



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:46 am BST

PDB ID : 6MGG  
Title : Succinyl-CoA synthase from *Francisella tularensis*, phosphorylated, in complex with CoA  
Authors : Osipiuk, J.; Maltseva, N.; Jedrzejczak, R.; Satchell, K.J.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2018-09-13  
Resolution : 1.78 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](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.

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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

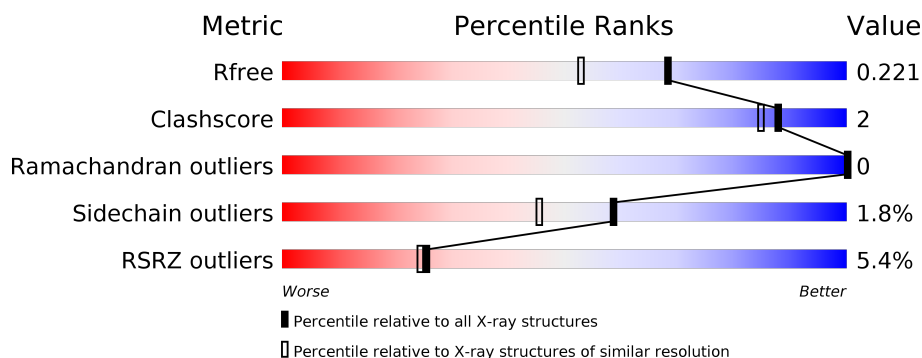
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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  $\geq 3$ , 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	296	<div> <div>4%</div> <div>95%</div> <div>• •</div> </div>
1	C	296	<div> <div>96%</div> <div>•</div> </div>
2	B	387	<div> <div>5%</div> <div>94%</div> <div>6%</div> </div>
2	D	387	<div> <div>11%</div> <div>88%</div> <div>7%</div> <div>• •</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11352 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 Succinate–CoA ligase [ADP-forming] subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	P	S	0	3	0
			2163	1377	359	417	1	9			
1	C	295	Total	C	N	O	P	S	0	3	0
			2182	1388	363	421	1	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	VAL	ALA	engineered mutation	UNP A0A0G2RQ73
A	291	GLU	-	expression tag	UNP A0A0G2RQ73
A	292	ASN	-	expression tag	UNP A0A0G2RQ73
A	293	LEU	-	expression tag	UNP A0A0G2RQ73
A	294	TYR	-	expression tag	UNP A0A0G2RQ73
A	295	PHE	-	expression tag	UNP A0A0G2RQ73
A	296	GLN	-	expression tag	UNP A0A0G2RQ73
C	85	VAL	ALA	engineered mutation	UNP A0A0G2RQ73
C	291	GLU	-	expression tag	UNP A0A0G2RQ73
C	292	ASN	-	expression tag	UNP A0A0G2RQ73
C	293	LEU	-	expression tag	UNP A0A0G2RQ73
C	294	TYR	-	expression tag	UNP A0A0G2RQ73
C	295	PHE	-	expression tag	UNP A0A0G2RQ73
C	296	GLN	-	expression tag	UNP A0A0G2RQ73

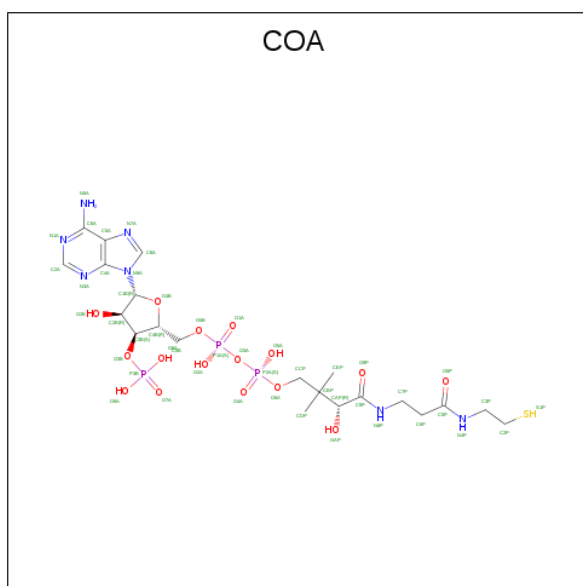
- Molecule 2 is a protein called Succinate–CoA ligase [ADP-forming] subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	387	Total	C	N	O	S		0	8	0
			2966	1880	505	568	13				
2	D	370	Total	C	N	O	S		0	10	0
			2850	1813	481	544	12				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	THR	ALA	engineered mutation	UNP Q5NHF3
D	69	THR	ALA	engineered mutation	UNP Q5NHF3

- Molecule 3 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	220	Total	O	0	1
			221	221		
6	B	323	Total	O	0	0
			323	323		
6	C	293	Total	O	0	0
			293	293		
6	D	240	Total	O	0	0
			240	240		

### 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.

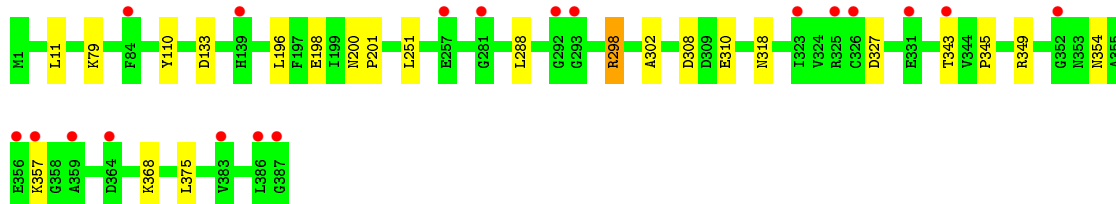
- Molecule 1: Succinate–CoA ligase [ADP-forming] subunit alpha



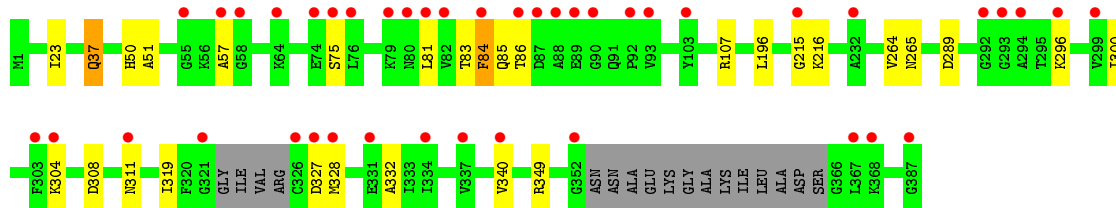
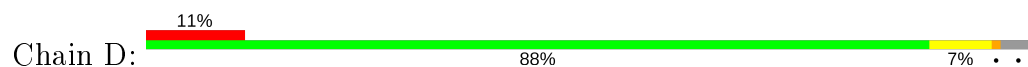
- Molecule 1: Succinate–CoA ligase [ADP-forming] subunit alpha



- Molecule 2: Succinate–CoA ligase [ADP-forming] subunit beta



- Molecule 2: Succinate–CoA ligase [ADP-forming] subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.91Å 158.34Å 73.58Å 90.00° 111.73° 90.00°	Depositor
Resolution (Å)	38.18 – 1.78 38.15 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.18-1.78) 99.6 (38.15-1.78)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.176 , 0.214 0.185 , 0.221	Depositor DCC
$R_{free}$ test set	6633 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11352	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, MG, EDO, NEP

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	0.62	0/2194	0.70	0/2973
1	C	0.70	0/2214	0.73	0/2998
2	B	0.59	0/3028	0.71	0/4082
2	D	0.60	0/2915	0.75	0/3927
All	All	0.62	0/10351	0.72	0/13980

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	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	ARG	Sidechain
2	B	298	ARG	Sidechain

## 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	2163	0	2219	5	0
1	C	2182	0	2232	6	0
2	B	2966	0	3048	12	0
2	D	2850	0	2929	20	0
3	A	48	0	32	0	0
3	C	48	0	32	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	B	8	0	12	0	0
5	D	8	0	12	0	0
6	A	221	0	0	1	0
6	B	323	0	0	1	0
6	C	293	0	0	1	0
6	D	240	0	0	0	0
All	All	11352	0	10516	42	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 2.

All (42) 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)
2:B:368:LYS:HE3	2:D:311:ASN:ND2	2.19	0.57
2:D:85:GLN:O	2:D:86:THR:HB	2.08	0.54
2:D:50:HIS:O	2:D:51:ALA:HB2	2.07	0.54
2:D:23:ILE:CD1	2:D:37:GLN:HG2	2.40	0.52
1:C:132:GLU:OE2	6:C:601:HOH:O	2.19	0.52
1:C:156:THR:HA	1:C:159:TYR:CD2	2.47	0.50
2:D:83:THR:C	2:D:85:GLN:H	2.15	0.49
2:D:296:LYS:O	2:D:300:ILE:HG13	2.13	0.48
2:B:327:ASP:HB3	2:B:357:LYS:HG2	1.93	0.48
2:D:23:ILE:HD11	2:D:37:GLN:HG2	1.95	0.48
1:C:193:LYS:HG2	1:C:221:TYR:OH	2.15	0.47
2:B:310:GLU:H	2:B:310:GLU:CD	2.18	0.47
2:D:300:ILE:CG2	2:D:304:LYS:HE3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:LEU:C	2:D:196:LEU:HD23	2.36	0.46
2:B:251:LEU:HD21	2:B:298:ARG:HG2	1.98	0.46
2:B:288:LEU:HD21	2:B:302:ALA:HB1	1.97	0.45
1:A:213:THR:CG2	1:A:256:LYS:HE2	2.47	0.45
2:D:84:PHE:CE1	2:D:85:GLN:HG3	2.53	0.44
1:A:118:ARG:NH2	1:A:190[B]:GLU:OE2	2.50	0.44
1:C:267:GLU:HG2	1:C:273:TYR:HE1	1.83	0.44
2:B:200:ASN:HA	2:B:201:PRO:HA	1.85	0.44
1:A:209:GLU:OE2	1:A:247:NEP:ND1	2.51	0.43
2:D:57:ALA:O	2:D:81:LEU:HD11	2.18	0.43
2:B:110:TYR:CE1	2:B:198:GLU:HG3	2.53	0.43
2:B:11:LEU:HD23	2:B:11:LEU:C	2.39	0.42
2:D:265:ASN:OD1	2:D:319:ILE:HA	2.20	0.42
2:D:296:LYS:HA	2:D:332:ALA:HB1	2.02	0.42
2:D:300:ILE:HG22	2:D:304:LYS:HE3	2.01	0.42
1:A:292:ASN:ND2	6:A:607:HOH:O	2.51	0.42
2:B:196:LEU:HD12	2:B:196:LEU:C	2.41	0.41
2:D:264:VAL:O	2:D:289:ASP:HA	2.21	0.41
2:B:345:PRO:HA	6:B:630:HOH:O	2.21	0.41
1:C:12:LEU:O	1:C:69:SER:HA	2.21	0.41
2:D:340:VAL:O	2:D:340:VAL:HG12	2.21	0.41
1:A:156:THR:HA	1:A:159:TYR:CD2	2.56	0.41
1:C:17:THR:OG1	3:C:501:COA:O8A	2.36	0.40
2:D:83:THR:C	2:D:85:GLN:N	2.74	0.40
2:B:318:ASN:HD21	2:B:375:LEU:HD11	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/296 (99%)	284 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	295/296 (100%)	286 (97%)	9 (3%)	0	100	100
2	B	393/387 (102%)	390 (99%)	3 (1%)	0	100	100
2	D	374/387 (97%)	360 (96%)	14 (4%)	0	100	100
All	All	1355/1366 (99%)	1320 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/227 (100%)	224 (99%)	3 (1%)	69	59
1	C	229/227 (101%)	227 (99%)	2 (1%)	78	72
2	B	316/308 (103%)	311 (98%)	5 (2%)	62	51
2	D	305/308 (99%)	295 (97%)	10 (3%)	38	21
All	All	1077/1070 (101%)	1057 (98%)	20 (2%)	59	43

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	LYS
1	A	256	LYS
1	A	267	GLU
2	B	79	LYS
2	B	133	ASP
2	B	308	ASP
2	B	349	ARG
2	B	354	ASN
1	C	50	ASP
1	C	134	LYS
2	D	37	GLN
2	D	75	SER
2	D	84	PHE

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Mol	Chain	Res	Type
2	D	107	ARG
2	D	216[A]	LYS
2	D	216[B]	LYS
2	D	308	ASP
2	D	327	ASP
2	D	328	MET
2	D	349	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	26	HIS
1	C	14	GLN
2	D	176	ASN
2	D	311	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	NEP	A	247	1,4	10,14,15	6.23	4 (40%)	5,20,22	1.75	1 (20%)
1	NEP	C	247	1,4	10,14,15	2.95	2 (20%)	5,20,22	2.64	4 (80%)

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	NEP	A	247	1,4	-	1/5/12/14	0/1/1/1
1	NEP	C	247	1,4	-	1/5/12/14	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	NEP	P-O3P	19.07	1.64	1.47
1	C	247	NEP	P-O3P	7.71	1.54	1.47
1	C	247	NEP	CD2-CG	4.00	1.42	1.36
1	A	247	NEP	CD2-CG	3.21	1.41	1.36
1	A	247	NEP	CD2-NE2	-2.20	1.35	1.39
1	A	247	NEP	P-O1P	-2.05	1.50	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	247	NEP	CB-CG-CD2	3.35	134.84	127.95
1	C	247	NEP	O1P-P-O3P	-3.14	106.65	113.44
1	A	247	NEP	CB-CA-C	-3.03	105.78	111.47
1	C	247	NEP	CB-CA-C	-2.65	106.50	111.47
1	C	247	NEP	O2P-P-O1P	2.27	115.50	106.57

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	247	NEP	CA-CB-CG-CD2
1	C	247	NEP	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	247	NEP	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	EDO	D	502	-	3,3,3	0.72	0	2,2,2	0.24	0
5	EDO	B	401	-	3,3,3	0.65	0	2,2,2	0.35	0
3	COA	C	501	-	41,50,50	1.08	3 (7%)	52,75,75	1.60	11 (21%)
3	COA	A	501	-	41,50,50	1.02	3 (7%)	52,75,75	1.38	8 (15%)
5	EDO	B	402	-	3,3,3	0.40	0	2,2,2	0.48	0
5	EDO	D	501	-	3,3,3	0.34	0	2,2,2	0.40	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	EDO	D	502	-	-	0/1/1/1	-
5	EDO	B	401	-	-	0/1/1/1	-
3	COA	C	501	-	-	1/44/64/64	0/3/3/3
3	COA	A	501	-	-	1/44/64/64	0/3/3/3
5	EDO	B	402	-	-	0/1/1/1	-
5	EDO	D	501	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	COA	P3B-O3B	3.43	1.65	1.59
3	A	501	COA	C5A-C4A	2.68	1.48	1.40
3	A	501	COA	C4A-N3A	2.63	1.39	1.35
3	A	501	COA	O4B-C1B	2.44	1.44	1.41
3	C	501	COA	C4A-N3A	2.36	1.38	1.35
3	C	501	COA	C2A-N3A	2.28	1.35	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	COA	N3A-C2A-N1A	-5.20	120.55	128.68
3	C	501	COA	C5A-C6A-N6A	-4.20	113.96	120.35
3	A	501	COA	N3A-C2A-N1A	-3.85	122.66	128.68
3	A	501	COA	O4B-C1B-C2B	-3.62	101.63	106.93
3	A	501	COA	CEP-CBP-CAP	3.59	115.05	108.82
3	C	501	COA	C1B-N9A-C4A	-3.36	120.74	126.64
3	C	501	COA	O8A-P3B-O7A	3.06	122.67	110.68
3	A	501	COA	C2A-N1A-C6A	2.76	123.47	118.75
3	C	501	COA	O5A-P2A-O4A	2.72	125.71	112.24
3	C	501	COA	N6A-C6A-N1A	2.69	124.16	118.57
3	C	501	COA	O2B-C2B-C3B	2.52	118.32	111.17
3	C	501	COA	O2A-P1A-O1A	2.51	124.65	112.24
3	A	501	COA	N6A-C6A-N1A	2.34	123.43	118.57
3	C	501	COA	O9P-C9P-N8P	-2.34	117.97	122.99
3	A	501	COA	C7P-C6P-C5P	-2.21	108.68	112.36
3	A	501	COA	O6A-P2A-O4A	-2.20	100.47	109.07
3	C	501	COA	P2A-O3A-P1A	-2.14	125.47	132.83
3	C	501	COA	O4B-C4B-C3B	2.13	109.43	104.87
3	A	501	COA	CEP-CBP-CDP	-2.02	105.05	109.17

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	COA	O4B-C4B-C5B-O5B
5	D	501	EDO	O1-C1-C2-O2
3	A	501	COA	O4B-C4B-C5B-O5B

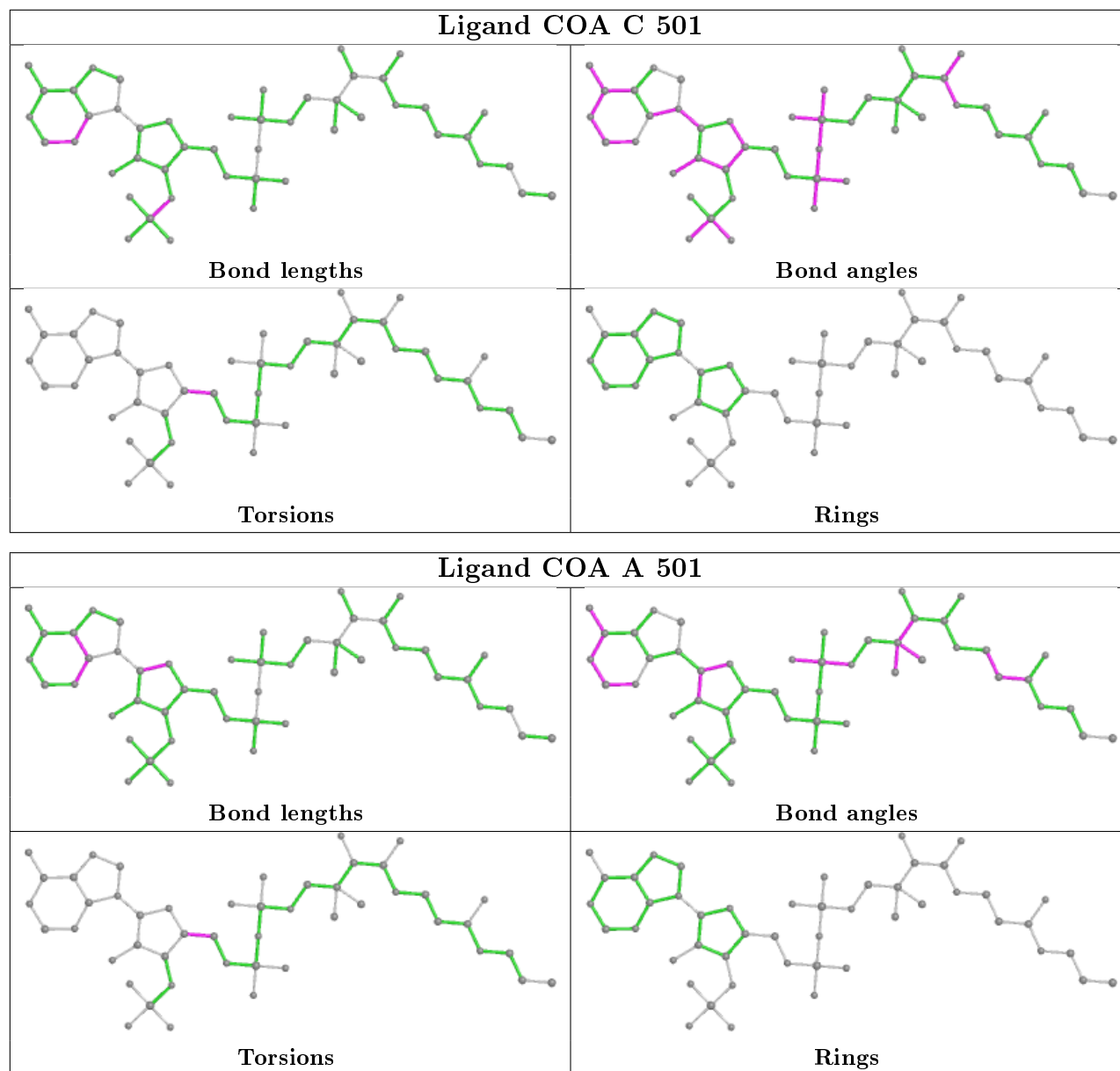
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	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, 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	292/296 (98%)	0.03	11 (3%) 40 39	14, 25, 39, 55	0
1	C	294/296 (99%)	-0.15	1 (0%) 94 93	12, 19, 29, 52	0
2	B	387/387 (100%)	0.12	19 (4%) 29 28	12, 27, 48, 64	0
2	D	370/387 (95%)	0.44	42 (11%) 5 4	12, 31, 59, 79	0
All	All	1343/1366 (98%)	0.13	73 (5%) 25 24	12, 24, 49, 79	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	84	PHE	7.8
2	D	292	GLY	7.4
2	D	367	LEU	7.1
2	D	82	VAL	6.4
2	B	387	GLY	5.1
2	D	352	GLY	5.0
2	D	58	GLY	4.8
2	D	326	CYS	4.7
1	C	255	GLY	4.7
2	D	293	GLY	4.6
2	D	75	SER	4.5
2	B	386	LEU	4.4
2	D	328	MET	4.3
1	A	255	GLY	4.3
2	D	334	ILE	4.3
1	A	293	LEU	4.2
2	B	326	CYS	4.1
2	D	103	TYR	4.1
2	B	325	ARG	4.0
2	D	89	GLU	3.9
2	B	323	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	327	ASP	3.8
2	D	294	ALA	3.6
2	D	81	LEU	3.6
2	D	55	GLY	3.5
1	A	292	ASN	3.4
2	D	76	LEU	3.4
2	D	215[A]	GLY	3.4
2	D	340	VAL	3.4
2	B	257[A]	GLU	3.3
1	A	268	ALA	3.2
2	D	88	ALA	3.1
2	B	293	GLY	3.1
2	D	57	ALA	3.0
2	B	84	PHE	3.0
2	D	368	LYS	2.9
2	D	87	ASP	2.9
2	B	357	LYS	2.8
2	D	86	THR	2.8
2	B	352	GLY	2.7
2	D	311	ASN	2.7
2	D	92	PRO	2.7
1	A	290	TRP	2.7
2	D	74	GLU	2.6
1	A	179	GLY	2.6
1	A	291	GLU	2.5
1	A	178	ILE	2.5
2	B	383	VAL	2.5
2	D	90	GLY	2.5
2	D	337	VAL	2.4
2	D	321	GLY	2.4
2	D	80	ASN	2.4
2	B	139	HIS	2.4
2	B	359	ALA	2.4
2	D	296	LYS	2.3
2	B	292	GLY	2.3
2	D	79	LYS	2.3
2	B	343[A]	THR	2.3
2	B	364	ASP	2.2
1	A	254	GLY	2.2
2	D	303	PHE	2.2
2	D	232	ALA	2.2
2	D	93	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	294	TYR	2.2
2	B	331	GLU	2.2
2	D	299	VAL	2.2
2	B	281	GLY	2.1
2	B	356	GLU	2.1
1	A	157	LEU	2.1
2	D	331	GLU	2.1
2	D	304	LYS	2.0
2	D	64	LYS	2.0
2	D	387	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	NEP	A	247	14/15	0.93	0.12	20,24,26,29	4
1	NEP	C	247	14/15	0.95	0.09	16,19,23,23	4

## 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, 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.

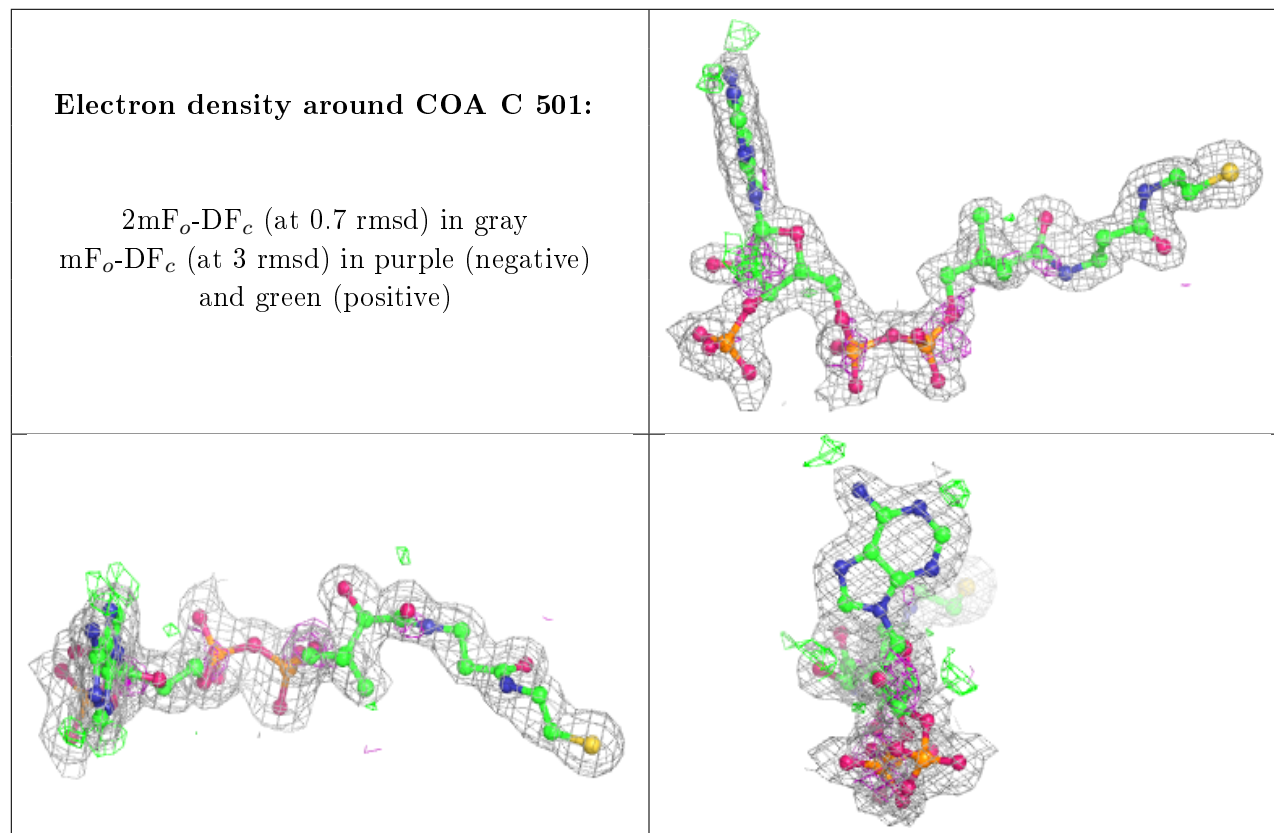
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	B	402	4/4	0.90	0.09	37,37,38,38	0
5	EDO	D	502	4/4	0.92	0.09	28,29,30,31	0
3	COA	C	501	48/48	0.93	0.12	25,27,29,30	0
3	COA	A	501	48/48	0.94	0.10	23,25,27,29	0
5	EDO	D	501	4/4	0.95	0.09	33,33,34,35	0
5	EDO	B	401	4/4	0.97	0.06	20,20,21,21	0

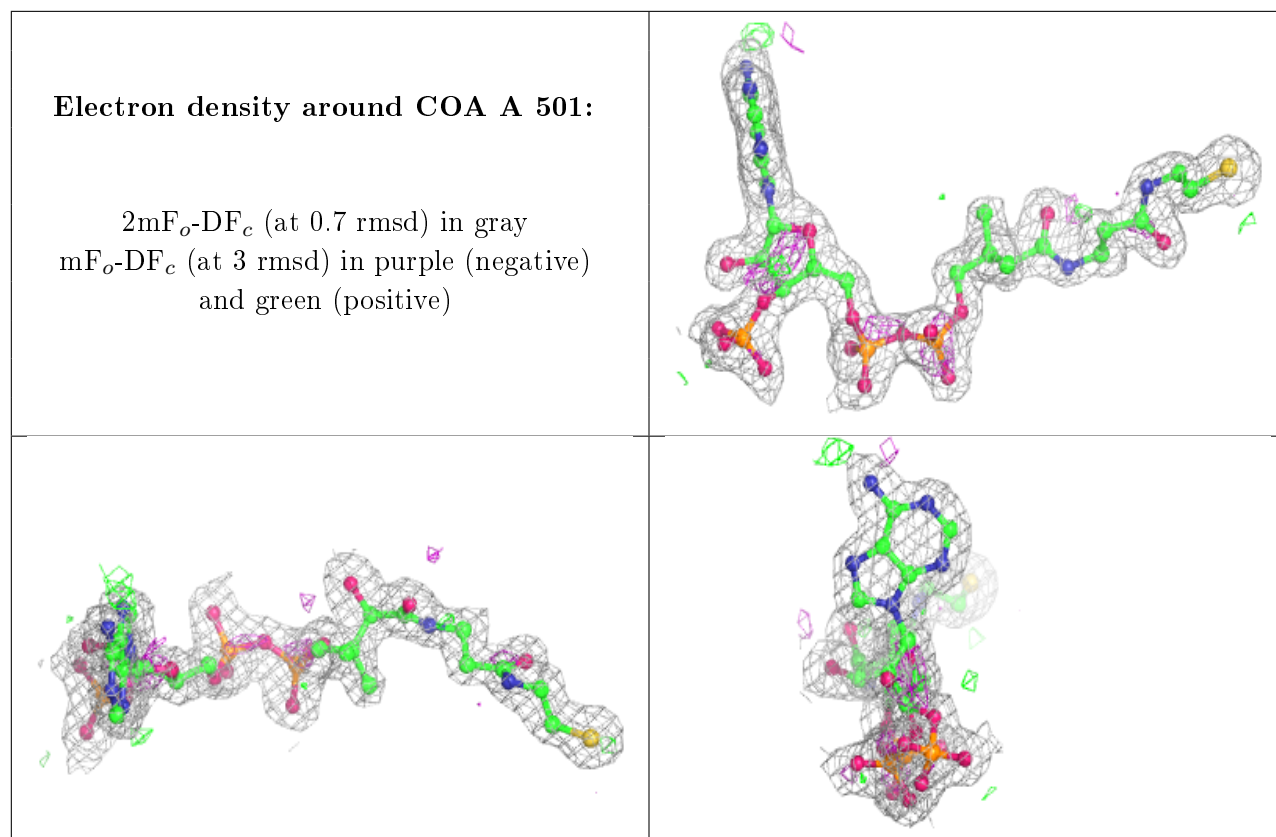
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	502	1/1	0.97	0.03	29,29,29,29	0
4	MG	C	502	1/1	0.98	0.04	25,25,25,25	0

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.