



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:56 AM UTC

PDB ID : 2WL4 / pdb\_00002w14  
Title : BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. COMPLEX OF THE H348A MUTANT WITH COENZYME A.  
Authors : Merilainen, G.; Poikela, V.; Kursula, P.; Wierenga, R.K.  
Deposited on : 2009-06-22  
Resolution : 1.80 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

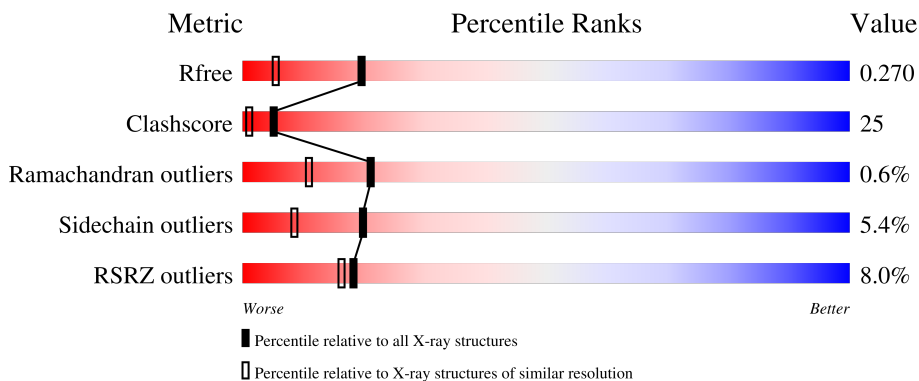
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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  $\geq 3$ , 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	392	
2	B	392	
3	C	392	
4	D	392	

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	SO4	A	1401	-	-	X	-
5	SO4	B	1398	-	-	X	-
5	SO4	D	1394	-	-	X	-
7	CL	C	1396	-	-	X	-
7	CL	D	1399	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12721 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	389	2837	1765	511	539	22	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	ALA	SEE REMARK 999	UNP P07097
A	348	ALA	HIS	engineered mutation	UNP P07097

- Molecule 2 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	389	2843	1770	509	543	21	0	7	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	129	ARG	ALA	SEE REMARK 999	UNP P07097
B	348	ALA	HIS	engineered mutation	UNP P07097

- Molecule 3 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	389	2816	1747	509	539	21	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	129	ARG	ALA	SEE REMARK 999	UNP P07097
C	348	ALA	HIS	engineered mutation	UNP P07097

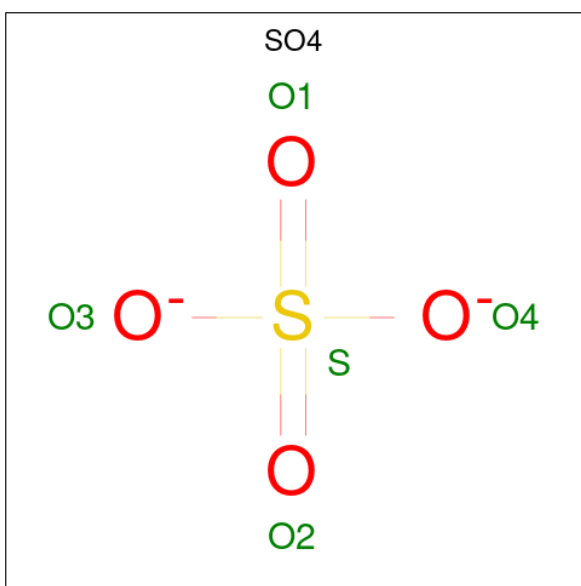
- Molecule 4 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	389	2828	1755	513	539	21	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	ALA	SEE REMARK 999	UNP P07097
D	348	ALA	HIS	engineered mutation	UNP P07097

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



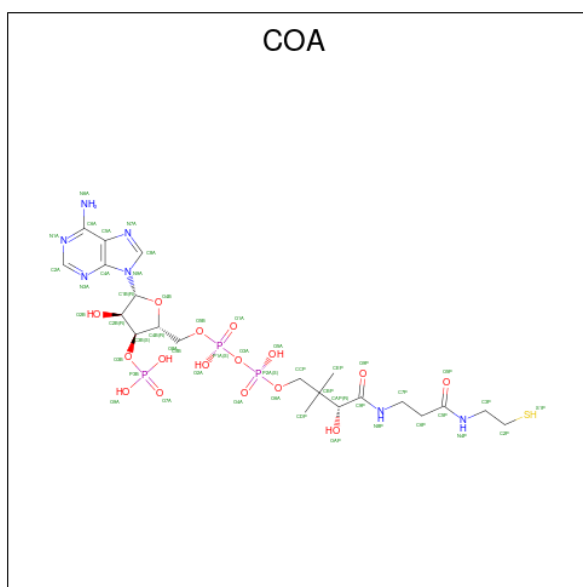
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
5	A	1	5	4	1	0	0
5	A	1	5	4	1	0	0
5	A	1	5	4	1	0	0
5	A	1	5	4	1	0	0
5	A	1	5	4	1	0	0
5	A	1	5	4	1	0	0

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

- Molecule 6 is COENZYME A (CCD ID: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	B	1	1	1	0	0
7	C	1	1	1	0	0
7	D	1	1	1	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
8	C	2	2	2	0	0
8	D	1	1	1	0	0

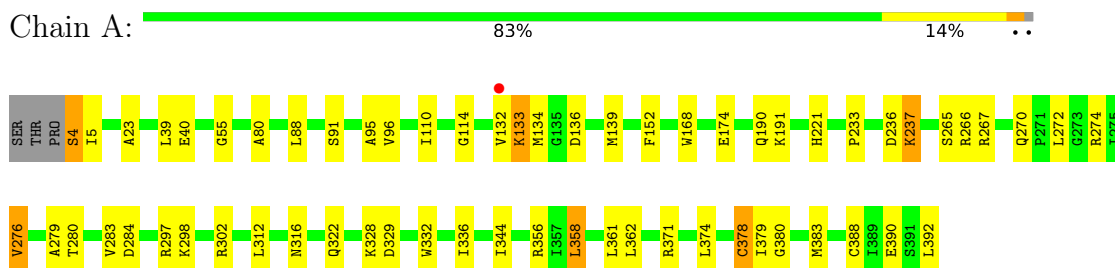
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	426	Total 426	O 426	0	0
9	B	407	Total 407	O 407	0	0
9	C	149	Total 149	O 149	0	0
9	D	188	Total 188	O 188	0	0

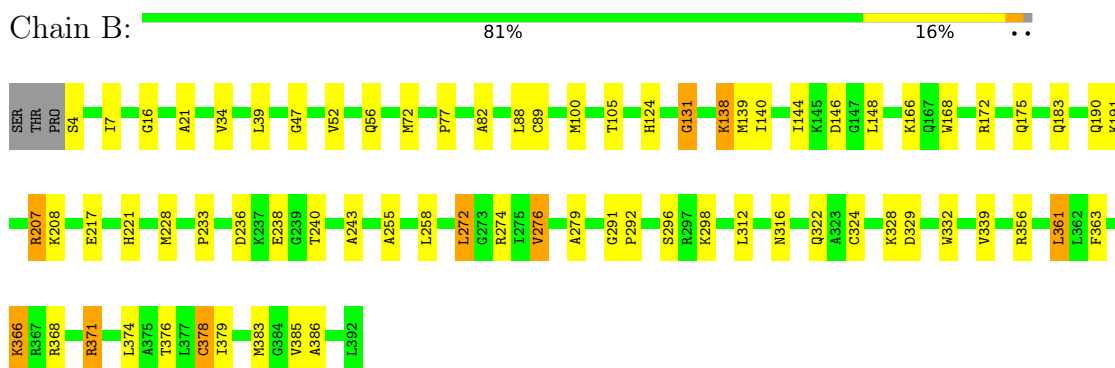
### 3 Residue-property plots [i](#)

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.

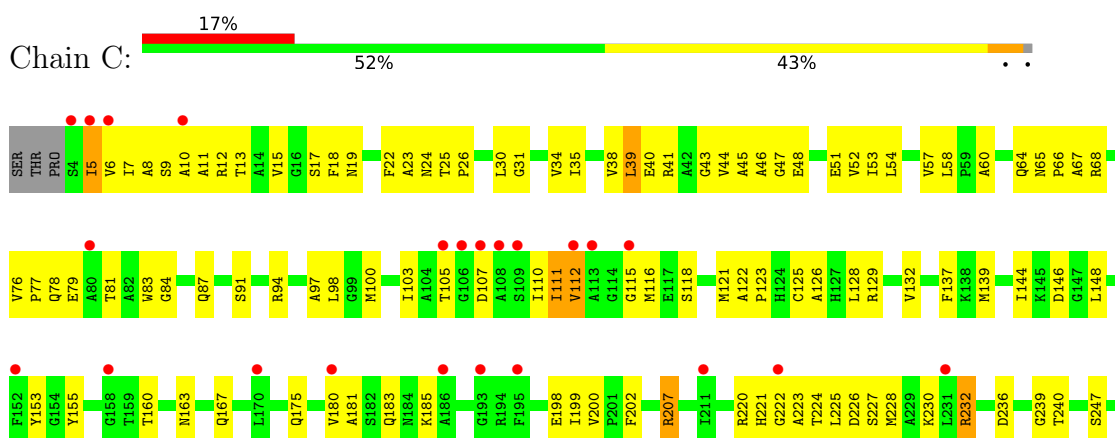
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE

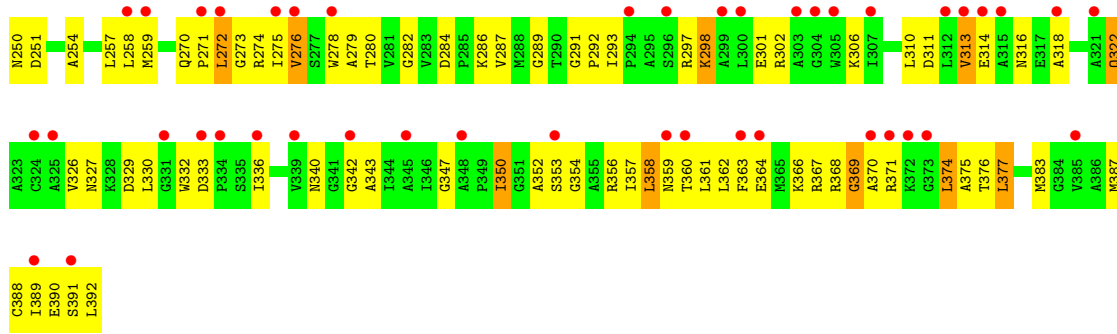


- Molecule 2: ACETYL-COA ACETYLTRANSFERASE

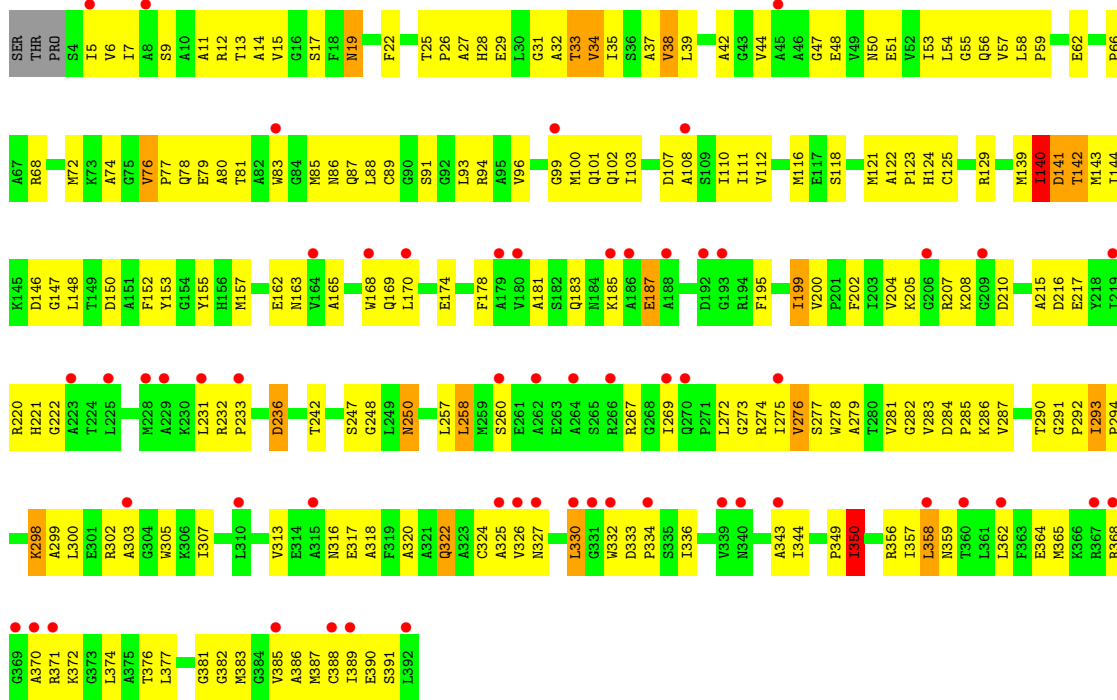


- Molecule 3: ACETYL-COA ACETYLTRANSFERASE





● Molecule 4: ACETYL-COA ACETYLTRANSFERASE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.31Å 79.14Å 149.41Å 90.00° 92.68° 90.00°	Depositor
Resolution (Å)	19.61 – 1.80 19.61 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.61-1.80) 86.6 (19.61-1.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 1.80Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.231 , 0.270 0.232 , 0.270	Depositor DCC
$R_{free}$ test set	9051 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.7	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 81.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	0.159 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	12721	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, SO4, CL, COA, CSO, CSD

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	0.65	0/2884	0.88	0/3892
2	B	0.64	0/2888	0.89	0/3896
3	C	0.34	0/2864	0.80	2/3867 (0.1%)
4	D	0.37	0/2869	0.79	2/3870 (0.1%)
All	All	0.52	0/11505	0.84	4/15525 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	140	ILE	N-CA-C	6.08	121.98	109.34
3	C	313	VAL	N-CA-C	5.64	115.99	108.27
4	D	250	ASN	N-CA-C	5.13	116.88	109.07
3	C	250	ASN	N-CA-C	5.04	116.85	109.24

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	2837	0	2870	58	0
2	B	2843	0	2882	77	0
3	C	2816	0	2825	212	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2828	0	2848	239	0
5	A	45	0	0	9	0
5	B	40	0	0	2	0
5	C	20	0	0	0	0
5	D	20	0	0	5	0
6	A	48	0	32	1	0
6	B	48	0	32	6	0
7	B	1	0	0	0	0
7	C	1	0	0	7	0
7	D	1	0	0	7	0
8	C	2	0	0	0	0
8	D	1	0	0	0	0
9	A	426	0	0	22	0
9	B	407	0	0	25	0
9	C	149	0	0	40	0
9	D	188	0	0	78	0
All	All	12721	0	11489	569	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 25.

The worst 5 of 569 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)
3:C:64:GLN:HG2	4:D:88:LEU:HD11	1.42	1.00
2:B:296:SER:OG	2:B:376[B]:THR:HG21	1.62	0.99
3:C:298:LYS:HE2	3:C:302:ARG:HE	1.24	0.99
4:D:140:ILE:CD1	4:D:141:ASP:H	1.76	0.98
3:C:356:ARG:HH21	3:C:357:ILE:HG22	1.25	0.97

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	391/392 (100%)	376 (96%)	15 (4%)	0	100	100
2	B	392/392 (100%)	378 (96%)	13 (3%)	1 (0%)	36	25
3	C	389/392 (99%)	350 (90%)	36 (9%)	3 (1%)	16	6
4	D	389/392 (99%)	352 (90%)	31 (8%)	6 (2%)	8	2
All	All	1561/1568 (100%)	1456 (93%)	95 (6%)	10 (1%)	21	11

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	140	ILE
4	D	141	ASP
4	D	330	LEU
4	D	350	ILE
2	B	131	GLY

### 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	279/277 (101%)	266 (95%)	13 (5%)	23	11
2	B	280/276 (101%)	269 (96%)	11 (4%)	28	16
3	C	277/278 (100%)	259 (94%)	18 (6%)	15	5
4	D	277/277 (100%)	259 (94%)	18 (6%)	15	5
All	All	1113/1108 (100%)	1053 (95%)	60 (5%)	20	8

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	111	ILE
4	D	322	GLN
3	C	298	LYS

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Mol	Chain	Res	Type
4	D	298	LYS
4	D	359	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	24	ASN
4	D	184	ASN
4	D	163	ASN
2	B	316	ASN
4	D	19	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	CSD	A	378	1	4,7,8	10.08	1 (25%)	1,8,10	1.97	0
2	CSD	B	378	2	4,7,8	9.80	1 (25%)	1,8,10	2.44	1 (100%)
2	CSO	B	89	2	3,6,7	0.60	0	1,6,8	1.65	0
4	CSO	D	89	4	3,6,7	0.62	0	1,6,8	0.18	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	CSD	A	378	1	-	0/2/6/8	-
2	CSD	B	378	2	-	0/2/6/8	-
2	CSO	B	89	2	-	0/1/5/7	-
4	CSO	D	89	4	-	1/1/5/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	378	CSD	OD1-SG	20.12	1.65	1.47
2	B	378	CSD	OD1-SG	19.56	1.65	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	378	CSD	OD1-SG-CB	2.44	110.10	105.60

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	89	CSO	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	378	CSD	1	0
2	B	378	CSD	2	0
2	B	89	CSO	2	0
4	D	89	CSO	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 6 are monoatomic - leaving 27 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
5	SO4	C	1399	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	A	1394	-	4,4,4	0.26	0	6,6,6	0.17	0
5	SO4	D	1397	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	B	1402	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	D	1395	-	4,4,4	0.25	0	6,6,6	0.05	0
5	SO4	C	1398	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	B	1399	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	D	1396	-	4,4,4	0.22	0	6,6,6	0.13	0
5	SO4	B	1395	-	4,4,4	0.26	0	6,6,6	0.11	0
5	SO4	B	1396	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	B	1403	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	B	1398	-	4,4,4	0.25	0	6,6,6	0.18	0
5	SO4	A	1398	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	A	1401	-	4,4,4	0.23	0	6,6,6	0.23	0
5	SO4	B	1397	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	C	1393	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	C	1397	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	D	1394	-	4,4,4	0.24	0	6,6,6	0.08	0
6	COA	B	1401	-	47,50,50	1.68	8 (17%)	69,75,75	1.73	10 (14%)
5	SO4	B	1404	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	A	1399	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	A	1395	-	4,4,4	0.24	0	6,6,6	0.08	0
6	COA	A	1402	-	47,50,50	1.64	7 (14%)	69,75,75	1.59	10 (14%)
5	SO4	A	1400	-	4,4,4	0.26	0	6,6,6	0.14	0
5	SO4	A	1403	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	A	1396	-	4,4,4	0.30	0	6,6,6	0.11	0
5	SO4	A	1397	-	4,4,4	0.23	0	6,6,6	0.05	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
6	COA	B	1401	-	-	7/48/64/64	0/3/3/3
6	COA	A	1402	-	-	4/48/64/64	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1401	COA	P3B-O7A	6.42	1.70	1.50
6	A	1402	COA	P3B-O7A	6.42	1.70	1.50
6	B	1401	COA	P3B-O8A	4.21	1.70	1.54
6	A	1402	COA	P3B-O8A	4.12	1.70	1.54
6	B	1401	COA	C5A-C4A	3.91	1.46	1.39

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1401	COA	C5A-C4A-N3A	-6.13	118.28	126.72
6	B	1401	COA	N3A-C4A-N9A	5.80	137.03	127.17
6	A	1402	COA	C5A-C4A-N3A	-5.72	118.84	126.72
6	A	1402	COA	N3A-C4A-N9A	5.62	136.73	127.17
6	B	1401	COA	C7P-C6P-C5P	-4.66	104.63	112.39

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1402	COA	C2P-C3P-N4P-C5P
6	B	1401	COA	C5B-O5B-P1A-O1A
6	B	1401	COA	C5B-O5B-P1A-O2A
6	B	1401	COA	C5B-O5B-P1A-O3A
6	B	1401	COA	O4B-C4B-C5B-O5B

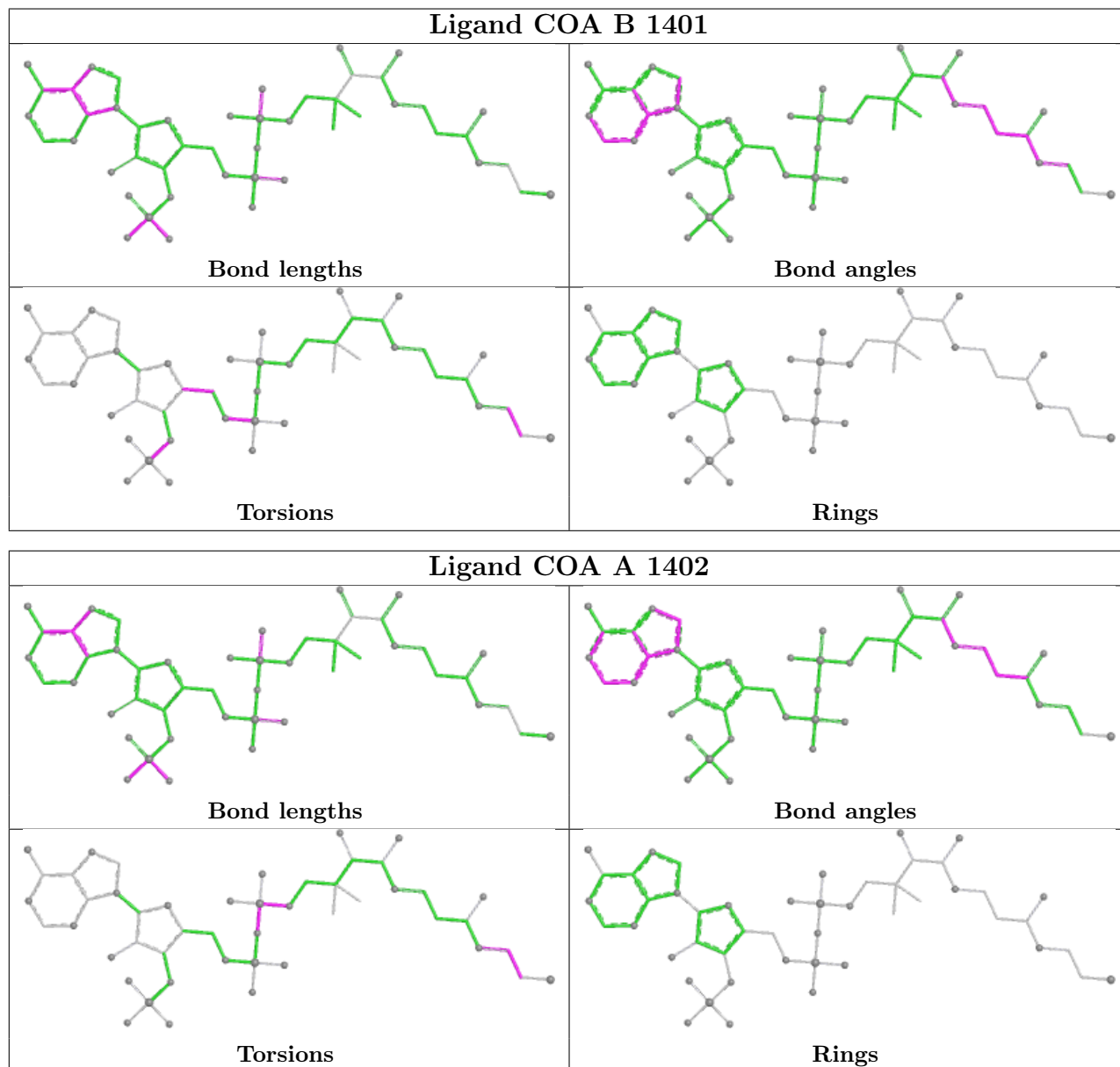
There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1394	SO4	1	0
5	D	1397	SO4	1	0
5	D	1396	SO4	1	0
5	B	1398	SO4	2	0
5	A	1401	SO4	7	0
5	D	1394	SO4	3	0
6	B	1401	COA	6	0
6	A	1402	COA	1	0
5	A	1400	SO4	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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	388/392 (98%)	-1.27	1 (0%) 90   90	5, 13, 33, 69	5 (1%)
2	B	387/392 (98%)	-1.27	0 100   100	4, 13, 31, 79	7 (1%)
3	C	389/392 (99%)	1.16	66 (16%) 4   3	23, 65, 100, 125	1 (0%)
4	D	388/392 (98%)	0.84	57 (14%) 6   4	20, 60, 118, 148	3 (0%)
All	All	1552/1568 (98%)	-0.13	124 (7%) 18   16	4, 37, 97, 148	16 (1%)

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	299	ALA	4.9
3	C	315	ALA	4.7
4	D	330	LEU	4.5
4	D	325	ALA	3.8
4	D	367	ARG	3.8

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	CSO	D	89	7/8	0.97	0.08	36,42,63,77	0
2	CSO	B	89	7/8	0.99	0.04	4,10,34,73	0
2	CSD	B	378	8/9	1.00	0.04	4,9,24,109	0
1	CSD	A	378	8/9	1.00	0.03	7,13,23,32	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95<sup>th</sup> 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.

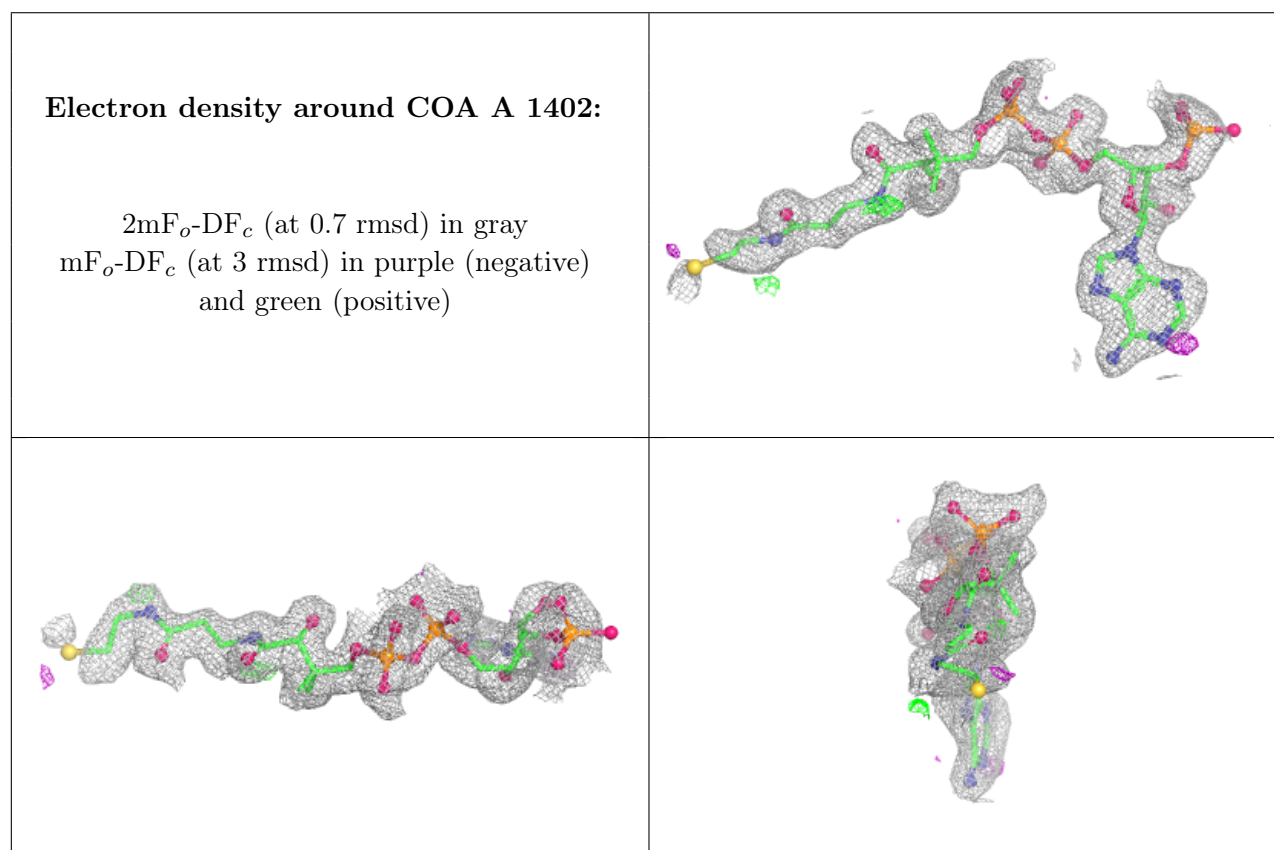
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	D	1395	5/5	0.90	0.09	89,89,90,91	0
5	SO4	C	1398	5/5	0.93	0.09	96,97,97,98	0
5	SO4	B	1403	5/5	0.93	0.09	86,87,88,89	0
5	SO4	B	1404	5/5	0.94	0.10	77,77,79,82	0
5	SO4	A	1403	5/5	0.95	0.09	94,94,95,98	0
5	SO4	C	1393	5/5	0.95	0.11	108,108,109,109	0
5	SO4	C	1397	5/5	0.95	0.07	84,84,85,86	0
5	SO4	B	1402	5/5	0.95	0.07	75,75,76,76	0
5	SO4	D	1394	5/5	0.95	0.11	63,70,71,75	0
5	SO4	A	1398	5/5	0.95	0.09	71,78,79,81	0
5	SO4	D	1397	5/5	0.95	0.18	120,121,122,123	0
5	SO4	A	1400	5/5	0.96	0.09	60,60,69,75	0
5	SO4	B	1399	5/5	0.96	0.06	78,78,80,81	0
5	SO4	C	1399	5/5	0.96	0.08	90,91,94,94	0
8	NA	C	1395	1/1	0.96	0.09	60,60,60,60	0
5	SO4	A	1395	5/5	0.97	0.07	46,54,58,59	0
5	SO4	D	1396	5/5	0.97	0.06	52,59,70,71	0
5	SO4	A	1399	5/5	0.97	0.10	95,99,101,101	0
7	CL	D	1399	1/1	0.97	0.12	80,80,80,80	0
5	SO4	B	1397	5/5	0.97	0.07	66,66,71,73	0
5	SO4	A	1397	5/5	0.98	0.06	47,48,56,56	0
5	SO4	B	1398	5/5	0.98	0.05	45,51,56,57	0
6	COA	A	1402	48/48	0.98	0.06	21,32,63,131	0
6	COA	B	1401	48/48	0.98	0.05	20,36,80,112	0
5	SO4	B	1395	5/5	0.98	0.05	47,50,52,55	0
5	SO4	B	1396	5/5	0.98	0.06	45,49,57,63	0
8	NA	D	1398	1/1	0.98	0.04	38,38,38,38	0
7	CL	C	1396	1/1	0.99	0.05	58,58,58,58	0
5	SO4	A	1396	5/5	0.99	0.04	31,39,50,57	0
8	NA	C	1394	1/1	0.99	0.04	34,34,34,34	0
5	SO4	A	1401	5/5	0.99	0.07	28,44,49,50	0
5	SO4	A	1394	5/5	0.99	0.03	41,43,48,48	0

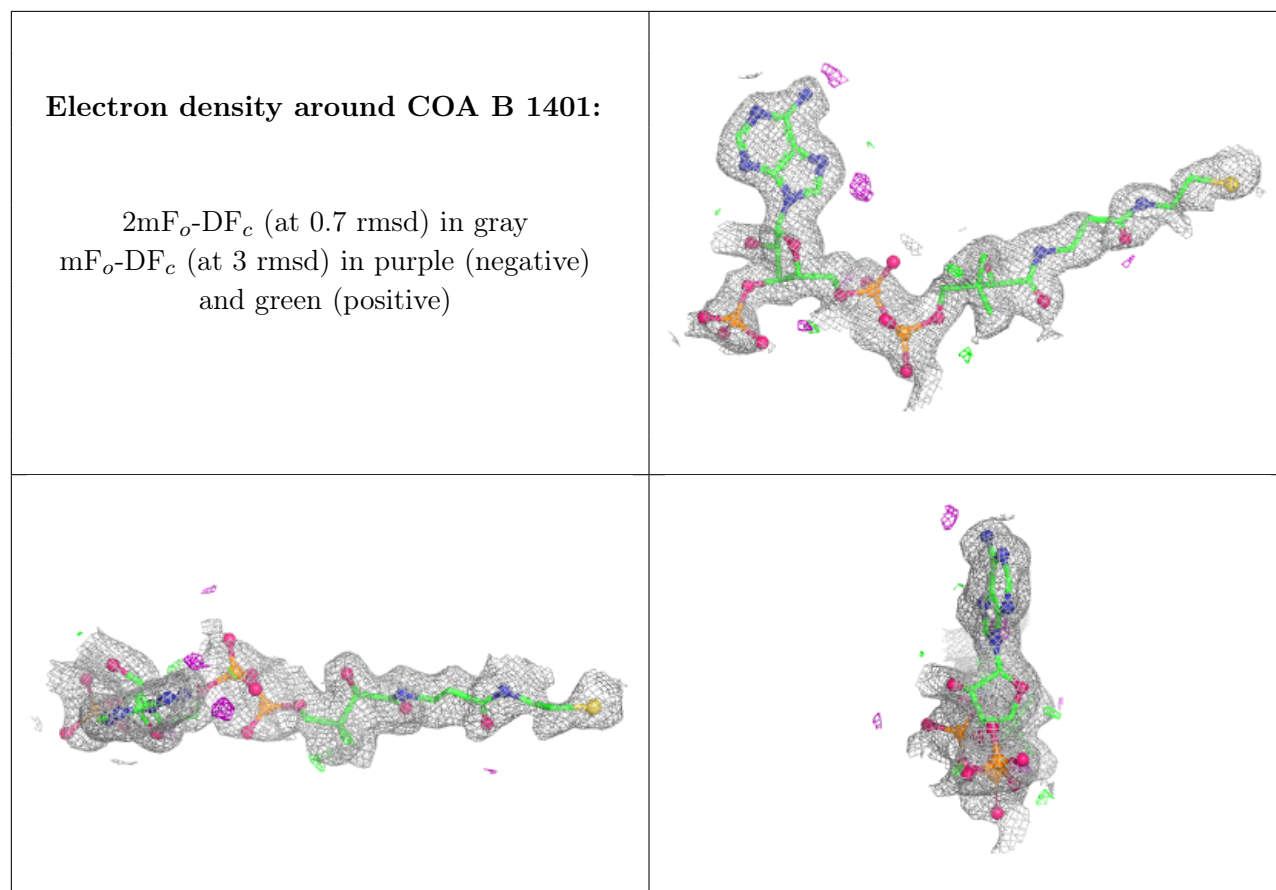
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CL	B	1400	1/1	1.00	0.04	28,28,28,28	0

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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.