



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 10:13 AM EDT

PDB ID : 7LDT
Title : Zoogloea ramigera biosynthetic thiolase Q183Y/Y218E mutant, RbCl soak
Authors : Marshall, A.C.; Bruning, J.B.
Deposited on : 2021-01-14
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 types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

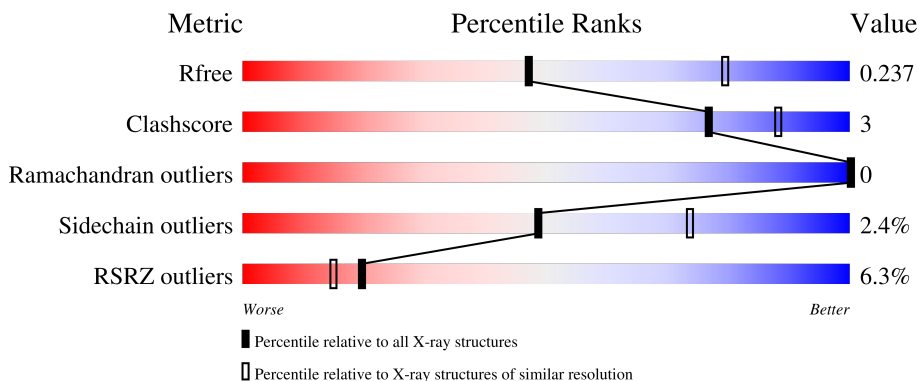
1 Overall quality at a glance i

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	 3% 89% 9% .
1	B	399	 2% 89% 8% ..
1	C	399	 5% 91% 7% .
1	D	399	 14% 88% 9% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	COA	D	401	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12259 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
			Total	C	N	O	S			
1	A	390	2817	1751	505	540	21	0	0	0
1	B	390	2812	1748	505	538	21	0	0	0
1	C	390	2809	1745	507	536	21	0	0	0
1	D	386	2737	1701	490	526	20	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

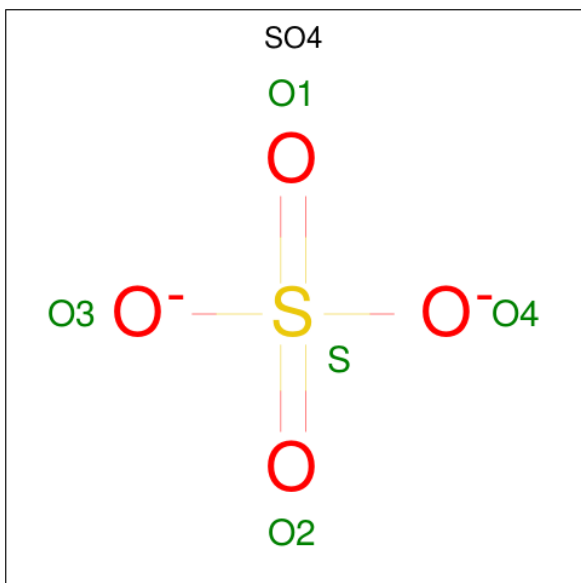
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P07097
A	-5	HIS	-	expression tag	UNP P07097
A	-4	HIS	-	expression tag	UNP P07097
A	-3	HIS	-	expression tag	UNP P07097
A	-2	HIS	-	expression tag	UNP P07097
A	-1	HIS	-	expression tag	UNP P07097
A	0	HIS	-	expression tag	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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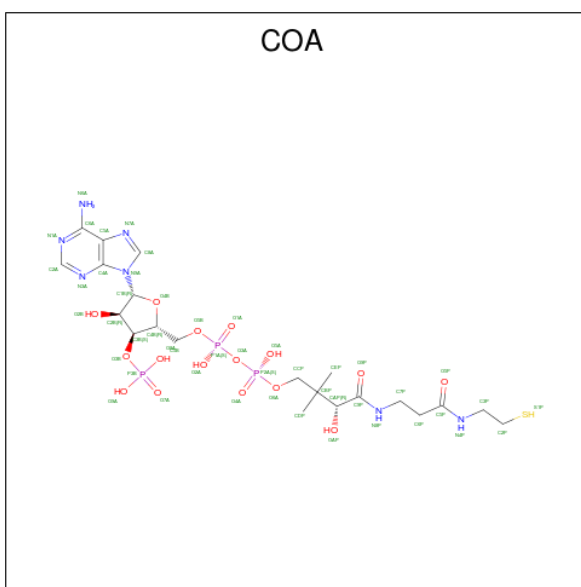
Chain	Residue	Modelled	Actual	Comment	Reference
B	218	GLU	TYR	engineered mutation	UNP P07097
C	-6	MET	-	initiating methionine	UNP P07097
C	-5	HIS	-	expression tag	UNP P07097
C	-4	HIS	-	expression tag	UNP P07097
C	-3	HIS	-	expression tag	UNP P07097
C	-2	HIS	-	expression tag	UNP P07097
C	-1	HIS	-	expression 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	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: $C_{21}H_{36}N_7O_{16}P_3S$) (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
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 RUBIDIUM ION (three-letter code: RB) (formula: Rb) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Rb 1 1	0	0

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

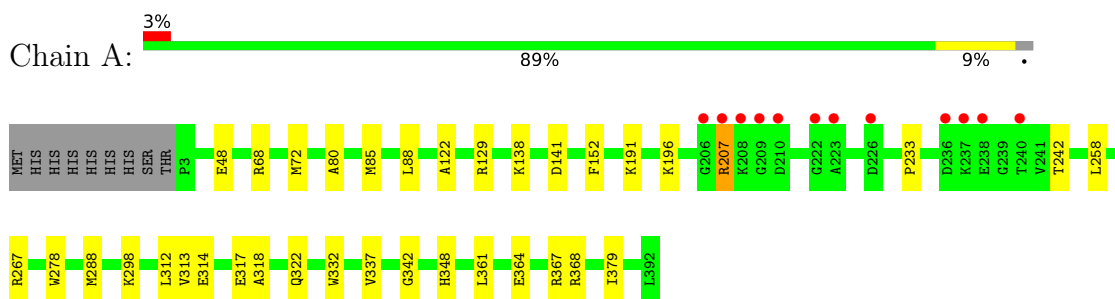
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	310	Total 310	O 310	0	0
5	B	301	Total 301	O 301	0	0
5	C	143	Total 143	O 143	0	0
5	D	114	Total 114	O 114	0	0

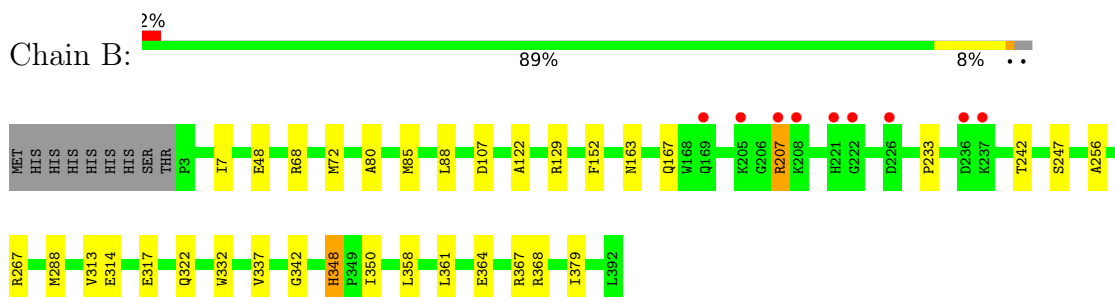
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

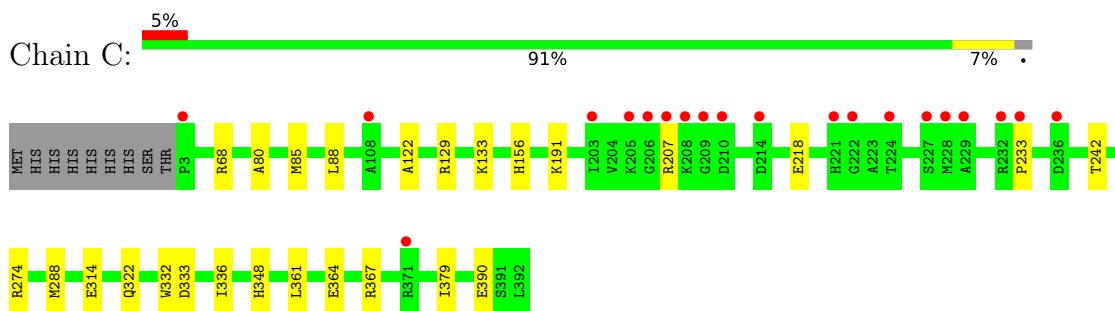
- Molecule 1: Acetyl-CoA acetyltransferase



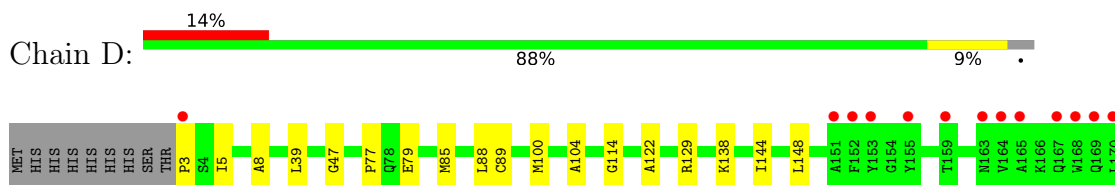
- Molecule 1: Acetyl-CoA acetyltransferase

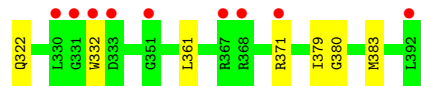
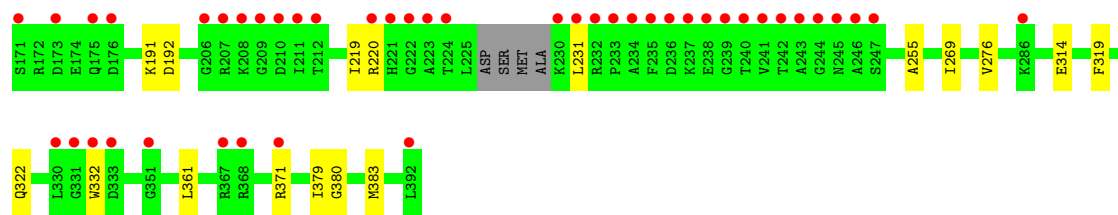


- Molecule 1: Acetyl-CoA acetyltransferase



- 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	84.24Å 79.76Å 150.58Å 90.00° 93.71° 90.00°	Depositor
Resolution (Å)	34.82 – 2.60 34.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.82-2.60) 99.5 (34.82-2.60)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.195 , 0.238 0.194 , 0.237	Depositor DCC
R_{free} test set	3118 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtrriage
Anisotropy	1.102	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12259	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.44% 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, RB, 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	0.25	0/2849	0.46	0/3846
1	B	0.26	0/2844	0.46	0/3840
1	C	0.25	0/2841	0.44	0/3837
1	D	0.26	0/2767	0.44	0/3744
All	All	0.26	0/11301	0.45	0/15267

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	2817	0	2812	24	0
1	B	2812	0	2806	20	0
1	C	2809	0	2800	14	0
1	D	2737	0	2678	20	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	48	0	32	1	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	1	0
3	D	48	0	32	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	310	0	0	2	0
5	B	301	0	0	0	0
5	C	143	0	0	1	0
5	D	114	0	0	3	0
All	All	12259	0	11224	67	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 (67) 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:A:207:ARG:HE	1:A:207:ARG:H	1.43	0.64
1:D:191:LYS:NZ	5:D:506:HOH:O	2.34	0.61
1:B:364:GLU:OE1	1:B:367:ARG:NH1	2.33	0.61
1:D:77:PRO:HB2	1:D:79:GLU:OE1	2.03	0.58
1:C:85:MET:HA	1:D:85:MET:HA	1.85	0.57
1:A:196:LYS:NZ	5:A:508:HOH:O	2.37	0.57
1:B:314:GLU:HG3	1:B:361:LEU:HB2	1.87	0.56
1:C:129:ARG:HH21	1:D:122:ALA:HB3	1.70	0.56
1:A:85:MET:HA	1:B:85:MET:HA	1.87	0.56
1:C:122:ALA:HB3	1:D:129:ARG:HH21	1.71	0.55
1:D:8:ALA:HB1	1:D:269:ILE:HG21	1.91	0.52
1:D:47:GLY:HA2	1:D:77:PRO:HG3	1.92	0.52
1:A:364:GLU:OE1	1:A:367:ARG:NH1	2.32	0.51
1:D:3:PRO:HG2	1:D:104:ALA:HA	1.94	0.50
1:A:318:ALA:HB1	3:A:403:COA:H22	1.93	0.50
1:B:68:ARG:NH1	1:B:80:ALA:O	2.45	0.49
1:A:129:ARG:HH21	1:B:122:ALA:HB3	1.76	0.49
1:A:138:LYS:HD2	1:D:138:LYS:HD2	1.94	0.49
1:B:207:ARG:H	1:B:207:ARG:CD	2.26	0.49
1:C:88:LEU:HB2	1:C:379:ILE:HG23	1.96	0.48
1:D:231:LEU:HD11	3:D:401:COA:C5A	2.44	0.48
1:D:144:ILE:HD13	1:D:148:LEU:HD12	1.96	0.47
1:A:88:LEU:HB2	1:A:379:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HB2	1:B:379:ILE:HG23	1.97	0.47
1:C:274:ARG:NH2	1:C:390:GLU:OE1	2.48	0.47
1:C:133:LYS:H	1:C:133:LYS:HD2	1.80	0.46
1:D:89:SCY:OCD	1:D:380:GLY:N	2.38	0.46
1:A:312:LEU:HD11	1:A:368:ARG:HD2	1.97	0.46
1:D:138:LYS:NZ	5:D:515:HOH:O	2.48	0.46
1:B:317:GLU:CD	1:B:342:GLY:HA3	2.36	0.46
1:D:5:ILE:HG13	1:D:100:MET:HG2	1.96	0.46
1:A:233:PRO:HA	1:A:242:THR:HG22	1.98	0.46
1:A:364:GLU:HA	1:A:367:ARG:HG2	1.97	0.46
1:D:88:LEU:HB2	1:D:379:ILE:HG23	1.98	0.45
1:B:313:VAL:HB	1:B:337:VAL:HG22	1.97	0.45
1:D:371:ARG:NH1	5:D:516:HOH:O	2.48	0.45
1:A:313:VAL:HB	1:A:337:VAL:HG22	1.99	0.45
1:A:364:GLU:O	1:A:368:ARG:HG2	2.16	0.45
1:C:233:PRO:HA	1:C:242:THR:HG22	1.98	0.45
1:B:7:ILE:HG23	1:B:256:ALA:HB1	1.98	0.45
1:B:48:GLU:OE1	1:B:267:ARG:NH2	2.38	0.45
1:A:207:ARG:HE	1:A:207:ARG:N	2.13	0.44
1:A:368:ARG:NH2	5:A:526:HOH:O	2.51	0.44
1:A:314:GLU:HG3	1:A:361:LEU:HB2	2.00	0.43
1:A:141:ASP:OD1	1:B:129:ARG:NH2	2.43	0.43
1:A:317:GLU:CD	1:A:342:GLY:HA3	2.39	0.43
1:B:247:SER:HB2	1:B:348:HIS:HB2	1.99	0.43
1:C:68:ARG:NH1	1:C:80:ALA:O	2.50	0.43
1:A:152:PHE:CZ	1:B:72:MET:HG3	2.53	0.43
1:A:68:ARG:NH1	1:A:80:ALA:O	2.48	0.43
1:B:163:ASN:O	1:B:167:GLN:HG3	2.19	0.42
1:C:156:HIS:HE1	3:C:401:COA:H71	1.84	0.42
1:A:72:MET:HG3	1:B:152:PHE:CZ	2.55	0.42
1:B:364:GLU:O	1:B:368:ARG:HG2	2.20	0.42
1:A:122:ALA:HB3	1:B:129:ARG:HH21	1.84	0.42
1:C:191:LYS:HB3	1:C:191:LYS:HE2	1.84	0.41
1:C:218:GLU:HB2	5:C:514:HOH:O	2.21	0.41
1:C:314:GLU:HG3	1:C:361:LEU:HB2	2.03	0.41
1:A:278:TRP:NE1	1:B:107:ASP:OD2	2.52	0.41
1:C:333:ASP:O	1:C:336:ILE:HG12	2.20	0.41
1:C:364:GLU:OE1	1:C:367:ARG:NH1	2.53	0.41
1:A:48:GLU:OE1	1:A:267:ARG:NH2	2.45	0.41
1:D:114:GLY:HA3	1:D:255:ALA:HA	2.02	0.41
1:D:319:PHE:O	1:D:322:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:GLU:HG3	1:D:361:LEU:HB2	2.02	0.40
1:D:379:ILE:HB	1:D:383:MET:HB2	2.03	0.40
1:B:233:PRO:HA	1:B:242:THR:HG22	2.03	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%)	378 (98%)	9 (2%)	0	100	100
1	B	387/399 (97%)	378 (98%)	9 (2%)	0	100	100
1	C	387/399 (97%)	377 (97%)	10 (3%)	0	100	100
1	D	381/399 (96%)	371 (97%)	10 (3%)	0	100	100
All	All	1542/1596 (97%)	1504 (98%)	38 (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	274/285 (96%)	266 (97%)	8 (3%)	42	68
1	B	273/285 (96%)	266 (97%)	7 (3%)	46	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	272/285 (95%)	267 (98%)	5 (2%)	59	80
1	D	258/285 (90%)	252 (98%)	6 (2%)	50	75
All	All	1077/1140 (94%)	1051 (98%)	26 (2%)	49	74

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	LYS
1	A	207	ARG
1	A	258	LEU
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	332	TRP
1	A	348	HIS
1	B	207	ARG
1	B	288	MET
1	B	322	GLN
1	B	332	TRP
1	B	348	HIS
1	B	350	ILE
1	B	358	LEU
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	192	ASP
1	D	219	ILE
1	D	220	ARG
1	D	276	VAL
1	D	332	TRP

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	D	89	1	7,8,9	0.92	0	3,9,11	0.86	0
1	SCY	C	89	1	7,8,9	0.88	0	3,9,11	0.78	0
1	SCY	B	89	1	7,8,9	0.91	0	3,9,11	0.82	0
1	SCY	A	89	1	7,8,9	0.89	0	3,9,11	0.79	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	D	89	1	-	0/5/7/9	-
1	SCY	C	89	1	-	0/5/7/9	-
1	SCY	B	89	1	-	0/5/7/9	-
1	SCY	A	89	1	-	0/5/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	B	401	-	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	0.06	0
2	SO4	C	402	-	4,4,4	0.13	0	6,6,6	0.07	0
3	COA	D	401	-	41,50,50	1.22	5 (12%)	52,75,75	1.48	9 (17%)
2	SO4	A	401	-	4,4,4	0.14	0	6,6,6	0.06	0
3	COA	C	401	-	41,50,50	1.22	5 (12%)	52,75,75	1.47	7 (13%)
3	COA	B	402	-	41,50,50	1.22	5 (12%)	52,75,75	1.44	8 (15%)
3	COA	A	403	-	41,50,50	1.21	4 (9%)	52,75,75	1.44	9 (17%)

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	B	402	-	-	1/44/64/64	0/3/3/3
3	COA	D	401	-	-	19/44/64/64	0/3/3/3
3	COA	A	403	-	-	9/44/64/64	0/3/3/3
3	COA	C	401	-	-	7/44/64/64	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	COA	O4B-C1B	3.95	1.46	1.41
3	A	403	COA	O4B-C1B	3.89	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	COA	O4B-C1B	3.69	1.46	1.41
3	B	402	COA	O4B-C1B	3.62	1.46	1.41
3	C	401	COA	C8A-N7A	-3.07	1.29	1.34
3	B	402	COA	C8A-N7A	-3.02	1.29	1.34
3	A	403	COA	C8A-N7A	-3.01	1.29	1.34
3	D	401	COA	C8A-N7A	-2.87	1.29	1.34
3	B	402	COA	C2B-C1B	2.24	1.57	1.53
3	D	401	COA	C4A-N3A	-2.13	1.32	1.35
3	D	401	COA	P3B-O8A	2.11	1.63	1.54
3	C	401	COA	P3B-O8A	2.10	1.63	1.54
3	B	402	COA	P3B-O8A	2.09	1.62	1.54
3	C	401	COA	C2B-C1B	2.08	1.56	1.53
3	B	402	COA	P3B-O9A	2.04	1.62	1.54
3	A	403	COA	P3B-O8A	2.03	1.62	1.54
3	A	403	COA	P3B-O9A	2.02	1.62	1.54
3	D	401	COA	C2B-C1B	2.01	1.56	1.53
3	C	401	COA	P3B-O9A	2.00	1.62	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	COA	P2A-O3A-P1A	-5.67	113.38	132.83
3	C	401	COA	P2A-O3A-P1A	-5.56	113.75	132.83
3	B	402	COA	P2A-O3A-P1A	-5.39	114.34	132.83
3	A	403	COA	P2A-O3A-P1A	-5.38	114.36	132.83
3	D	401	COA	N3A-C2A-N1A	-3.69	122.91	128.68
3	A	403	COA	N3A-C2A-N1A	-3.59	123.06	128.68
3	C	401	COA	N3A-C2A-N1A	-3.58	123.08	128.68
3	B	402	COA	N3A-C2A-N1A	-3.57	123.10	128.68
3	B	402	COA	O4B-C1B-C2B	-2.70	102.98	106.93
3	A	403	COA	CAP-C9P-N8P	2.61	121.77	116.58
3	D	401	COA	O4B-C1B-C2B	-2.60	103.13	106.93
3	D	401	COA	N6A-C6A-N1A	2.57	123.91	118.57
3	B	402	COA	CAP-C9P-N8P	2.54	121.64	116.58
3	C	401	COA	N6A-C6A-N1A	2.53	123.83	118.57
3	B	402	COA	N6A-C6A-N1A	2.49	123.74	118.57
3	A	403	COA	P1A-O5B-C5B	-2.46	107.27	121.68
3	A	403	COA	N6A-C6A-N1A	2.37	123.50	118.57
3	C	401	COA	CAP-C9P-N8P	2.32	121.21	116.58
3	A	403	COA	C6P-C5P-N4P	2.27	120.24	116.42
3	D	401	COA	C6P-C5P-N4P	2.25	120.21	116.42
3	D	401	COA	CAP-C9P-N8P	2.22	121.00	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	COA	O4B-C1B-C2B	-2.22	103.68	106.93
3	B	402	COA	P2A-O6A-CCP	-2.21	108.84	121.56
3	C	401	COA	C6P-C5P-N4P	2.19	120.11	116.42
3	D	401	COA	C1B-N9A-C4A	2.18	130.47	126.64
3	C	401	COA	P2A-O6A-CCP	-2.15	109.19	121.56
3	D	401	COA	P1A-O5B-C5B	-2.11	109.31	121.68
3	C	401	COA	P1A-O5B-C5B	-2.07	109.56	121.68
3	B	402	COA	P1A-O5B-C5B	-2.06	109.58	121.68
3	A	403	COA	O9P-C9P-N8P	-2.06	118.57	122.99
3	A	403	COA	P2A-O6A-CCP	-2.06	109.69	121.56
3	B	402	COA	O9P-C9P-N8P	-2.06	118.58	122.99
3	D	401	COA	P2A-O6A-CCP	-2.03	109.88	121.56

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	COA	O4B-C4B-C5B-O5B
3	A	403	COA	CCP-O6A-P2A-O3A
3	A	403	COA	CCP-O6A-P2A-O4A
3	C	401	COA	CCP-O6A-P2A-O3A
3	C	401	COA	CDP-CBP-CCP-O6A
3	C	401	COA	CEP-CBP-CCP-O6A
3	C	401	COA	CAP-CBP-CCP-O6A
3	D	401	COA	C3B-C4B-C5B-O5B
3	D	401	COA	O4B-C4B-C5B-O5B
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	D	401	COA	C2B-C3B-O3B-P3B
3	D	401	COA	C4B-C3B-O3B-P3B
3	D	401	COA	CDP-CBP-CCP-O6A
3	D	401	COA	CEP-CBP-CCP-O6A
3	D	401	COA	C4B-C5B-O5B-P1A
3	A	403	COA	CCP-O6A-P2A-O5A
3	C	401	COA	CCP-O6A-P2A-O5A
3	A	403	COA	CDP-CBP-CCP-O6A

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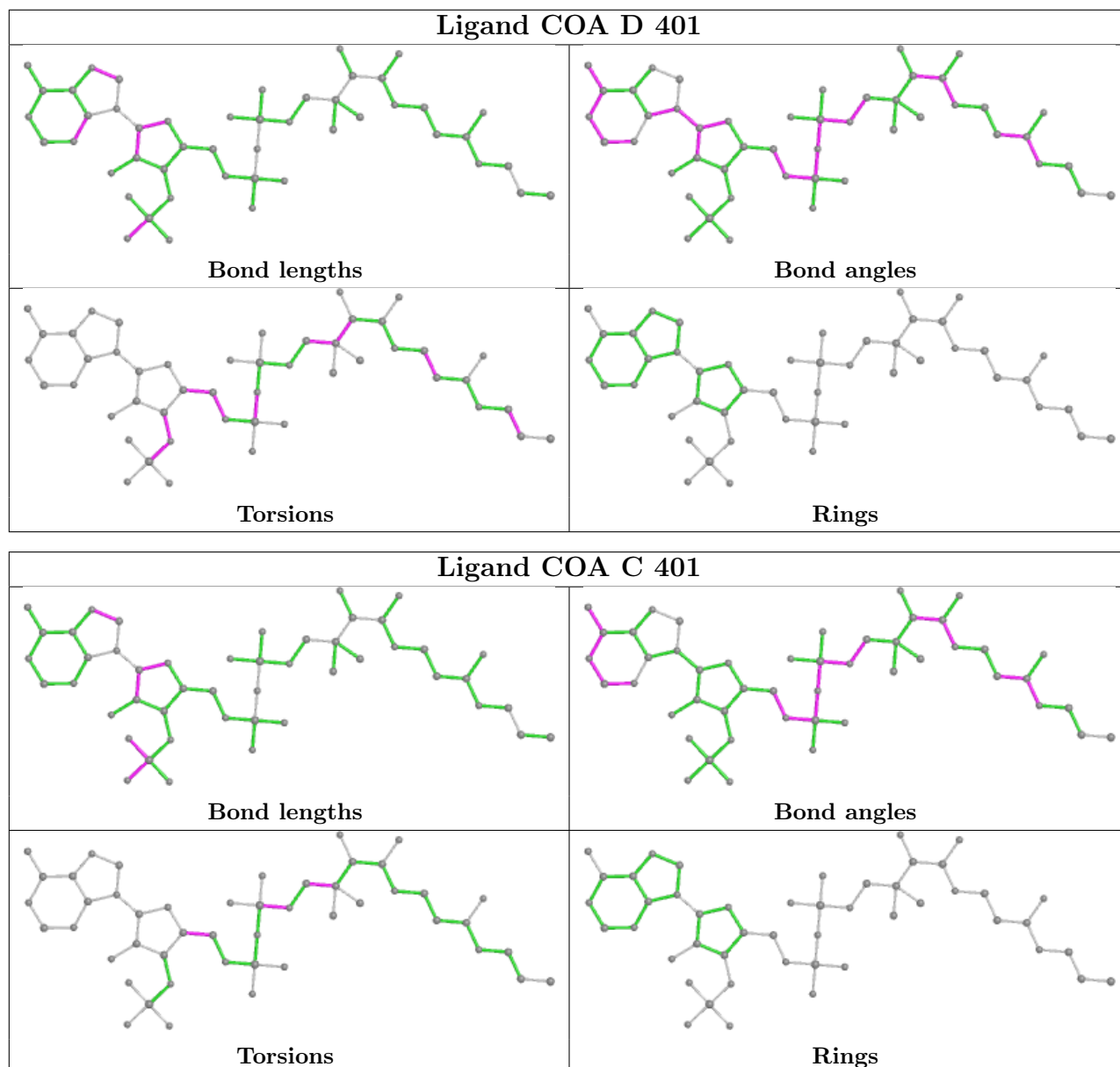
Mol	Chain	Res	Type	Atoms
3	A	403	COA	CEP-CBP-CCP-O6A
3	D	401	COA	C5P-C6P-C7P-N8P
3	A	403	COA	C3B-O3B-P3B-O7A
3	D	401	COA	C3B-O3B-P3B-O7A
3	A	403	COA	C3B-C4B-C5B-O5B
3	A	403	COA	C3B-O3B-P3B-O8A
3	D	401	COA	C3B-O3B-P3B-O8A
3	C	401	COA	O4B-C4B-C5B-O5B
3	D	401	COA	P2A-O3A-P1A-O2A
3	B	402	COA	CCP-O6A-P2A-O4A
3	C	401	COA	CCP-O6A-P2A-O4A

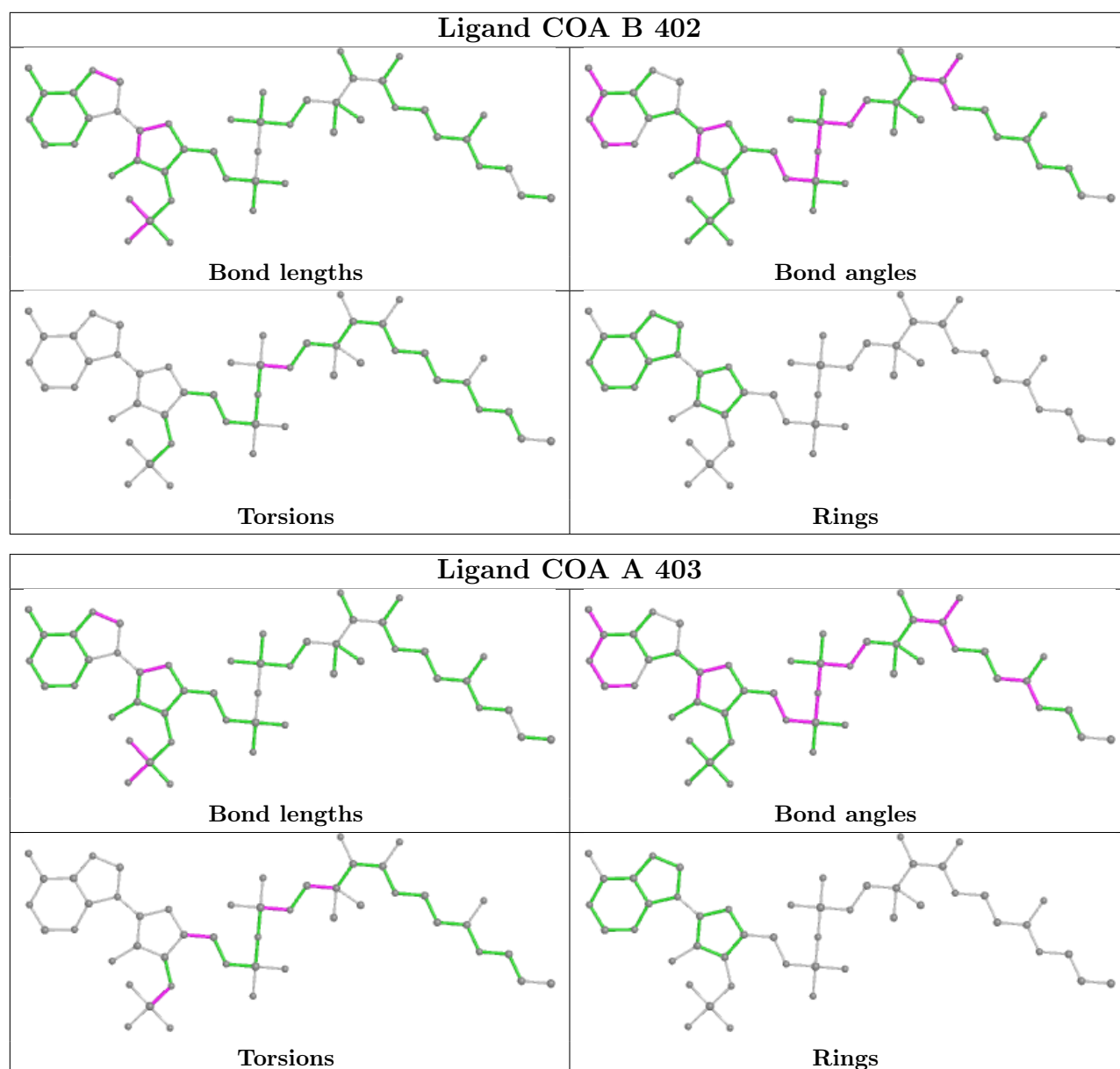
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	COA	1	0
3	C	401	COA	1	0
3	A	403	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%)	-0.19	12 (3%) 49 42	15, 26, 56, 78	0
1	B	389/399 (97%)	-0.20	9 (2%) 60 54	15, 26, 51, 82	0
1	C	389/399 (97%)	0.07	20 (5%) 28 22	26, 39, 67, 89	0
1	D	385/399 (96%)	0.69	57 (14%) 2 1	26, 49, 94, 119	0
All	All	1552/1596 (97%)	0.09	98 (6%) 20 15	15, 35, 71, 119	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	239	GLY	8.3
1	D	241	VAL	7.9
1	D	234	ALA	7.2
1	D	233	PRO	7.1
1	D	238	GLU	6.5
1	D	223	ALA	5.4
1	D	244	GLY	5.3
1	D	236	ASP	5.1
1	D	231	LEU	5.1
1	C	236	ASP	5.0
1	C	207	ARG	4.8
1	A	236	ASP	4.7
1	D	170	LEU	4.6
1	B	207	ARG	4.6
1	D	163	ASN	4.5
1	B	226	ASP	4.5
1	D	247	SER	4.4
1	D	392	LEU	4.1
1	D	207	ARG	4.1
1	D	242	THR	4.1
1	C	221	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	236	ASP	3.9
1	D	224	THR	3.7
1	C	222	GLY	3.7
1	D	232	ARG	3.7
1	D	206	GLY	3.7
1	D	237	LYS	3.7
1	D	240	THR	3.7
1	D	246	ALA	3.5
1	D	165	ALA	3.5
1	D	243	ALA	3.5
1	D	175	GLN	3.5
1	A	207	ARG	3.5
1	D	245	ASN	3.4
1	D	168	TRP	3.4
1	D	235	PHE	3.4
1	D	167	GLN	3.4
1	A	222	GLY	3.4
1	C	208	LYS	3.3
1	D	155	TYR	3.2
1	D	222	GLY	3.2
1	D	221	HIS	3.2
1	A	209	GLY	3.2
1	A	238	GLU	3.1
1	C	232	ARG	3.1
1	D	210	ASP	3.1
1	A	237	LYS	3.1
1	D	171	SER	3.0
1	D	169	GLN	3.0
1	D	208	LYS	3.0
1	C	206	GLY	3.0
1	D	230	LYS	3.0
1	D	3	PRO	3.0
1	D	330	LEU	2.9
1	B	222	GLY	2.9
1	B	169	GLN	2.9
1	A	210	ASP	2.9
1	A	226	ASP	2.9
1	D	173	ASP	2.9
1	D	331	GLY	2.9
1	B	208	LYS	2.9
1	D	151	ALA	2.9
1	C	205	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	220	ARG	2.8
1	D	153	TYR	2.8
1	A	208	LYS	2.6
1	C	210	ASP	2.6
1	C	229	ALA	2.5
1	B	221	HIS	2.5
1	D	286	LYS	2.5
1	C	224	THR	2.5
1	C	214	ASP	2.5
1	C	227	SER	2.5
1	D	209	GLY	2.5
1	B	237	LYS	2.5
1	C	233	PRO	2.4
1	A	223	ALA	2.4
1	A	240	THR	2.3
1	D	152	PHE	2.3
1	D	367	ARG	2.3
1	C	209	GLY	2.3
1	C	371	ARG	2.3
1	D	176	ASP	2.3
1	A	206	GLY	2.3
1	D	332	TRP	2.2
1	D	159	THR	2.2
1	C	3	PRO	2.2
1	D	212	THR	2.2
1	C	203	ILE	2.2
1	B	205	LYS	2.2
1	D	351	GLY	2.2
1	D	211	ILE	2.2
1	D	164	VAL	2.1
1	D	333	ASP	2.1
1	D	368	ARG	2.1
1	D	371	ARG	2.1
1	C	108	ALA	2.0
1	C	228	MET	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(Å ²)	Q<0.9
1	SCY	C	89	9/10	0.94	0.20	38,40,49,55	0
1	SCY	D	89	9/10	0.94	0.28	41,47,61,63	0
1	SCY	A	89	9/10	0.95	0.21	20,20,38,38	0
1	SCY	B	89	9/10	0.97	0.13	17,23,36,36	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

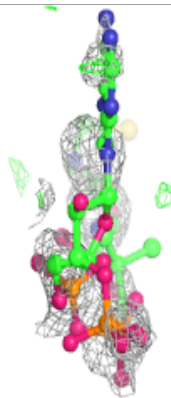
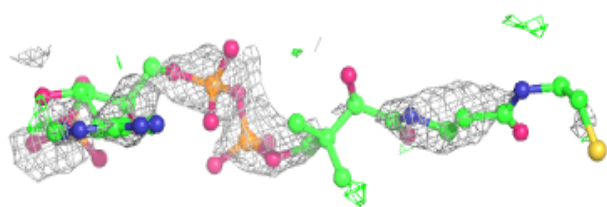
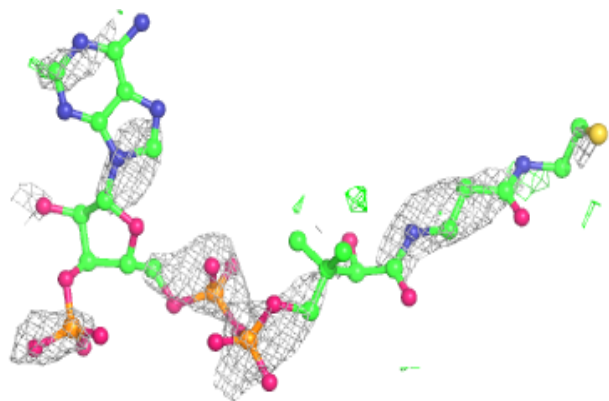
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	COA	D	401	48/48	0.59	0.46	72,106,112,113	48
3	COA	C	401	48/48	0.74	0.31	51,70,90,93	48
3	COA	B	402	48/48	0.77	0.25	25,52,83,84	48
4	RB	D	402	1/1	0.78	0.10	122,122,122,122	0
3	COA	A	403	48/48	0.81	0.26	34,44,65,66	48
2	SO4	C	402	5/5	0.84	0.23	106,106,107,108	0
2	SO4	A	401	5/5	0.89	0.47	86,86,87,88	0
2	SO4	A	402	5/5	0.91	0.26	102,102,103,104	0
2	SO4	B	401	5/5	0.94	0.21	76,79,80,81	0
4	RB	C	403	1/1	0.97	0.09	52,52,52,52	1
4	RB	B	403	1/1	0.98	0.07	36,36,36,36	1
4	RB	A	404	1/1	0.99	0.04	43,43,43,43	1

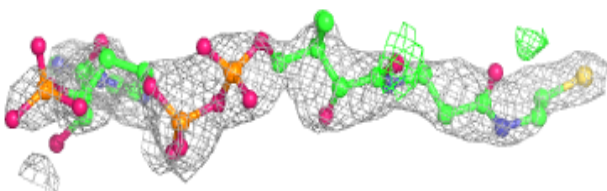
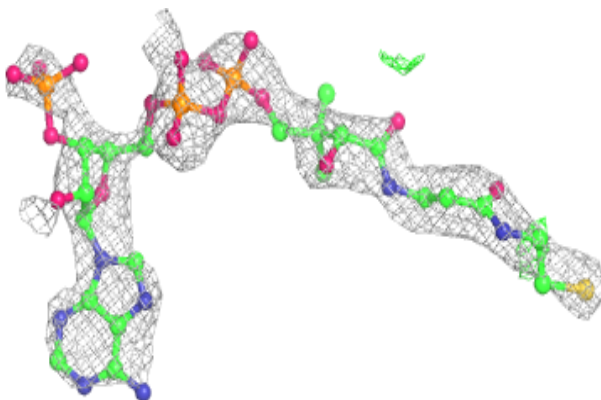
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

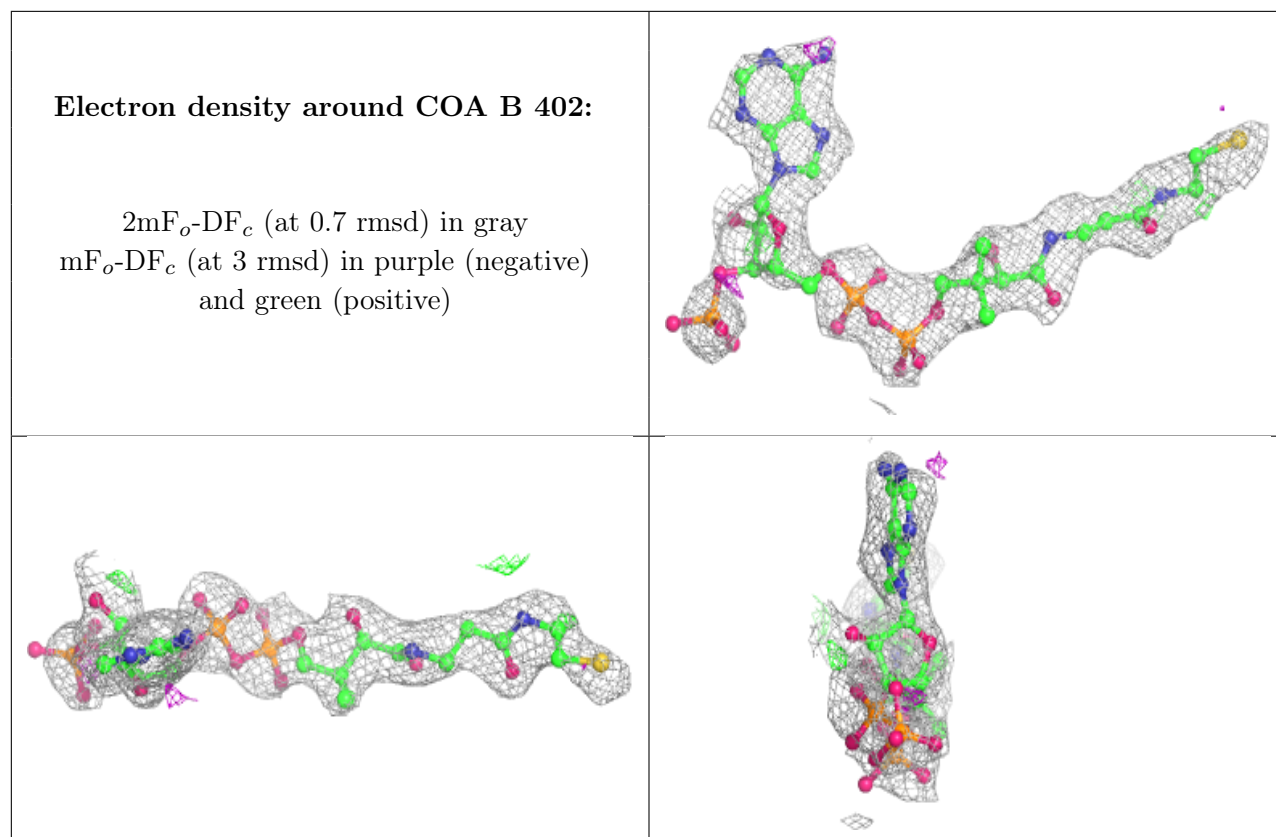
Electron density around COA D 401:

$2mF_o-DF_c$ (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:**

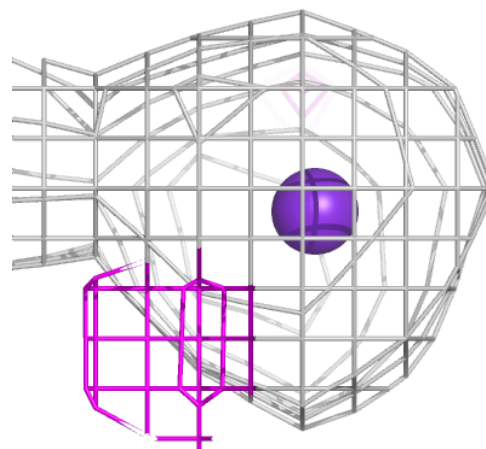
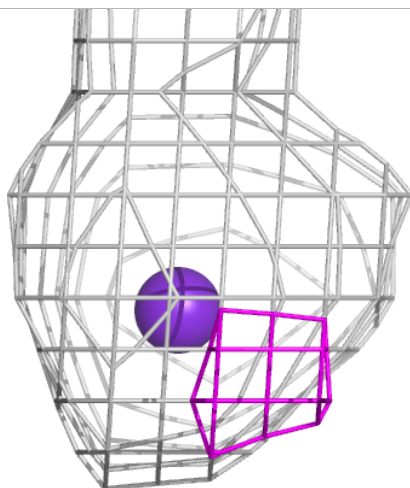
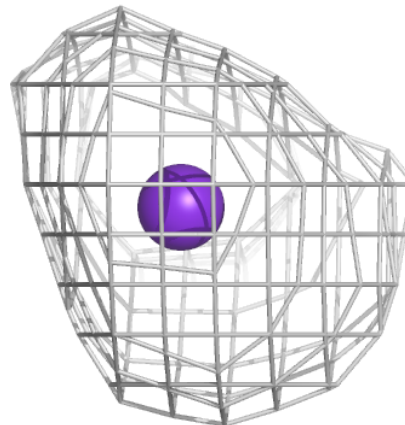
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

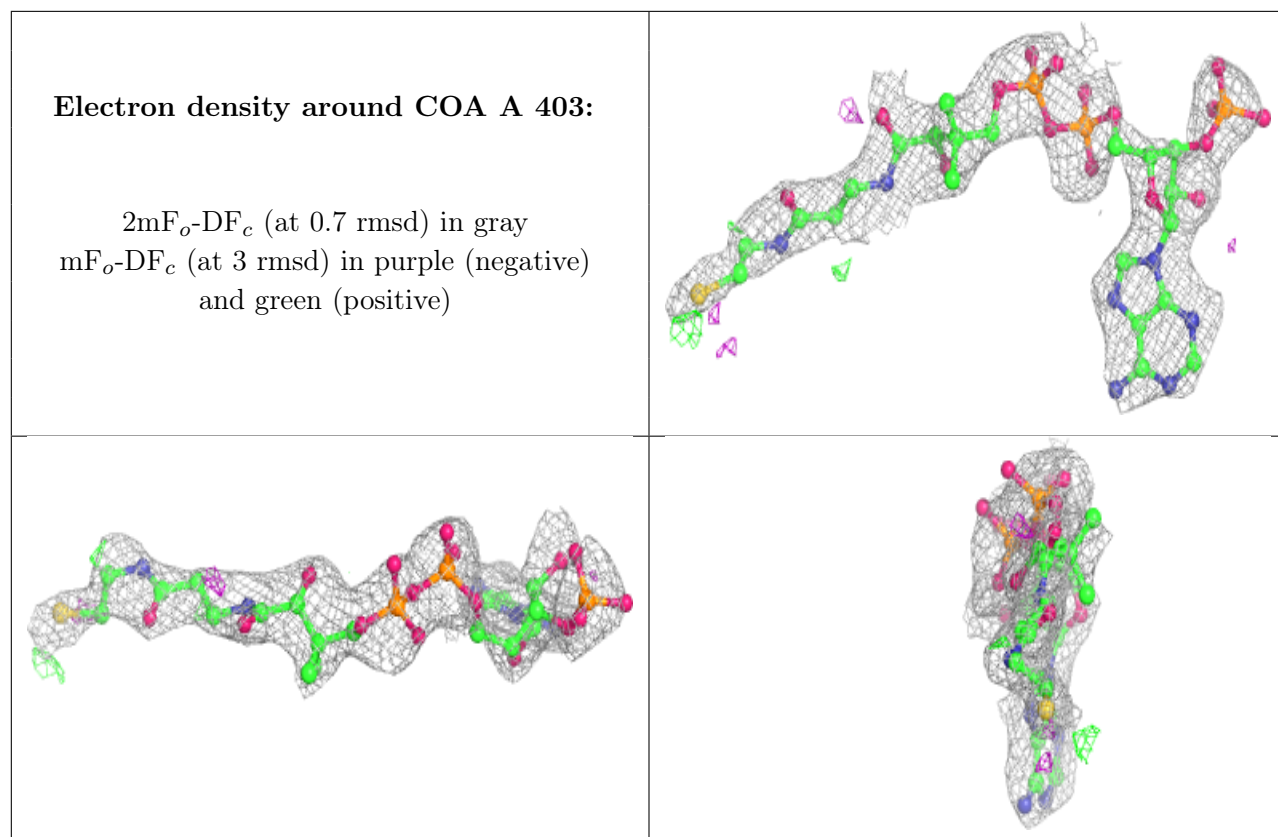




Electron density around RB D 402:

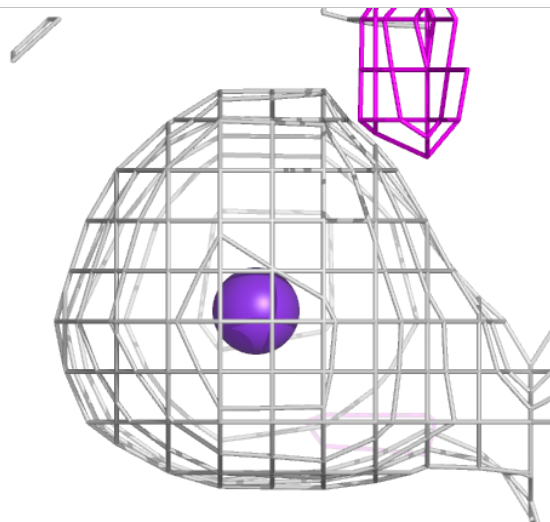
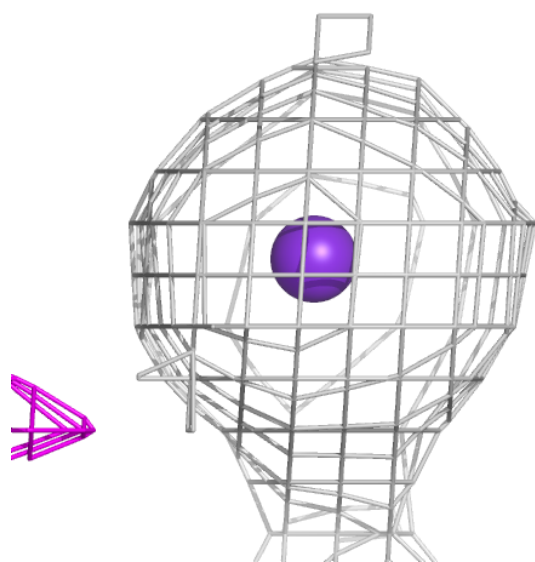
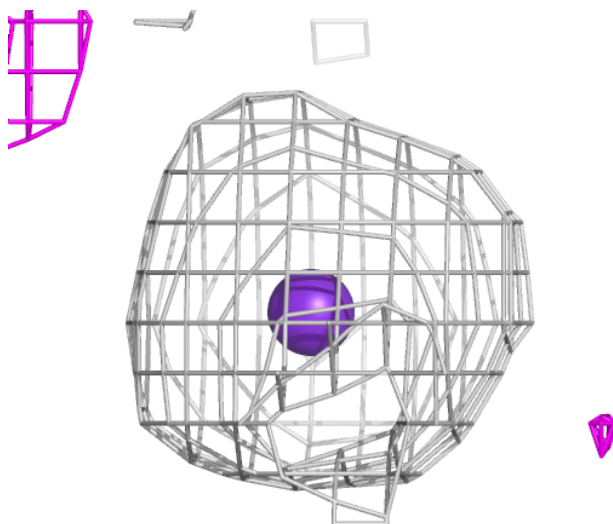
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





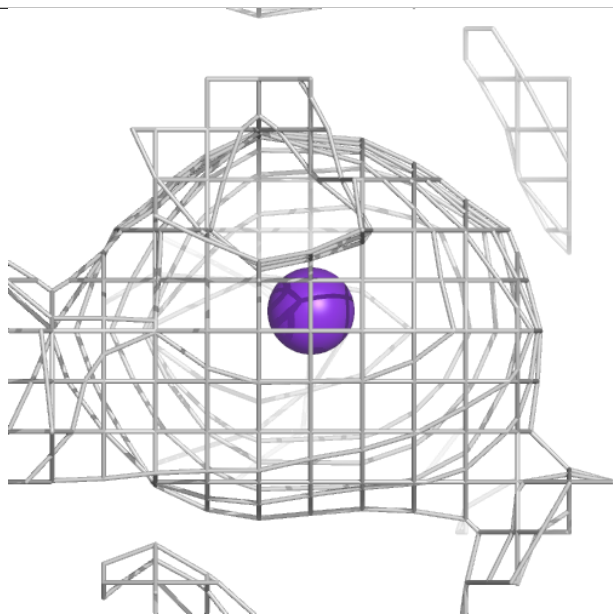
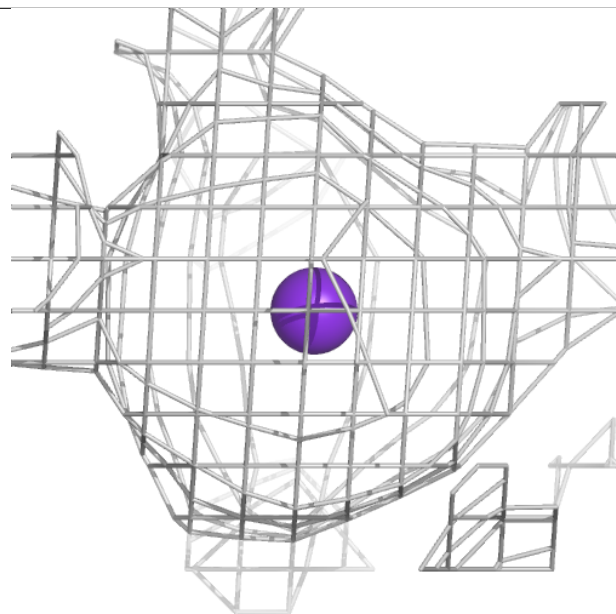
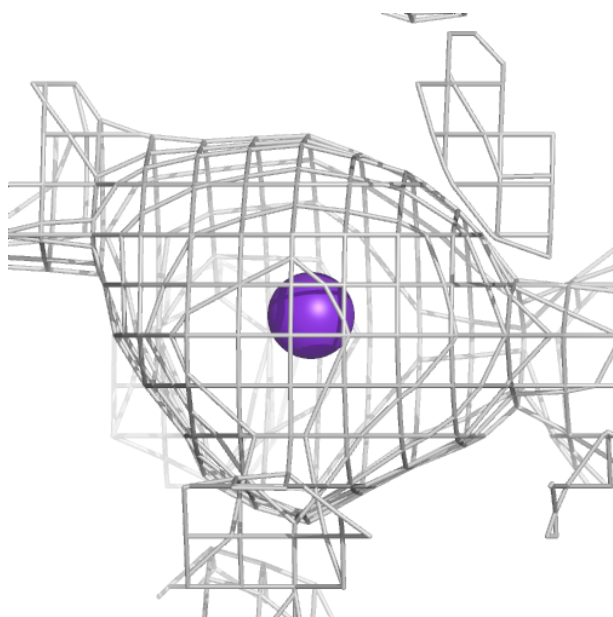
Electron density around RB C 403:

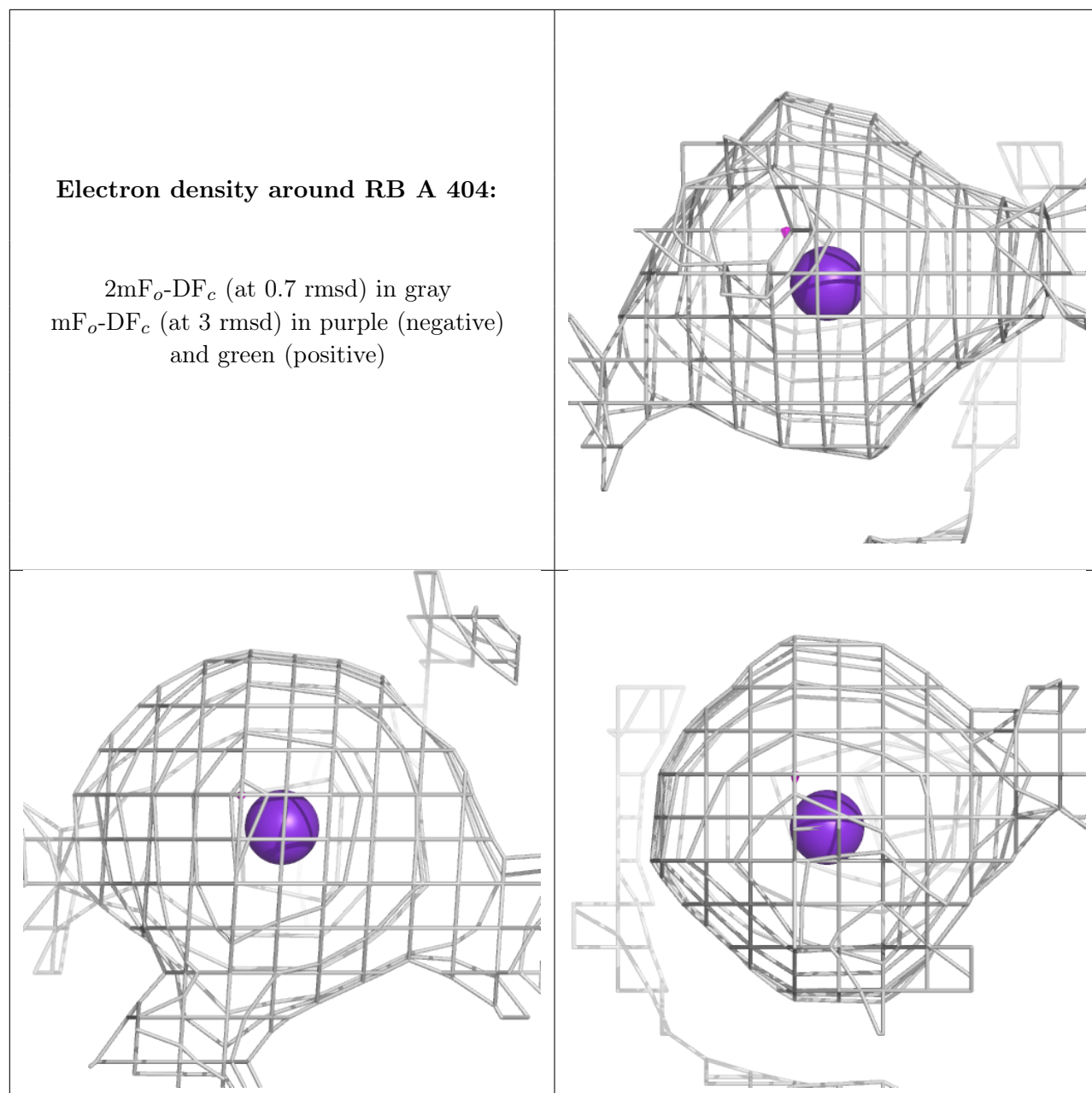
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around RB 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.