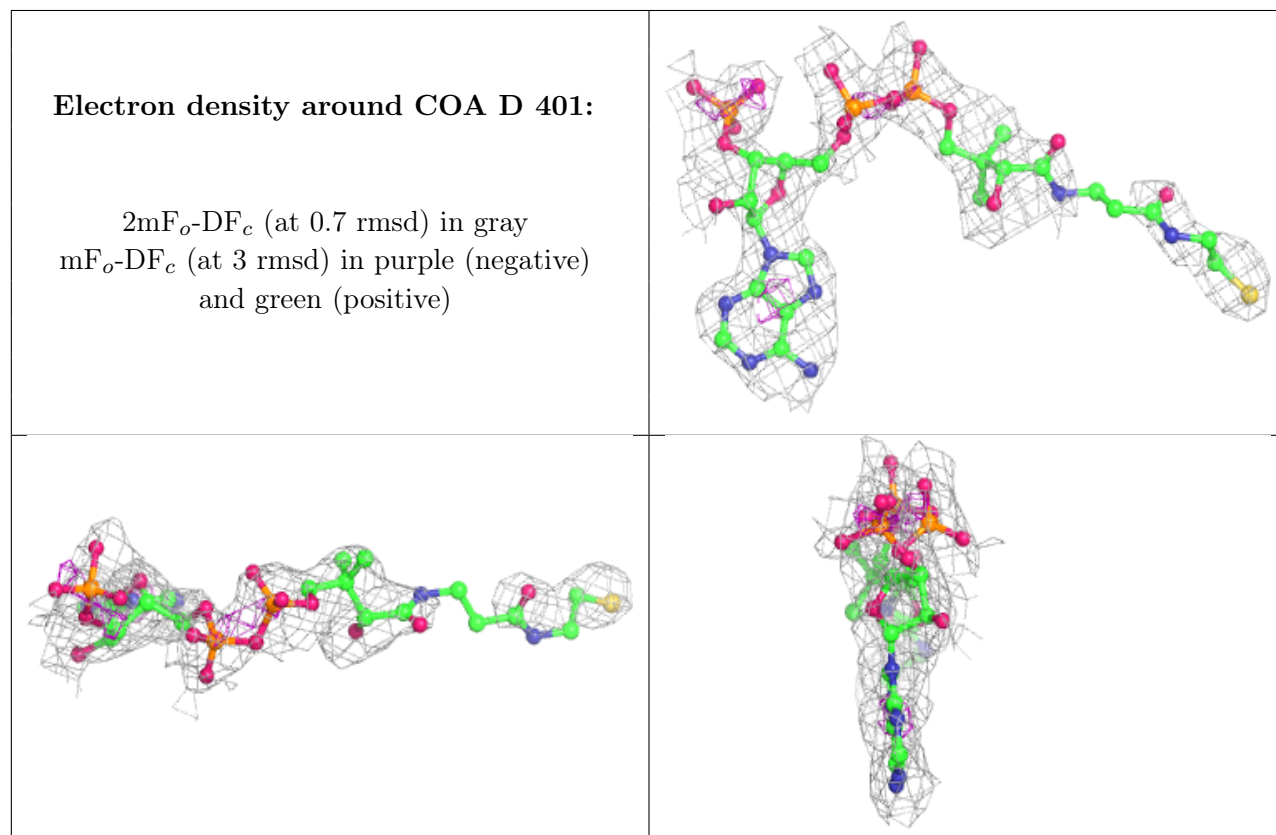
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COA	D	401	48/48	0.71	0.34	28,42,50,55	48
3	SO4	D	402	5/5	0.75	0.34	76,76,78,78	0

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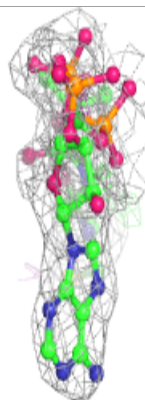
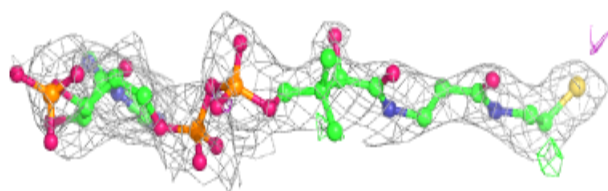
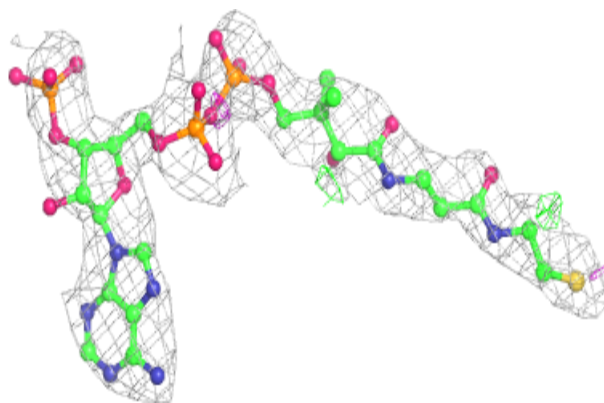
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	COA	A	801	48/48	0.83	0.26	41,54,75,85	0
2	COA	B	402	48/48	0.83	0.22	0,22,60,78	0
2	COA	C	401	48/48	0.85	0.23	20,28,40,44	0
3	SO4	B	401	5/5	0.90	0.19	51,52,54,55	0

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

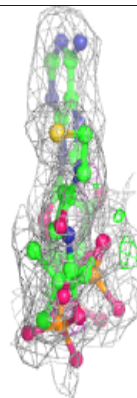
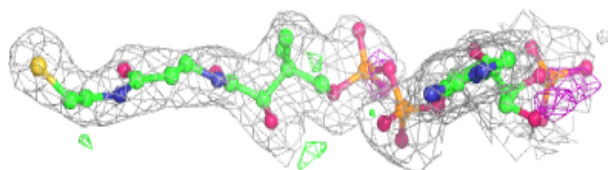
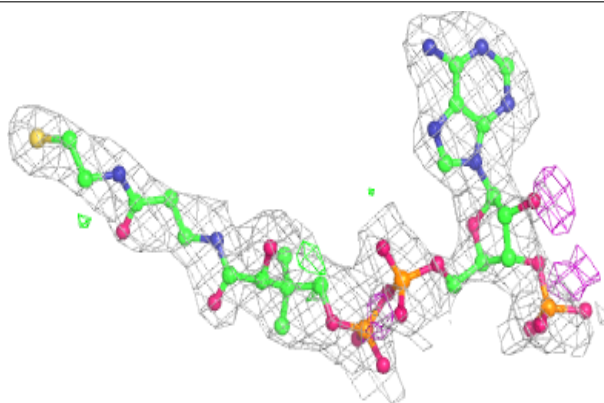


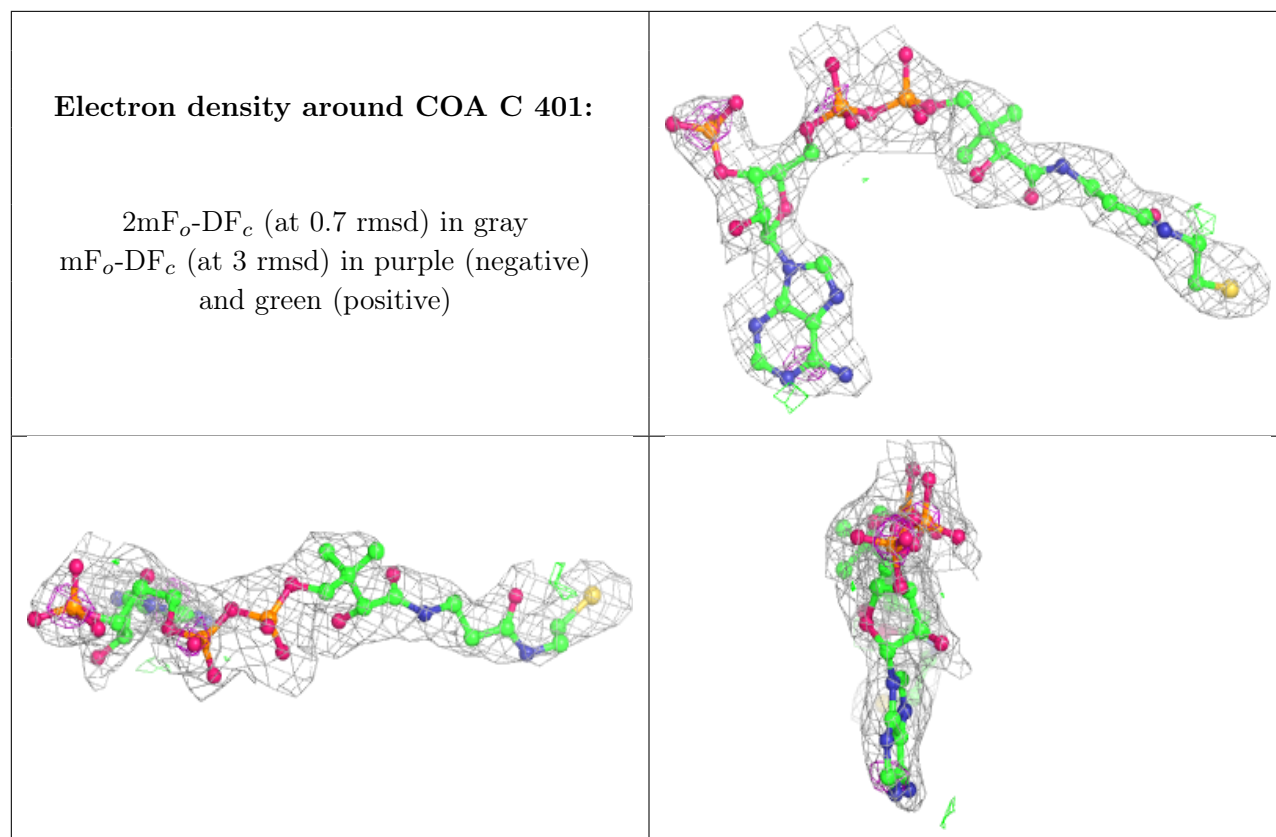
Electron density around COA A 801:

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

**Electron density around COA B 402:**

$2mF_o-DF_c$ (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.