



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 04:38 am BST

PDB ID : 1NL7
Title : Z. ramigera biosynthetic thiolase, acetylated enzyme complexed with CoA at pH 9.5
Authors : Kursula, P.; Wierenga, R.K.
Deposited on : 2003-01-06
Resolution : 1.90 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

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 : 2.11
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) : 2.11

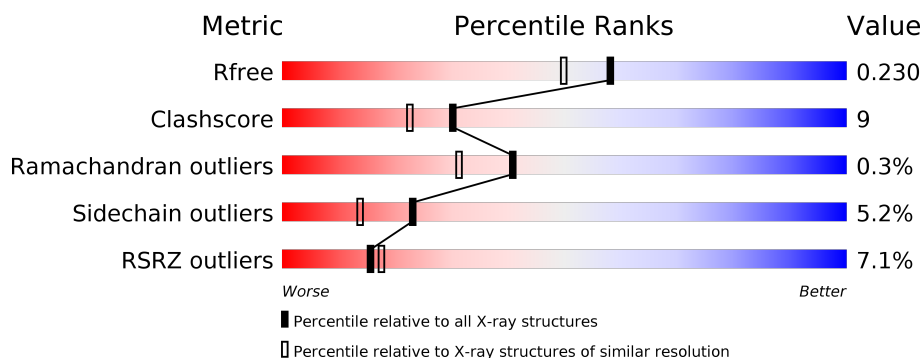
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	392	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 87% 11% .. </div> </div>
1	B	392	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 85% 13% .. </div> </div>
1	C	392	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 1%, green 92%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 84% 14% .. </div> </div>
1	D	392	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 20%, orange 1%, yellow 1%, green 78%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 76% 21% .. </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SCY	A	89	-	-	X	-
1	SCY	B	89	-	-	X	-
1	SCY	C	89	-	-	X	-
1	SCY	D	89	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12691 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	390	Total	C	N	O	S	0	1	0
			2825	1754	510	540	21			
1	B	390	Total	C	N	O	S	0	1	0
			2825	1754	510	540	21			
1	C	390	Total	C	N	O	S	0	1	0
			2825	1754	510	540	21			
1	D	390	Total	C	N	O	S	0	1	0
			2825	1754	510	540	21			

There are 12 discrepancies between the modelled and reference sequences:

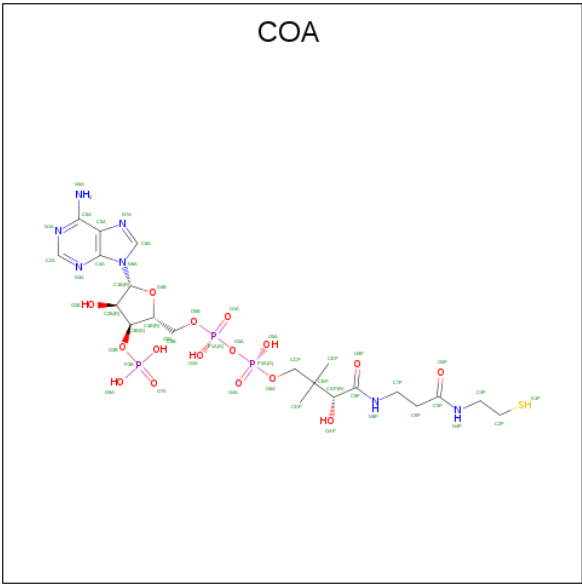
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	INSERTION	UNP P07097
A	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	10	ALA	-	INSERTION	UNP P07097
B	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	10	ALA	-	INSERTION	UNP P07097
C	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
C	129	ARG	ALA	CONFLICT	UNP P07097
D	10	ALA	-	INSERTION	UNP P07097
D	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
D	129	ARG	ALA	CONFLICT	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	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

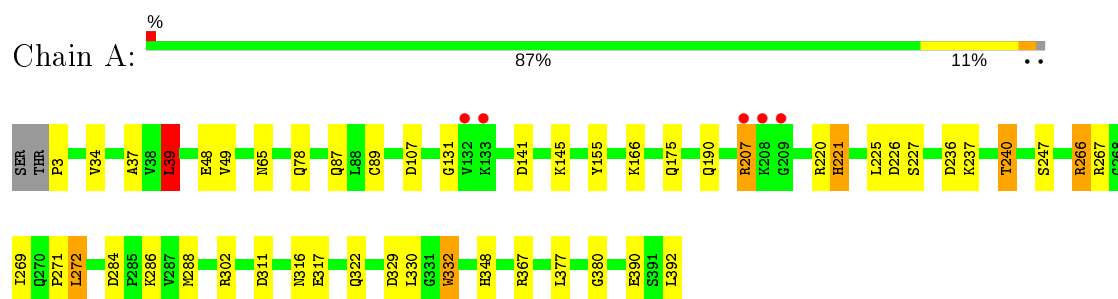
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	443	Total 443	O 443	0	0
4	B	446	Total 446	O 446	0	0
4	C	190	Total 190	O 190	0	0
4	D	196	Total 196	O 196	0	0

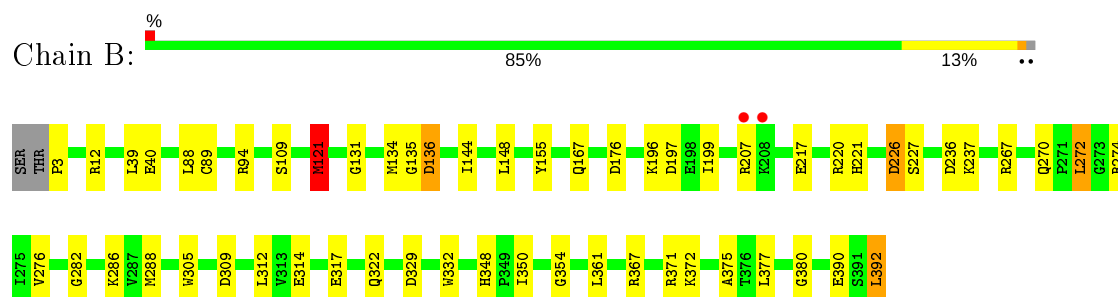
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

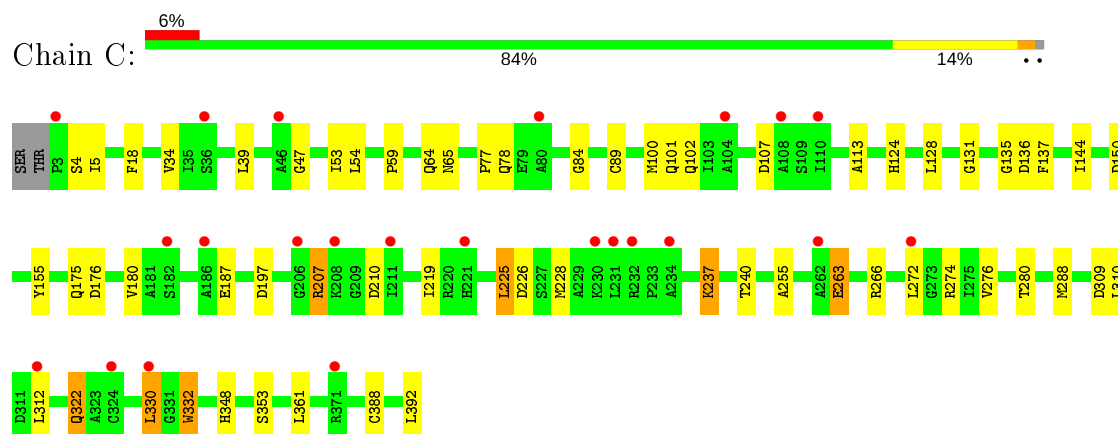
- Molecule 1: Acetyl-CoA acetyltransferase



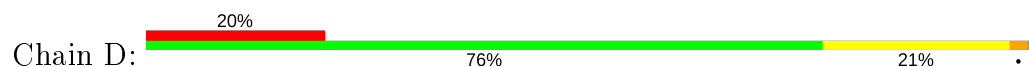
- Molecule 1: Acetyl-CoA acetyltransferase



- Molecule 1: Acetyl-CoA acetyltransferase



- Molecule 1: Acetyl-CoA acetyltransferase



SER	THR	P3	R12	V15	G16	S17	F18	A21	V34	I35	V38	L39	F40	R41	V49	L54	V57	L58	P59	T81	G84	Q87	L88	C89	A97	Q101	A104	T105	G106	D107	E117	H124	C125	R129	G130	G131	M134	G135	D136	I140												
D141	T142	M143	I144	D146	G147	L148	T149	D150	A151	F152	G153	G154	Y155	H156	M157	G158	T159	T160	M163	V164	A165	K166	Q167	W168	Q169	L170	S171	R172	D173	E174	Q175	D176	A177	F178	A179	Q183	E187	A188	A189	Q190	K191	D192	F195	K196	D197	E198	I199	V200	G206	R207	K208	D216
E217	T218	I219	R220	H221	D226	S227	W228	A229	K230	L231	R232	P233	A234	F235	D236	K237	L238	E239	T240	G244	W245	A246	S247	D251	G252	A253	G254	A255	A256	L257	L258	S265	T269	Q270	P271	R274	L275	V281	G282	V283	V286	W287	W288	G289	T290	P294	W305	K306	I307			
L310	D311	L312	N316	E317	A318	F319	Q322	A323	C324	A325	V326	N327	K328	D329	L330	G331	W332	V337	N338	V339	A343	I344	A345	I346	G347	H348	P349	I350	A352	S353	G354	A355	N359	T360	L361	L362	K366	R367	R368	R371	L374	L377	C378	G382	S391	L392						

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.37Å 79.06Å 148.88Å 90.00° 92.58° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 27.08 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-1.90) 85.1 (27.08-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.179 , 0.223 0.191 , 0.230	Depositor DCC
R_{free} test set	6714 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.124 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12691	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: COA, SCY, SO4

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	1.02	3/2861 (0.1%)	1.03	17/3861 (0.4%)
1	B	1.02	2/2861 (0.1%)	0.97	12/3861 (0.3%)
1	C	0.66	0/2861	0.83	7/3861 (0.2%)
1	D	0.61	0/2861	0.83	10/3861 (0.3%)
All	All	0.85	5/11444 (0.0%)	0.92	46/15444 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	VAL	CB-CG1	-7.47	1.37	1.52
1	B	317	GLU	CD-OE1	6.98	1.33	1.25
1	A	317	GLU	CD-OE1	6.50	1.32	1.25
1	B	109	SER	CB-OG	-6.37	1.33	1.42
1	A	37	ALA	CA-CB	5.28	1.63	1.52

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ARG	NE-CZ-NH2	-14.97	112.82	120.30
1	B	309	ASP	CB-CG-OD2	8.83	126.25	118.30
1	A	141	ASP	CB-CG-OD2	8.29	125.76	118.30
1	A	266	ARG	NE-CZ-NH1	8.25	124.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	ASP	CB-CG-OD2	7.68	125.21	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	135	GLY	Mainchain,Peptide

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	2825	0	2830	46	0
1	B	2825	0	2830	49	0
1	C	2825	0	2830	42	0
1	D	2825	0	2830	76	0
2	A	10	0	0	1	0
2	B	10	0	0	1	0
3	A	48	0	32	5	0
3	B	48	0	32	5	0
4	A	443	0	0	29	0
4	B	446	0	0	31	0
4	C	190	0	0	18	0
4	D	196	0	0	45	0
All	All	12691	0	11384	212	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 212 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:D:89:SCY:CD	4:D:393:HOH:O	1.64	1.32
1:C:89:SCY:CD	4:C:393:HOH:O	1.89	1.20
1:B:121:MET:SD	4:B:487:HOH:O	1.98	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLU:HB2	4:B:551:HOH:O	1.46	1.14
1:A:89:SCY:HE1	1:A:380:GLY:H	1.03	1.13

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	388/392 (99%)	372 (96%)	15 (4%)	1 (0%)	41	31
1	B	388/392 (99%)	378 (97%)	9 (2%)	1 (0%)	41	31
1	C	388/392 (99%)	367 (95%)	20 (5%)	1 (0%)	41	31
1	D	388/392 (99%)	369 (95%)	18 (5%)	1 (0%)	41	31
All	All	1552/1568 (99%)	1486 (96%)	62 (4%)	4 (0%)	41	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	350	ILE
1	A	207	ARG
1	C	4	SER
1	B	350	ILE

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	277/278 (100%)	265 (96%)	12 (4%)	29	19
1	B	277/278 (100%)	263 (95%)	14 (5%)	24	14
1	C	277/278 (100%)	264 (95%)	13 (5%)	26	16
1	D	277/278 (100%)	259 (94%)	18 (6%)	17	8
All	All	1108/1112 (100%)	1051 (95%)	57 (5%)	23	14

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	392	LEU
1	C	237	LYS
1	D	328	LYS
1	C	39	LEU
1	C	155	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	175	GLN
1	C	184	ASN
1	D	184	ASN
1	C	78	GLN
1	D	221	HIS

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	0.84	0	3,9,11	1.04	0
1	SCY	A	89	1	7,8,9	1.24	1 (14%)	3,9,11	2.17	1 (33%)
1	SCY	C	89	1	7,8,9	0.65	0	3,9,11	0.98	0
1	SCY	B	89	1	7,8,9	1.14	1 (14%)	3,9,11	1.90	1 (33%)

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	-	3/5/7/9	-
1	SCY	A	89	1	-	3/5/7/9	-
1	SCY	C	89	1	-	2/5/7/9	-
1	SCY	B	89	1	-	2/5/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	SCY	CD-SG	-2.50	1.60	1.75
1	B	89	SCY	CD-SG	-2.03	1.63	1.75

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	SCY	OCD-CD-CE	3.17	136.06	123.07
1	B	89	SCY	OCD-CD-SG	-2.71	110.57	122.60

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	89	SCY	OCD-CD-SG-CB
1	D	89	SCY	CE-CD-SG-CB
1	A	89	SCY	CA-CB-SG-CD
1	A	89	SCY	OCD-CD-SG-CB
1	A	89	SCY	CE-CD-SG-CB

There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	89	SCY	6	0
1	A	89	SCY	8	0
1	C	89	SCY	5	0
1	B	89	SCY	9	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	SO4	A	9722	-	4,4,4	0.18	0	6,6,6	0.44	0
2	SO4	A	9720	-	4,4,4	0.35	0	6,6,6	0.52	0
3	COA	A	1393	-	41,50,50	1.39	4 (9%)	52,75,75	1.20	5 (9%)
2	SO4	B	9721	-	4,4,4	0.39	0	6,6,6	0.67	0
2	SO4	B	9719	-	4,4,4	0.16	0	6,6,6	0.32	0
3	COA	B	5939	-	41,50,50	1.45	5 (12%)	52,75,75	1.32	5 (9%)

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	5939	-	-	8/44/64/64	0/3/3/3
3	COA	A	1393	-	-	8/44/64/64	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1393	COA	P3B-O8A	4.33	1.71	1.54
3	B	5939	COA	P3B-O8A	4.28	1.71	1.54
3	B	5939	COA	P3B-O9A	4.20	1.71	1.54
3	A	1393	COA	P3B-O9A	4.12	1.70	1.54
3	B	5939	COA	P2A-O5A	3.57	1.72	1.55

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5939	COA	C1B-N9A-C4A	-5.26	117.40	126.64
3	A	1393	COA	N3A-C2A-N1A	-4.15	122.19	128.68
3	B	5939	COA	N3A-C2A-N1A	-3.57	123.10	128.68
3	A	1393	COA	C1B-N9A-C4A	-3.03	121.32	126.64
3	B	5939	COA	C5A-C6A-N6A	2.85	124.68	120.35

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1393	COA	C3B-O3B-P3B-O7A
3	A	1393	COA	CCP-O6A-P2A-O3A
3	A	1393	COA	C2P-C3P-N4P-C5P
3	B	5939	COA	C5B-O5B-P1A-O3A
3	B	5939	COA	CCP-O6A-P2A-O3A

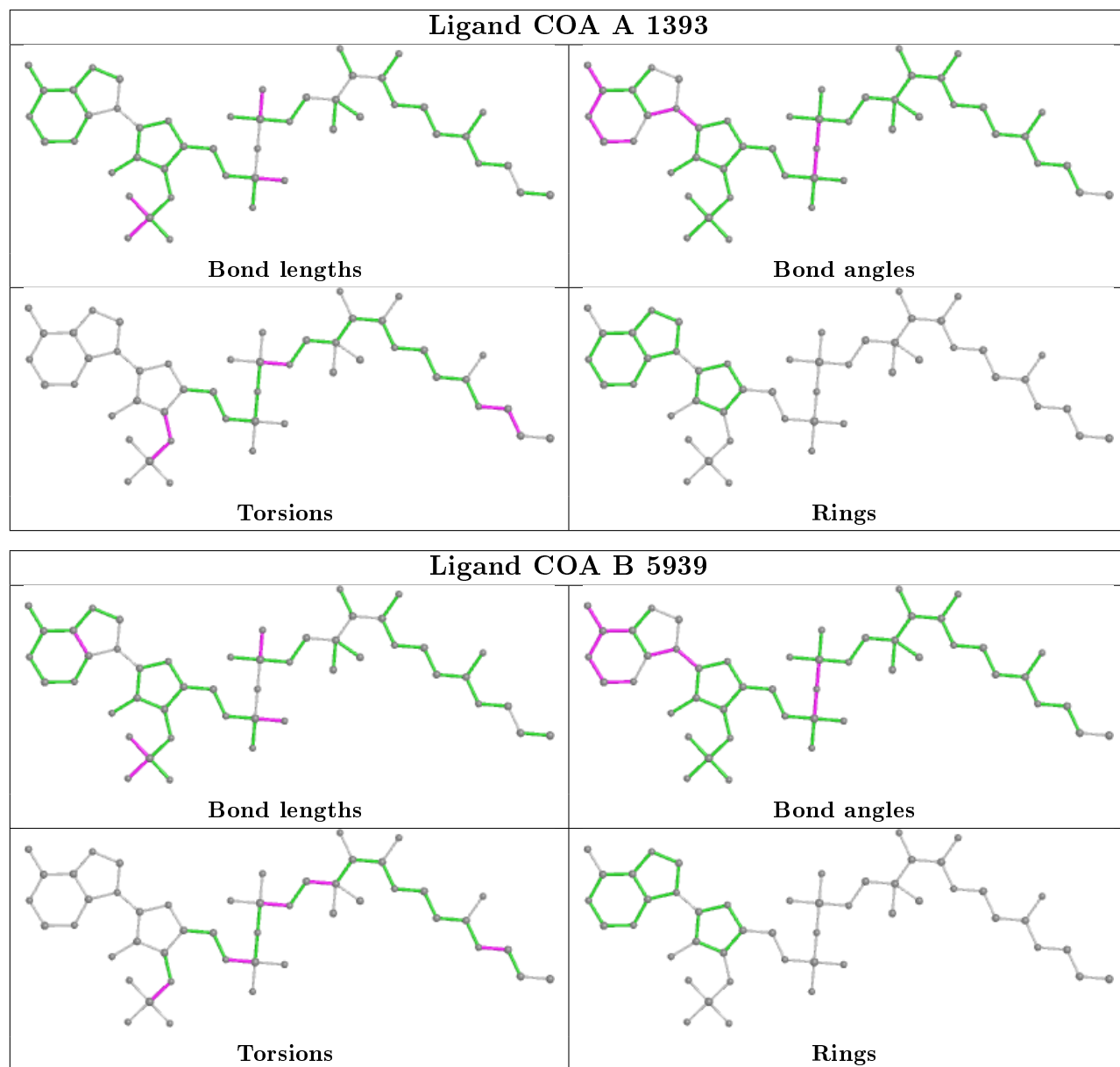
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9720	SO4	1	0
3	A	1393	COA	5	0
2	B	9721	SO4	1	0
3	B	5939	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 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 [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, 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	389/392 (99%)	-0.34	5 (1%) 77 79	10, 15, 30, 54	0
1	B	389/392 (99%)	-0.34	2 (0%) 91 92	10, 15, 30, 59	0
1	C	389/392 (99%)	0.45	23 (5%) 22 25	3, 17, 26, 51	0
1	D	389/392 (99%)	1.08	80 (20%) 1 1	4, 17, 32, 50	0
All	All	1556/1568 (99%)	0.21	110 (7%) 16 17	3, 16, 30, 59	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	392	LEU	7.2
1	D	331	GLY	7.2
1	D	153	TYR	7.0
1	D	238	GLU	6.5
1	D	221	HIS	5.8

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, 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	0.89	0.20	15,19,38,41	0
1	SCY	D	89	9/10	0.93	0.13	9,14,27,30	0
1	SCY	A	89	9/10	0.94	0.10	12,17,31,35	0
1	SCY	B	89	9/10	0.95	0.10	11,15,33,37	0

6.3 Carbohydrates [i](#)

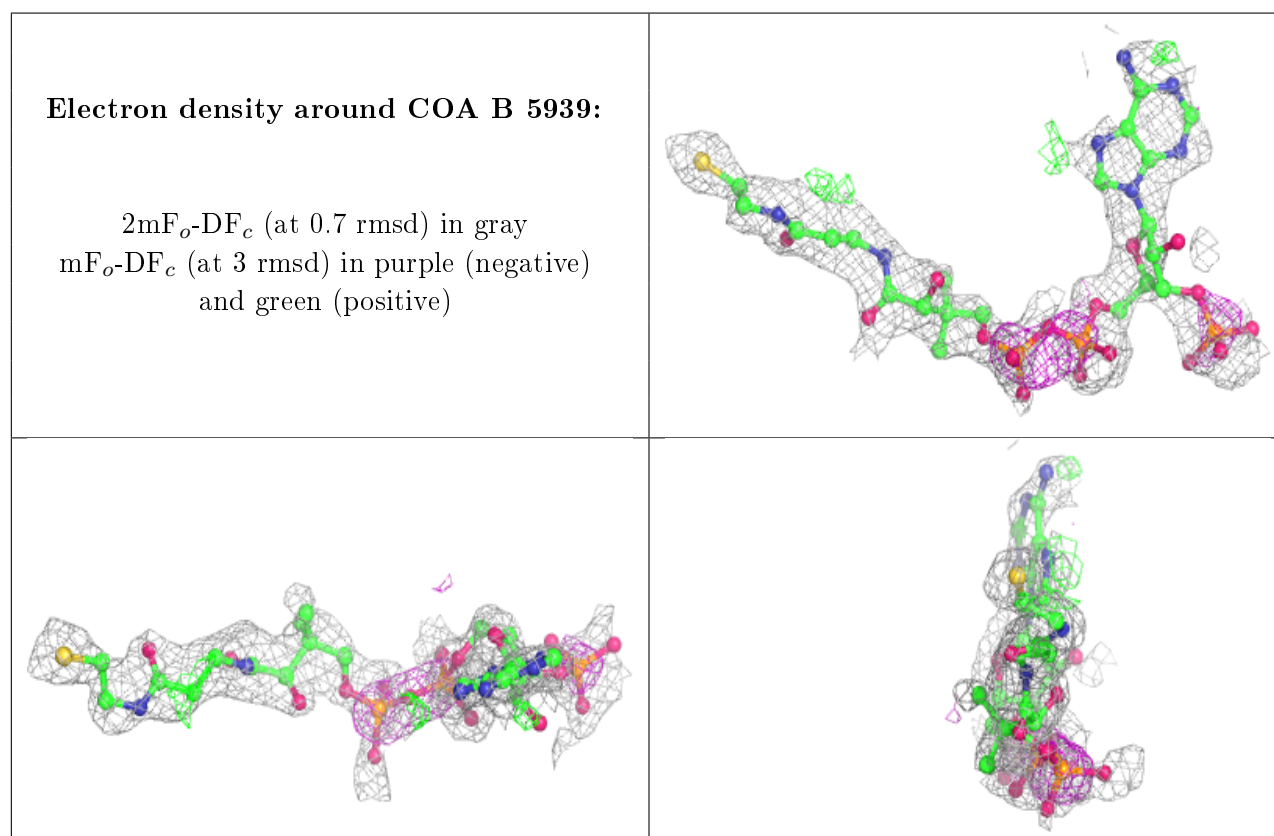
There are no carbohydrates in this entry.

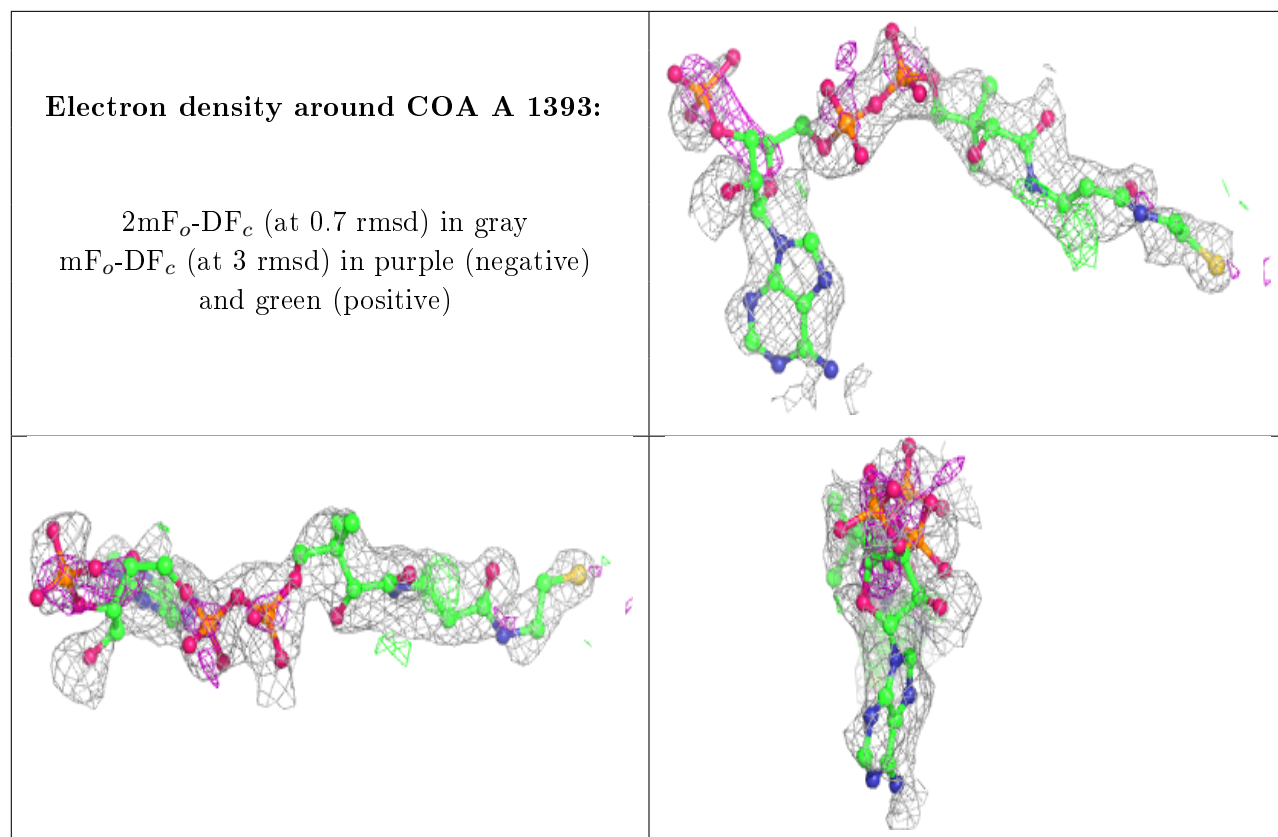
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	COA	B	5939	48/48	0.60	0.26	60,75,82,83	0
3	COA	A	1393	48/48	0.65	0.25	60,73,82,83	0
2	SO4	A	9722	5/5	0.94	0.11	66,67,67,68	0
2	SO4	B	9719	5/5	0.96	0.14	77,78,79,79	0
2	SO4	B	9721	5/5	0.97	0.11	45,46,47,50	0
2	SO4	A	9720	5/5	0.99	0.09	47,48,51,51	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.