W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 07:26 PM EDT

PDB ID	:	4PSX
Title	:	Crystal structure of histone acetyltransferase complex
Authors	:	Yang, M.; Li, Y.
Deposited on	:	2014-03-08
Resolution	:	2.51 Å(reported)

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

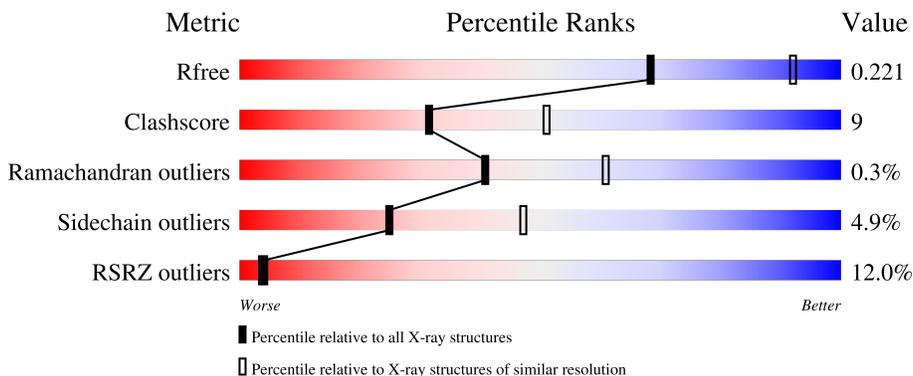|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.51 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	Percentile Ranks	Value
Rfree		0.221
Clashscore		9
Ramachandran outliers		0.3%
Sidechain outliers		4.9%
RSRZ outliers		12.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	320	12% / 78% / 18% / · ·
1	D	320	8% / 78% / 17% / · ·
2	B	401	9% / 72% / 17% / · / 10%
2	E	401	9% / 72% / 17% / · / 10%
3	C	48	29% / 50% / 31% / 19%

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Mol	Chain	Length	Quality of chain
3	F	48	21% 52% 21% • 23%
4	P	15	40% 53% 7% 7% 33%
4	Y	15	53% 53% 20% 7% 20%

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
5	COA	A	401	-	-	-	X
5	COA	D	401	-	-	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 12392 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 Histone acetyltransferase type B catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2603	1679	426	494	4			
1	D	313	Total	C	N	O	S	0	0	0
			2603	1679	426	494	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q12341
A	2	SER	-	expression tag	UNP Q12341
A	3	ALA	-	expression tag	UNP Q12341
A	4	ASN	-	expression tag	UNP Q12341
A	5	ASP	-	expression tag	UNP Q12341
A	6	PHE	-	expression tag	UNP Q12341
A	320	SER	-	expression tag	UNP Q12341
D	1	MET	-	expression tag	UNP Q12341
D	2	SER	-	expression tag	UNP Q12341
D	3	ALA	-	expression tag	UNP Q12341
D	4	ASN	-	expression tag	UNP Q12341
D	5	ASP	-	expression tag	UNP Q12341
D	6	PHE	-	expression tag	UNP Q12341
D	320	SER	-	expression tag	UNP Q12341

- Molecule 2 is a protein called Histone acetyltransferase type B subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	361	Total	C	N	O	S	0	0	0
			2868	1808	484	566	10			
2	E	361	Total	C	N	O	S	0	0	0
			2868	1808	484	566	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP P39984
B	2	GLU	-	expression tag	UNP P39984
B	3	ASN	-	expression tag	UNP P39984
B	4	GLN	-	expression tag	UNP P39984
B	5	GLU	-	expression tag	UNP P39984
B	6	LYS	-	expression tag	UNP P39984
B	7	PRO	-	expression tag	UNP P39984
B	143	THR	VAL	engineered mutation	UNP P39984
B	390	GLY	-	expression tag	UNP P39984
B	391	GLY	-	expression tag	UNP P39984
B	392	PRO	-	expression tag	UNP P39984
B	393	PRO	-	expression tag	UNP P39984
B	394	LYS	-	expression tag	UNP P39984
B	395	VAL	-	expression tag	UNP P39984
B	396	ASN	-	expression tag	UNP P39984
B	397	LYS	-	expression tag	UNP P39984
B	398	ASP	-	expression tag	UNP P39984
B	399	ILE	-	expression tag	UNP P39984
B	400	ILE	-	expression tag	UNP P39984
B	401	SER	-	expression tag	UNP P39984
E	1	MET	-	expression tag	UNP P39984
E	2	GLU	-	expression tag	UNP P39984
E	3	ASN	-	expression tag	UNP P39984
E	4	GLN	-	expression tag	UNP P39984
E	5	GLU	-	expression tag	UNP P39984
E	6	LYS	-	expression tag	UNP P39984
E	7	PRO	-	expression tag	UNP P39984
E	143	THR	VAL	engineered mutation	UNP P39984
E	390	GLY	-	expression tag	UNP P39984
E	391	GLY	-	expression tag	UNP P39984
E	392	PRO	-	expression tag	UNP P39984
E	393	PRO	-	expression tag	UNP P39984
E	394	LYS	-	expression tag	UNP P39984
E	395	VAL	-	expression tag	UNP P39984
E	396	ASN	-	expression tag	UNP P39984
E	397	LYS	-	expression tag	UNP P39984
E	398	ASP	-	expression tag	UNP P39984
E	399	ILE	-	expression tag	UNP P39984
E	400	ILE	-	expression tag	UNP P39984
E	401	SER	-	expression tag	UNP P39984

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	39	Total 294	C 180	N 70	O 44	0	0	0
3	F	37	Total 280	C 171	N 67	O 42	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
C	21	VAL	ILE	engineered mutation	UNP P02309
F	21	VAL	ILE	engineered mutation	UNP P02309

- Molecule 4 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Y	12	Total 90	C 52	N 21	O 17	0	0	0
4	P	10	Total 79	C 46	N 19	O 14	0	0	0

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).
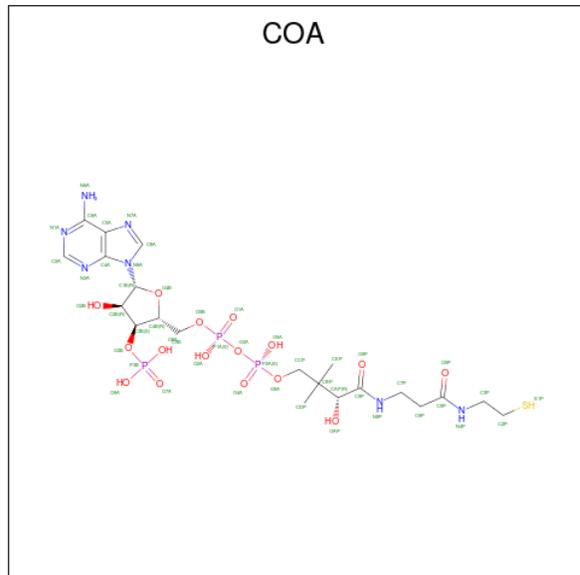
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
5	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

• Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
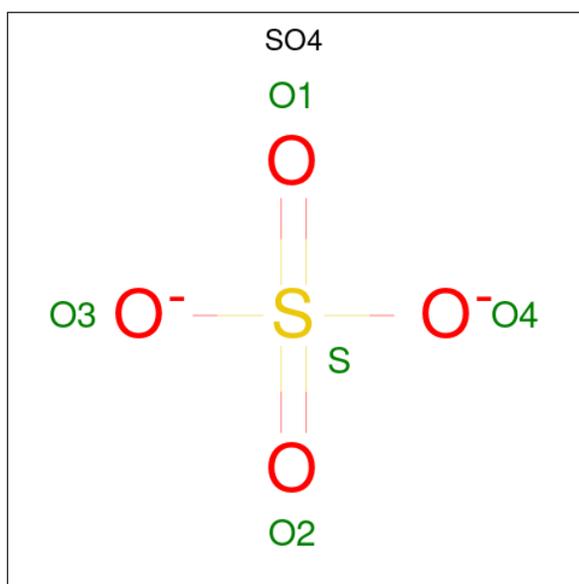
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 5	O 4	S 1	0	0

• Molecule 7 is water.

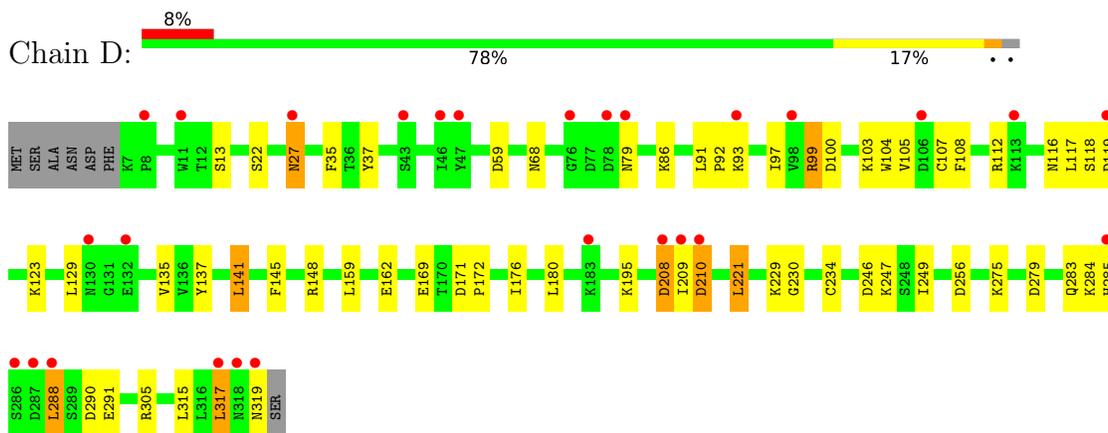| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	125	Total 125	O 125	0	0
7	B	153	Total 153	O 153	0	0
7	C	19	Total 19	O 19	0	0
7	D	122	Total 122	O 122	0	0
7	E	167	Total 167	O 167	0	0
7	F	18	Total 18	O 18	0	0
7	Y	1	Total 1	O 1	0	0
7	P	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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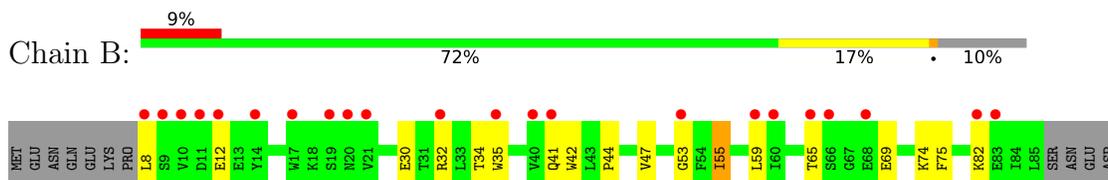
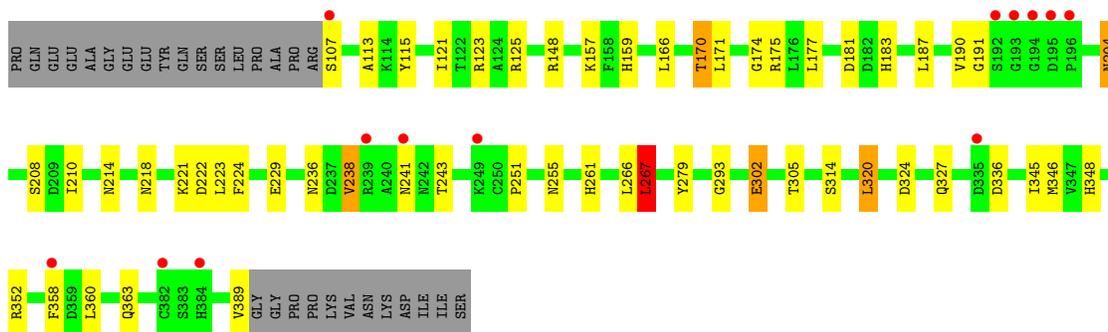• Molecule 1: Histone acetyltransferase type B catalytic subunit
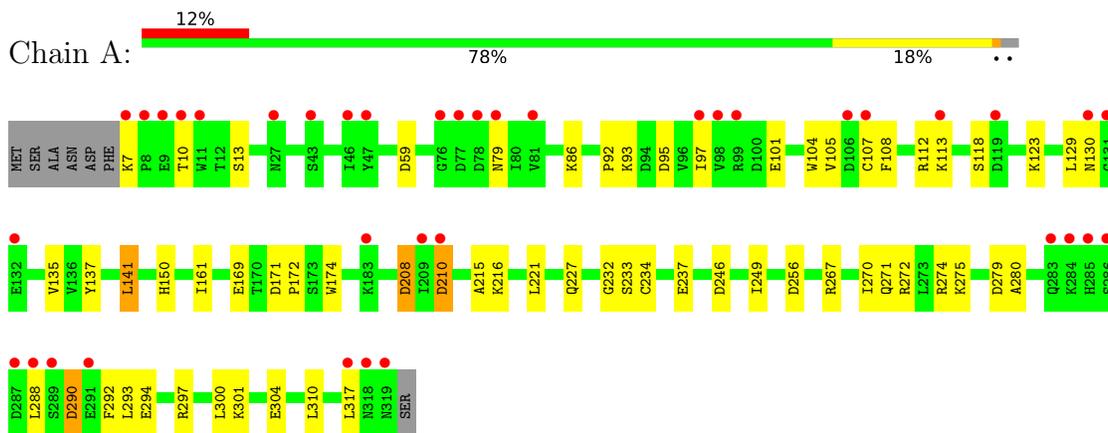
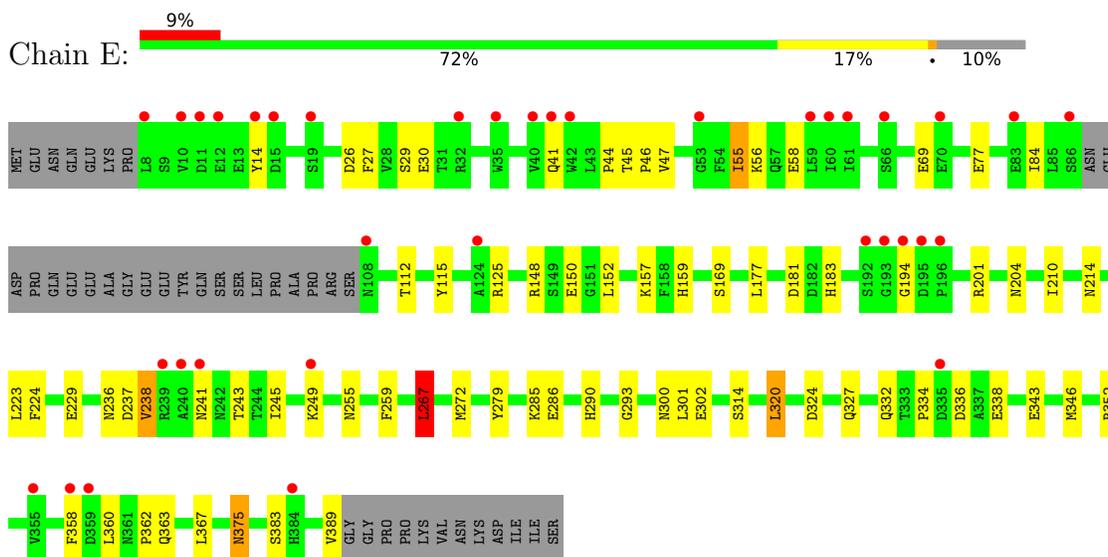• Molecule 1: Histone acetyltransferase type B catalytic subunit

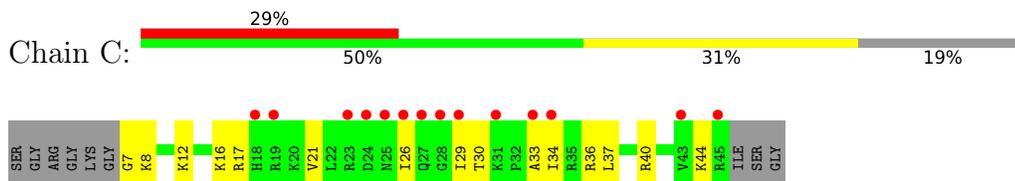• Molecule 2: Histone acetyltransferase type B subunit 2

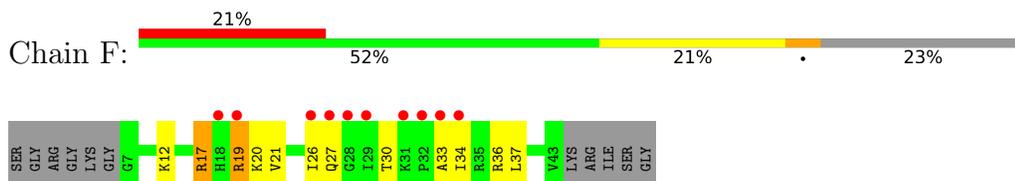PRO GLN GLU GLU ALA GLY GLU GLU TYR GLN SER SER LEU PRO ALA PRO ARG S107 A113 K114 Y115 I121 T122 R123 A124 R125 R148 K157 F158 H159 L166 T170 L171 G174 R175 L176 L177 D181 D182 H183 L187 V190 G191 S192 G193 G194 D195 P196 N204

S208 D209 I210 N214 N218 K221 D222 L223 F224 E229 N236 D237 V238 R239 A240 N241 N242 T243 K249 C250 P251 N255 H261 L266 L267 Y279 G293 E302 T305 S314 L320 D324 Q327 D335 D336 I345 M346 V347 H348

R352 F358 D359 L360 Q363 C382 S383 H384 V389 GLY GLY PRO PRO LYS VAL ASN LYS ASP ILE ILE SER

• Molecule 2: Histone acetyltransferase type B subunit 2

Chain E:

9%
72%   17%   •   10%

MET GLU ASN GLN GLU LYS PRO L8 S9 V10 D11 E12 E13 Y14 D15 S19 D26 F27 V28 S29 E30 T31 R32 W35 V40 Q41 W42 L43 P44 T45 P46 V47 G53 F54 I55 K56 Q57 E58 L59 I60 I61 S66 E69 E70 E77 E83 I84 L85 S86 ASN GLU

ASP PRO GLN GLU GLU ALA GLY GLU GLU TYR GLN SER SER LEU PRO ALA PRO ARG SER N108 T112 Y115 A124 R125 R148 S149 E150 G151 L152 K157 F158 H159 S169 L177 D181 D182 H183 S192 G193 G194 D195 P196 R201 N204 I210 N214

L223 F224 E229 N236 D237 V238 R239 A240 N241 N242 T243 T244 I245 K249 N255 F259 L267 M272 Y279 K285 E286 H290 G293 N300 L301 E302 S314 L320 D324 Q327 Q332 T333 P334 D335 D336 A337 E338 E343 M346 R352

V355 F358 D359 L360 N361 P362 Q363 L367 N375 S383 H384 V389 GLY GLY PRO PRO LYS VAL ASN LYS ASP ILE ILE SER

• Molecule 3: Histone H4

Chain C:

29%
50%   31%   19%

SER GLY ARG GLY LYS GLY G7 K8 K12 K16 R17 H18 R19 K20 V21 L22 R23 D24 N25 I26 Q27 G28 I29 T30 K31 P32 A33 I34 R35 L37 R40 V43 K44 R45 ILE SER GLY

• Molecule 3: Histone H4

Chain F:

21%
52%   21%   •   23%

SER GLY ARG GLY LYS GLY G7 K12 R17 H18 R19 K20 V21 I26 Q27 G28 I29 T30 K31 P32 A33 I34 R35 R36 L37 V43 LYS ARG ILE SER GLY

• Molecule 4: Histone H3

Chain Y:

53%
53%   20%   7%   20%

A1 R2 Q5 T6 A7 R8 K9 S10 T11 G12 GLY LYS ALA

• Molecule 4: Histone H3

Chain P:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.55Å 85.33Å 114.51Å 75.97° 72.40° 66.06°	Depositor
Resolution (Å)	38.60 – 2.51 38.62 – 2.51	Depositor EDS
% Data completeness (in resolution range)	75.7 (38.60-2.51) 75.7 (38.62-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.181 , 0.223 0.181 , 0.221	Depositor DCC
R_{free} test set	3338 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 62.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12392	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.47	0/2665	0.59	0/3602
1	D	0.48	0/2665	0.58	0/3602
2	B	0.47	0/2938	0.64	1/4001 (0.0%)
2	E	0.46	0/2938	0.62	1/4001 (0.0%)
3	C	0.42	0/295	0.62	0/386
3	F	0.46	0/281	0.71	0/368
4	P	0.35	0/78	0.60	0/101
4	Y	0.35	0/89	0.57	0/116
All	All	0.47	0/11949	0.61	2/16177 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	267	LEU	CA-CB-CG	6.88	131.12	115.30
2	B	267	LEU	CA-CB-CG	6.66	130.61	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2603	0	2550	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2603	0	2550	47	0
2	B	2868	0	2744	51	0
2	E	2868	0	2744	48	0
3	C	294	0	332	9	0
3	F	280	0	317	10	0
4	P	79	0	91	3	0
4	Y	90	0	101	5	0
5	A	48	0	32	5	0
5	D	48	0	32	8	0
6	B	5	0	0	0	0
7	A	125	0	0	11	0
7	B	153	0	0	18	0
7	C	19	0	0	3	0
7	D	122	0	0	18	0
7	E	167	0	0	16	0
7	F	18	0	0	4	0
7	P	1	0	0	0	0
7	Y	1	0	0	0	0
All	All	12392	0	11493	210	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 9.

The worst 5 of 210 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:107:CYS:SG	7:A:592:HOH:O	2.25	0.94
3:F:17:ARG:HG3	7:F:103:HOH:O	1.71	0.89
1:A:150:HIS:ND1	7:A:532:HOH:O	2.07	0.88
2:E:194:GLY:O	7:E:620:HOH:O	1.95	0.83
1:A:232:GLY:HA3	5:A:401:COA:H132	1.62	0.82

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	311/320 (97%)	300 (96%)	11 (4%)	0	100	100
1	D	311/320 (97%)	305 (98%)	5 (2%)	1 (0%)	41	61
2	B	357/401 (89%)	340 (95%)	16 (4%)	1 (0%)	41	61
2	E	357/401 (89%)	342 (96%)	14 (4%)	1 (0%)	41	61
3	C	37/48 (77%)	34 (92%)	3 (8%)	0	100	100
3	F	35/48 (73%)	33 (94%)	2 (6%)	0	100	100
4	P	8/15 (53%)	8 (100%)	0	0	100	100
4	Y	10/15 (67%)	9 (90%)	0	1 (10%)	0	0
All	All	1426/1568 (91%)	1371 (96%)	51 (4%)	4 (0%)	41	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	99	ARG
4	Y	11	THR
2	B	293	GLY
2	E	293	GLY

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	288/294 (98%)	277 (96%)	11 (4%)	33	58
1	D	288/294 (98%)	276 (96%)	12 (4%)	30	54
2	B	323/358 (90%)	307 (95%)	16 (5%)	24	46
2	E	323/358 (90%)	310 (96%)	13 (4%)	31	56
3	C	27/33 (82%)	23 (85%)	4 (15%)	3	5
3	F	26/33 (79%)	21 (81%)	5 (19%)	1	2
4	P	8/10 (80%)	7 (88%)	1 (12%)	4	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Y	9/10 (90%)	8 (89%)	1 (11%)	6	11
All	All	1292/1390 (93%)	1229 (95%)	63 (5%)	25	47

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	21	VAL
2	E	389	VAL
1	D	159	LEU
2	E	375	ASN
3	F	26	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	108	ASN
2	E	255	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

3 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	$\#|Z| > 2$
5	COA	D	401	-	41,50,50	1.74	6 (14%)	52,75,75	1.76	11 (21%)
5	COA	A	401	-	41,50,50	1.72	6 (14%)	52,75,75	1.53	7 (13%)
6	SO4	B	501	-	4,4,4	0.25	0	6,6,6	0.09	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
5	COA	D	401	-	-	19/44/64/64	0/3/3/3
5	COA	A	401	-	-	16/44/64/64	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	COA	C5P-N4P	6.54	1.48	1.33
5	A	401	COA	C5P-N4P	6.35	1.47	1.33
5	A	401	COA	C9P-N8P	5.26	1.45	1.33
5	D	401	COA	C9P-N8P	4.61	1.43	1.33
5	D	401	COA	C6A-N6A	3.73	1.47	1.34

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	401	COA	N3A-C2A-N1A	-6.25	118.91	128.68
5	A	401	COA	N3A-C2A-N1A	-5.67	119.81	128.68
5	A	401	COA	O6A-CCP-CBP	-4.40	103.48	110.55
5	D	401	COA	O4B-C1B-C2B	-3.65	101.60	106.93
5	D	401	COA	C6P-C5P-N4P	3.63	122.53	116.42

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	COA	C3B-C4B-C5B-O5B
5	A	401	COA	CCP-O6A-P2A-O3A
5	A	401	COA	OAP-CAP-CBP-CCP

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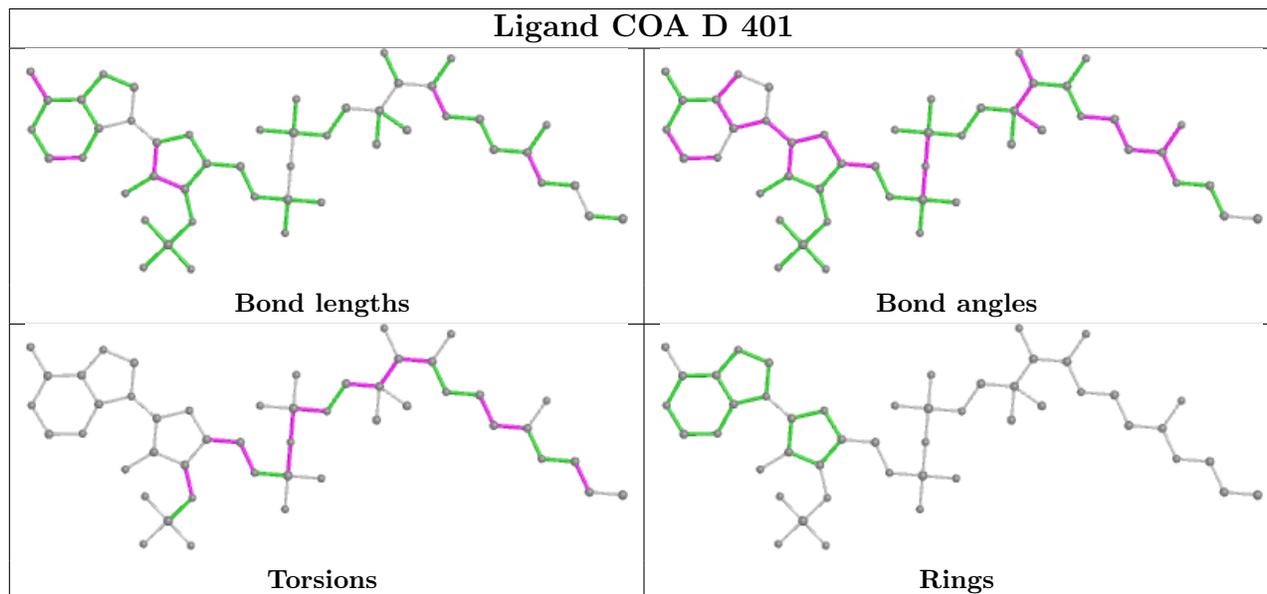| Mol	Chain	Res	Type	Atoms
5	A	401	COA	C9P-CAP-CBP-CCP
5	A	401	COA	OAP-CAP-CBP-CDP

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	401	COA	8	0
5	A	401	COA	5	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 then 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.

Ligand COA D 401

Bond lengths   Bond angles

Torsions   Rings

Ligand COA A 401

Bond lengths

Bond angles

Torsions

Rings
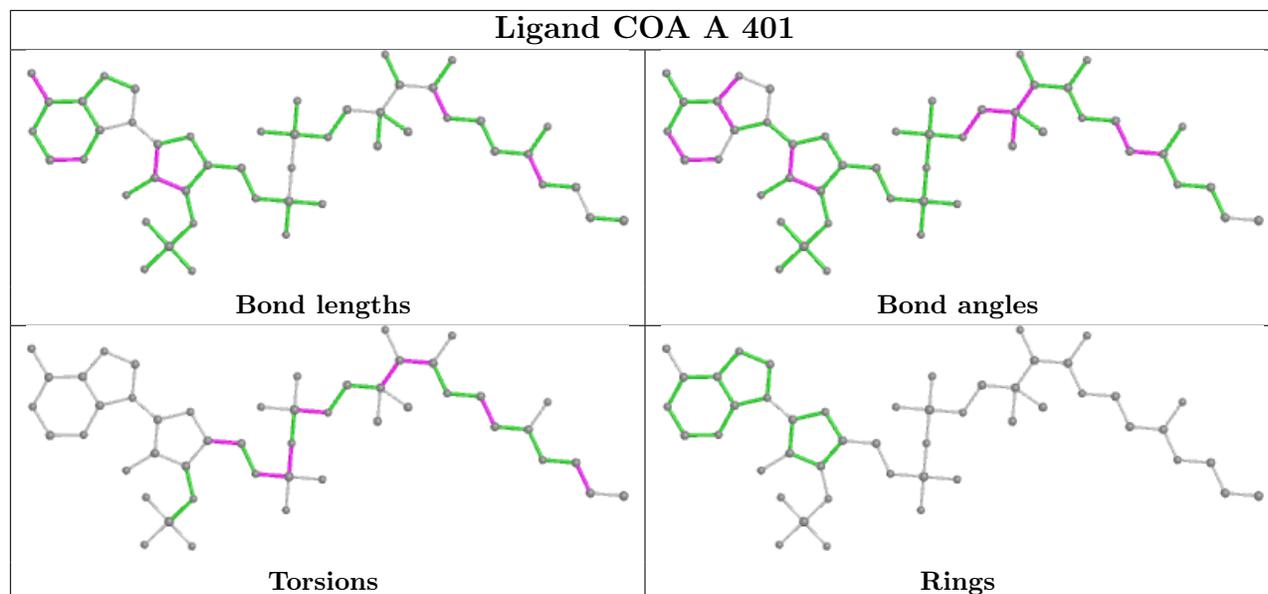
5.7 Other polymers ⓘ

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	313/320 (97%)	0.82	38 (12%)	4	4	52, 76, 122, 158	0
1	D	313/320 (97%)	0.66	27 (8%)	10	10	49, 75, 113, 149	0
2	B	361/401 (90%)	0.69	35 (9%)	7	7	51, 72, 110, 150	0
2	E	361/401 (90%)	0.79	36 (9%)	7	6	51, 73, 108, 152	0
3	C	39/48 (81%)	1.30	14 (35%)	0	0	59, 84, 154, 190	0
3	F	37/48 (77%)	1.37	10 (27%)	0	0	55, 81, 140, 175	0
4	P	10/15 (66%)	3.15	6 (60%)	0	0	85, 116, 128, 152	0
4	Y	12/15 (80%)	3.17	8 (66%)	0	0	90, 111, 132, 163	0
All	All	1446/1568 (92%)	0.81	174 (12%)	4	4	49, 75, 119, 190	0

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	ASP	9.2
1	A	76	GLY	8.9
3	C	26	ILE	7.9
1	A	79	ASN	7.1
1	A	286	SER	6.8

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

There are no non-standard protein/DNA/RNA residues in this entry.
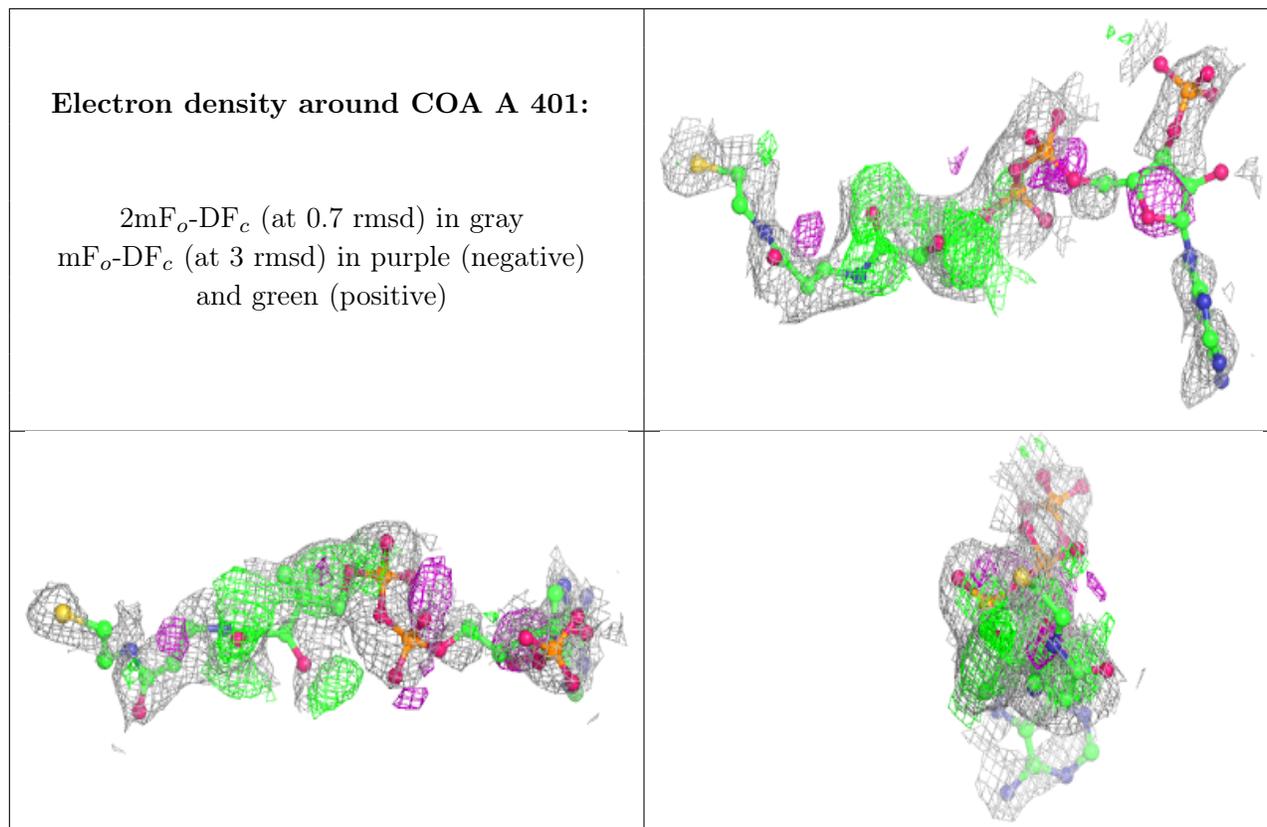
6.3 Carbohydrates ⓘ

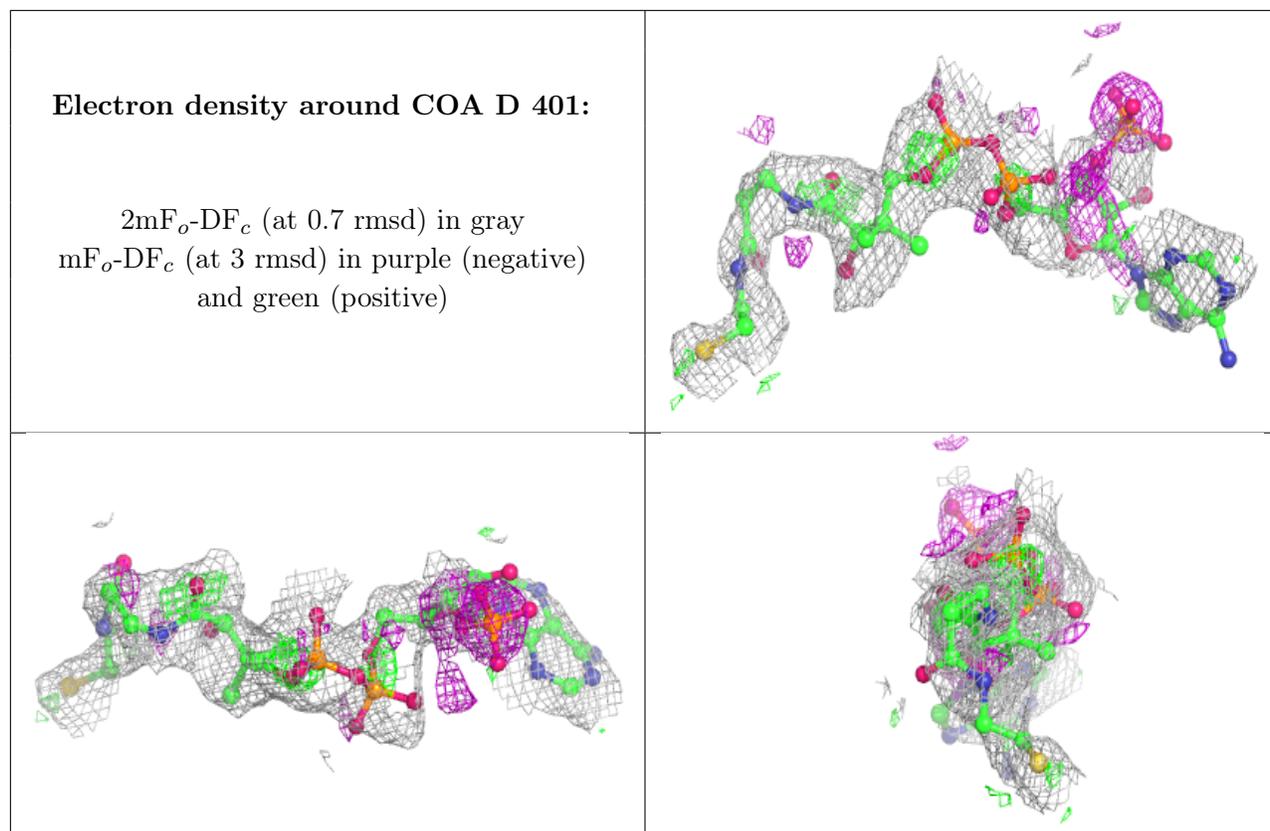There are no monosaccharides in this entry.

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
5	COA	A	401	48/48	0.29	0.50	137,138,141,141	0
5	COA	D	401	48/48	0.51	0.46	129,132,135,135	0
6	SO4	B	501	5/5	0.82	0.31	111,122,126,126	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 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 D 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.