

# Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2021 – 02:10 pm BST

PDB ID : 704R

Title: Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme

with Coenzyme A bound at the thiolase active sites and additional binding

site (CoA(HAD/KAT))

Authors: Dalwani, S.; Wierenga, R.K.; Venkatesan, R.

Deposited on : 2021-04-07

Resolution : 2.79 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

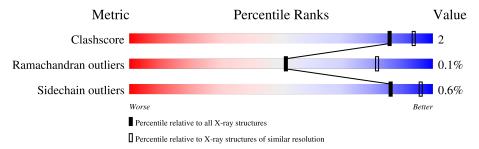
Validation Pipeline (wwPDB-VP) : 2.23.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.79 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{resolution range}( ext{Å}))$
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 >=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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain	
1	A	736	94%	5% •
1	В	736	94%	5% •
2	С	403	90%	10%
2	D	403	90%	8% •



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17229 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 3-hydroxyacyl-CoA dehydrogenase.

Mol	Chain	Residues		${f Atoms}$					AltConf	Trace
1	A	729	Total 5416	C 3425	N 933	O 1037	S 21	0	0	0
1	В	728	Total 5396	C 3414	N 929	O 1032	S 21	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP O53872
A	-14	GLY	_	expression tag	UNP O53872
A	-13	SER	-	expression tag	UNP O53872
A	-12	SER	-	expression tag	UNP O53872
A	-11	HIS	=	expression tag	UNP O53872
A	-10	HIS	-	expression tag	UNP O53872
A	-9	HIS	-	expression tag	UNP O53872
A	-8	HIS	_	expression tag	UNP O53872
A	-7	HIS	-	expression tag	UNP O53872
A	-6	HIS	-	expression tag	UNP O53872
A	-5	SER	_	- expression tag	
A	-4	GLN	_	expression tag	UNP O53872
A	-3	ASP	_	expression tag	UNP O53872
A	-2	PRO	_	expression tag	UNP O53872
A	-1	ASN	_	expression tag	UNP O53872
A	0	SER	_	expression tag	UNP O53872
В	-15	MET	_	initiating methionine	UNP O53872
В	-14	GLY	_	expression tag	UNP O53872
В	-13	SER	-	expression tag	UNP O53872
В	-12	SER	-	expression tag	UNP O53872
В	-11	HIS	_	expression tag	UNP O53872
В	-10	HIS	_	expression tag	UNP O53872
В	-9	HIS	-	expression tag	UNP O53872
В	-8	HIS	-	expression tag	UNP O53872
В	-7	HIS	-	expression tag	UNP O53872



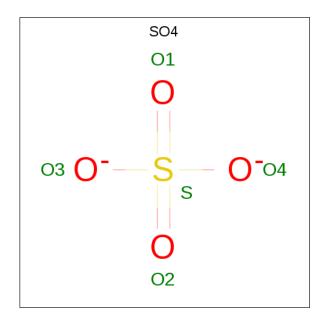
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Chain	Residue	Modelled	Actual	Comment	Reference
В	-6	HIS	_	expression tag	UNP O53872
В	-5	SER	-	expression tag	UNP O53872
В	-4	GLN	_	expression tag	UNP O53872
В	-3	ASP	-	expression tag	UNP O53872
В	-2	PRO	-	expression tag	UNP O53872
В	-1	ASN	-	expression tag	UNP O53872
В	0	SER	=	expression tag	UNP O53872

• Molecule 2 is a protein called Putative acyltransferase Rv0859.

Mol	Chain	Residues		Atoms					AltConf	Trace
9	С	402	Total	С	N	О	S	0	0	0
	402	2964	1852	524	573	15	0	0		
2	D	392	Total	С	N	О	S	0	0	0
	2 D	392	2901	1810	515	562	14	0	0	

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



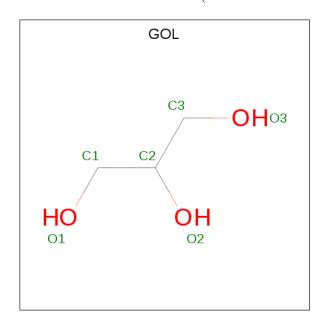
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

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Mol	Chain	$oxed{ \mathbf{Residues} }$	Atoms	ZeroOcc	AltConf
2			Total O S		
3	A	1	5 4 1	0	0
3	A	1	Total O S	0	0
	11	1	5 4 1	0	U
3	В	1	Total O S	0	0
			5 4 1 Total O S		
3	В	1	Total O S 5 4 1	0	0
			Total O S		
3	В	1	5 4 1	0	0
			Total O S		
3	В	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	0
3	В	1	Total O S	0	0
3	D	1		0	0
3	С	1	Total O S	0	0
		1	5 4 1	Ů,	0
3	$^{\rm C}$	1	Total O S	0	0
			5 4 1		
3	С	1	Total O S	0	0
			5 4 1 Total O S		
3	С	1	$\begin{bmatrix} 10tal & 0 & 5 \\ 5 & 4 & 1 \end{bmatrix}$	0	0
			Total O S		
3	С	1	5 4 1	0	0
2	0	7	Total O S	0	0
3	С	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	0
3	С	1	Total O S	0	0
	0	1	5 4 1	U	U
3	C	1	Total O S	0	0
		_	5 4 1		
3	D	1	Total O S	0	0
			5 4 1 Total O S		
3	D	1	$\begin{bmatrix} 10 & 10 & 10 & 10 \\ 5 & 4 & 1 \end{bmatrix}$	0	0
			Total O S		
3	D	1	5 4 1	0	0
	D	4	Total O S	0	0
3	D	1	5 4 1	0	0
3	D	1	Total O S	0	0
<u> </u>	ע	1	5 4 1	U	U
3	D	1	Total O S	0	0
		<u> </u>	5 4 1		

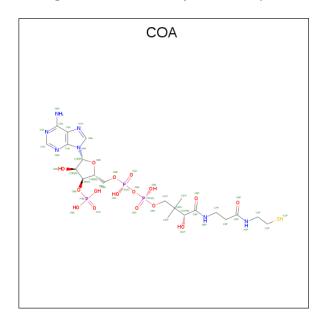


• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0

• Molecule 5 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	C	1	Total	С	N	О	Р	S	0	0
) 3		1	48	21	7	16	3	1	U	U



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Mol	Chain	Residues	${f Atoms}$						ZeroOcc	AltConf
5		C 1	Total	С	N	О	Р	S	0	0
5			48	21	7	16	3	1	0	U
5	D	1	Total	С	N	О	Р	S	0	0
5	ש	1	48	21	7	16	3	1		
5	5 D	1	Total	С	N	О	Р	S	0	0
3		1	48	21	7	16	3	1	0	

### • Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	64	Total O 64 64	0	0
6	В	78	Total O 78 78	0	0
6	С	58	Total O 58 58	0	0
6	D	29	Total O 29 29	0	0

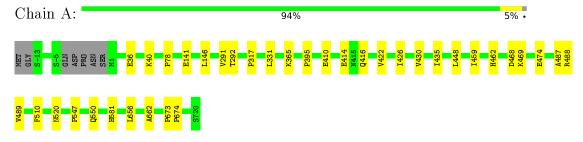


# 3 Residue-property plots (i)

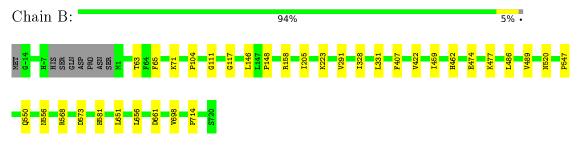
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

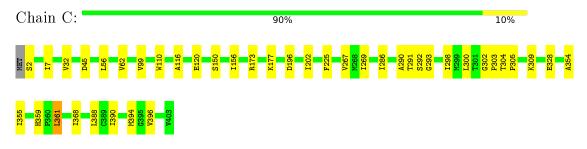
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase



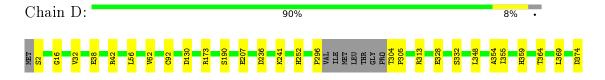
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase



• Molecule 2: Putative acyltransferase Rv0859



• Molecule 2: Putative acyltransferase Rv0859









# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	248.25Å 135.75Å 119.30Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 110.51° 90.00°	Depositor
Resolution (Å)	48.50 - 2.79	Depositor
% Data completeness	86.8 (48.50-2.79)	Depositor
(in resolution range)	00.0 (40.00 2.10)	Берозног
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PHENIX 1.18.2_3874	Depositor
$R, R_{free}$	0.178 , 0.216	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP



# 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: COA, SO4, GOL

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
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5
1	A	0.24	0/5519	0.40	0/7473
1	В	0.24	0/5501	0.40	0/7449
2	С	0.24	0/3009	0.43	0/4075
2	D	0.24	0/2943	0.41	0/3981
All	All	0.24	0/16972	0.41	0/22978

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	5416	0	5431	18	0
1	В	5396	0	5416	16	0
2	С	2964	0	2979	27	0
2	D	2901	0	2910	19	0
3	A	30	0	0	0	0
3	В	25	0	0	1	0
3	С	40	0	0	0	0
3	D	30	0	0	0	0
4	A	6	0	8	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	С	96	0	64	0	0
5	D	96	0	64	1	0
6	A	64	0	0	0	0
6	В	78	0	0	1	0
6	С	58	0	0	0	0
6	D	29	0	0	0	0
All	All	17229	0	16872	75	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 (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
2:C:2:SER:N	2:D:2:SER:HG	1.81	0.77
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.80	0.63
2:D:173:ARG:NH2	2:D:348:LEU:O	2.31	0.57
2:C:2:SER:N	2:D:2:SER:OG	2.37	0.57
2:C:291:THR:HG22	2:C:396:VAL:HG22	1.86	0.57
2:D:190:SER:OG	2:D:374:ASP:OD2	2.20	0.55
2:D:252:HIS:HE1	2:D:332:SER:H	1.54	0.55
2:C:150:SER:HB3	2:C:225:PHE:CG	2.42	0.54
1:B:459:ILE:HG21	1:B:489:VAL:HG21	1.88	0.54
2:D:369:LEU:HD12	2:D:386:ILE:HD13	1.90	0.53
2:C:62:VAL:HG12	2:D:62:VAL:HG12	1.91	0.53
2:D:92:CYS:SG	5:D:507:COA:S1P	3.01	0.53
1:A:459:ILE:HG21	1:A:489:VAL:HG21	1.91	0.52
2:D:354:ALA:HB1	2:D:359:HIS:HB2	1.91	0.52
1:A:547:PRO:HG2	1:A:550:GLN:HB3	1.92	0.51
2:C:390:ILE:HB	2:C:394:MET:HB2	1.92	0.51
2:C:196:ASP:HB3	2:C:202:ILE:HD11	1.93	0.50
1:B:158:ARG:NH1	6:B:902:HOH:O	2.44	0.50
2:C:99:VAL:HG13	2:C:269:ILE:HD11	1.94	0.49
2:D:38:GLU:HG3	2:D:42:ARG:HD2	1.95	0.49
2:C:390:ILE:HD11	2:C:396:VAL:HG23	1.94	0.49
1:B:63:THR:HA	1:B:111:GLY:HA3	1.93	0.49
1:A:426:ILE:HG22	1:A:430:VAL:HG13	1.96	0.48
1:B:547:PRO:HG2	1:B:550:GLN:HB3	1.95	0.47
1:B:477:LYS:HB2	1:B:486:LEU:HD11	1.96	0.47
1:B:146:LEU:HD22	1:B:291:VAL:HG22	1.96	0.47
2:C:156:ILE:HG12	2:C:298:ILE:HD11	1.97	0.47



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Continuea from prev		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	overlap (Å)
1:A:36:GLU:HG3	1:A:40:LYS:HE3	1.96	0.47
2:C:354:ALA:HB1	2:C:359:HIS:HB2	1.96	0.47
1:A:416:GLN:HG3	1:A:448:LEU:HD23	1.97	0.46
2:C:120:GLU:HG2	2:C:361:LEU:HB2	1.97	0.46
2:C:302:GLY:N	2:C:303:PRO:HD2	2.31	0.46
2:C:290:ALA:HB1	2:C:309:LYS:HD3	1.97	0.46
2:C:368:ILE:HD11	2:C:388:LEU:HD11	1.98	0.46
2:D:359:HIS:ND1	2:D:364:THR:OG1	2.41	0.45
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.99	0.44
1:A:331:LEU:HB2	1:A:410:GLU:HA	1.99	0.44
2:C:32:VAL:HG11	2:C:56:LEU:HD11	2.00	0.44
1:A:435:ILE:HD11	1:A:488:ARG:HD3	1.99	0.44
1:A:146:LEU:HD22	1:A:291:VAL:HG22	2.00	0.44
2:D:328:GLU:HB3	2:D:355:ILE:HG13	1.99	0.44
1:A:510:PHE:CD1	1:A:656:LEU:HD11	2.53	0.43
2:C:116:ALA:O	2:C:267:VAL:N	2.42	0.43
1:A:317:PRO:HG2	1:A:487:ALA:HB2	2.00	0.43
1:A:520:ASN:HB3	1:A:581:HIS:CE1	2.54	0.43
1:B:104:PRO:HG2	1:B:205:ILE:HG23	1.99	0.43
2:C:328:GLU:HB3	2:C:355:ILE:HG13	2.01	0.43
2:D:16:GLY:HA2	2:D:207:GLU:HG2	2.00	0.43
2:D:304:THR:HB	2:D:305:PRO:HD3	2.01	0.43
2:D:62:VAL:HG11	2:D:130:ASP:HA	2.00	0.43
2:D:241:LYS:NZ	2:D:296:PRO:HG2	2.34	0.43
1:A:468:ASP:OD1	1:A:468:ASP:N	2.52	0.42
1:A:331:LEU:HD13	1:A:422:VAL:HG12	2.00	0.42
1:A:673:PRO:HA	1:A:674:PRO:HD3	1.93	0.42
2:C:292:SER:HB3	2:C:293:GLY:H	1.71	0.42
1:B:520:ASN:HB3	1:B:581:HIS:CE1	2.54	0.42
1:A:78:PRO:HA	1:A:292:THR:HB	2.02	0.42
2:C:302:GLY:O	2:C:305:PRO:HD2	2.20	0.42
2:C:298:ILE:O	2:C:300:LEU:N	2.51	0.42
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.55	0.42
1:A:656:LEU:HD13	1:A:662:ALA:HB2	2.01	0.41
1:B:65:PHE:HB3	1:B:117:GLY:HA3	2.02	0.41
2:C:7:ILE:HD11	2:C:286:ILE:HD11	2.02	0.41
1:B:223:LYS:NZ	3:B:805:SO4:O4	2.51	0.41
2:C:110:TRP:O	2:D:313:ARG:NH1	2.54	0.41
1:B:698:VAL:HG13	1:B:714:PRO:HG3	2.02	0.41
1:B:651:LEU:HD23	1:B:656:LEU:HB2	2.04	0.40
2:D:32:VAL:HG11	2:D:56:LEU:HD11	2.03	0.40



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Atom-1	Atom-2	$egin{array}{l}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{array}$	$egin{array}{c}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{array}$
1:A:365:LYS:HD2	1:A:395:PRO:HD3	2.02	0.40
1:B:331:LEU:HD13	1:B:422:VAL:HG12	2.01	0.40
2:C:304:THR:HB	2:C:305:PRO:HD3	2.02	0.40
2:C:390:ILE:HD12	2:C:394:MET:HB3	2.03	0.40
1:B:328:ILE:HD13	1:B:407:PHE:HB3	2.02	0.40
1:B:568:ARG:HB3	1:B:568:ARG:HH11	1.86	0.40
2:C:173:ARG:NH1	2:C:177:LYS:HE2	2.36	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	${ m ntiles}$
1	A	725/736~(98%)	702 (97%)	23 (3%)	0	100	100
1	В	725/736~(98%)	706 (97%)	18 (2%)	1 (0%)	51	81
2	С	400/403~(99%)	386 (96%)	13 (3%)	1 (0%)	41	72
2	D	386/403~(96%)	373 (97%)	13 (3%)	0	100	100
All	All	$2236/2278 \ (98\%)$	2167 (97%)	67 (3%)	2 (0%)	51	81

#### All (2) Ramachandran outliers are listed below:

Mol	Chain	${f Res}$	$\mathbf{Type}$
2	С	361	LEU
1	В	148	PRO

#### 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	Percent	iles
1	A	556/566~(98%)	553 (100%)	3 (0%)	88 9	6
1	В	553/566~(98%)	549 (99%)	4 (1%)	84 9	5
2	С	308/310 (99%)	307 (100%)	1 (0%)	92 9	8
2	D	$302/310 \ (97\%)$	299 (99%)	3 (1%)	76 9	3
All	All	1719/1752 (98%)	1708 (99%)	11 (1%)	86 9	6

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	GLU
1	A	414	GLU
1	A	469	LYS
1	В	71	LYS
1	В	556	ASN
1	В	573	ASP
1	В	661	ASP
2	С	45	ASP
2	D	236	ASP
2	D	387	THR
2	D	388	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



### 5.6 Ligand geometry (i)

30 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	T	Chain	Dog	T in le	Во	Bond lengths			Bond angles			
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2		
3	SO4	С	507	-	4,4,4	0.14	0	6,6,6	0.05	0		
5	COA	С	508	-	41,50,50	0.60	0	52,75,75	0.75	2 (3%)		
3	SO4	С	502	-	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	В	803	-	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	D	508	-	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	С	501	-	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	D	501	_	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	В	805	_	4,4,4	0.14	0	6,6,6	0.04	0		
3	SO4	D	503	_	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	A	802	-	4,4,4	0.14	0	6,6,6	0.04	0		
3	SO4	С	506	_	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	В	804	_	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	В	802	_	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	С	505	_	4,4,4	0.14	0	6,6,6	0.05	0		
5	COA	D	506	-	41,50,50	0.58	0	52,75,75	0.76	2 (3%)		
5	COA	D	507	_	41,50,50	0.59	0	52,75,75	0.77	2 (3%)		
3	SO4	A	805	-	4,4,4	0.14	0	6,6,6	0.04	0		
3	SO4	A	803	-	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	С	503	-	4,4,4	0.14	0	6,6,6	0.05	0		
4	GOL	A	806	_	5,5,5	0.92	0	5,5,5	0.99	0		
3	SO4	A	801	_	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	С	504	-	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	D	504	_	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	D	502	_	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	A	807	-	4,4,4	0.14	0	6,6,6	0.05	0		
5	COA	С	509	-	41,50,50	0.60	0	52,75,75	0.79	2 (3%)		
3	SO4	A	804	-	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	С	510	-	4,4,4	0.14	0	6,6,6	0.05	0		
3	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.04	0		
3	SO4	В	801	-	4,4,4	0.14	0	6,6,6	0.04	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	507	-	-	11/44/64/64	0/3/3/3
5	COA	С	508	-	-	12/44/64/64	0/3/3/3
5	COA	С	509	-	-	4/44/64/64	0/3/3/3
4	$\operatorname{GOL}$	A	806	_	-	2/4/4/4	-
5	COA	D	506	_	-	0/44/64/64	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(^o)$	$Ideal(^{o})$
5	D	507	COA	O6A-CCP-CBP	-2.51	106.52	110.55
5	D	506	COA	O4B-C1B-C2B	-2.35	103.49	106.93
5	D	506	COA	C5A-C6A-N6A	2.35	123.92	120.35
5	С	508	COA	O4B-C1B-C2B	-2.30	103.57	106.93
5	D	507	COA	C5A-C6A-N6A	2.29	123.83	120.35
5	С	509	COA	C5A-C6A-N6A	2.27	123.80	120.35
5	С	508	COA	C5A-C6A-N6A	2.16	123.64	120.35
5	С	509	COA	O4B-C1B-C2B	-2.11	103.84	106.93

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	806	GOL	C1-C2-C3-O3
5	С	508	COA	P1A-O3A-P2A-O6A
5	С	508	COA	CCP-O6A-P2A-O3A
5	С	508	COA	OAP-CAP-CBP-CCP
5	С	508	COA	C9P-CAP-CBP-CCP
5	С	508	COA	OAP-CAP-CBP-CDP
5	С	508	COA	C9P-CAP-CBP-CDP
5	С	508	COA	OAP-CAP-CBP-CEP
5	С	508	COA	C9P-CAP-CBP-CEP
5	D	507	COA	C5B-O5B-P1A-O2A
5	D	507	COA	CCP-O6A-P2A-O4A
5	D	507	COA	CAP-CBP-CCP-O6A
5	С	508	COA	C6P-C5P-N4P-C3P
5	С	509	COA	C6P-C5P-N4P-C3P



Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	С	509	COA	O5P-C5P-N4P-C3P
5	С	508	COA	O5P-C5P-N4P-C3P
4	A	806	GOL	O2-C2-C3-O3
5	D	507	COA	CDP-CBP-CCP-O6A
5	D	507	COA	CEP-CBP-CCP-O6A
5	D	507	COA	C5B-O5B-P1A-O3A
5	С	508	COA	CCP-O6A-P2A-O4A
5	D	507	COA	C5B-O5B-P1A-O1A
5	С	509	COA	C2P-C3P-N4P-C5P
5	С	508	COA	C4B-C5B-O5B-P1A
5	D	507	COA	C4B-C5B-O5B-P1A
5	D	507	COA	O9P-C9P-CAP-OAP
5	D	507	COA	CCP-O6A-P2A-O3A
5	D	507	COA	C6P-C7P-N8P-C9P
5	С	509	COA	O4B-C4B-C5B-O5B

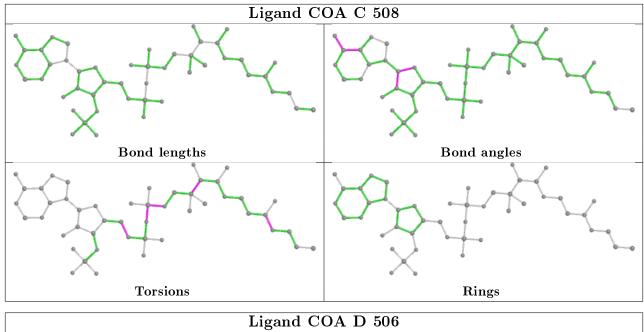
There are no ring outliers.

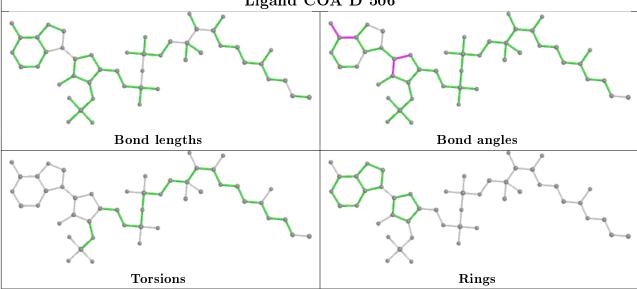
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	805	SO4	1	0
5	D	507	COA	1	0

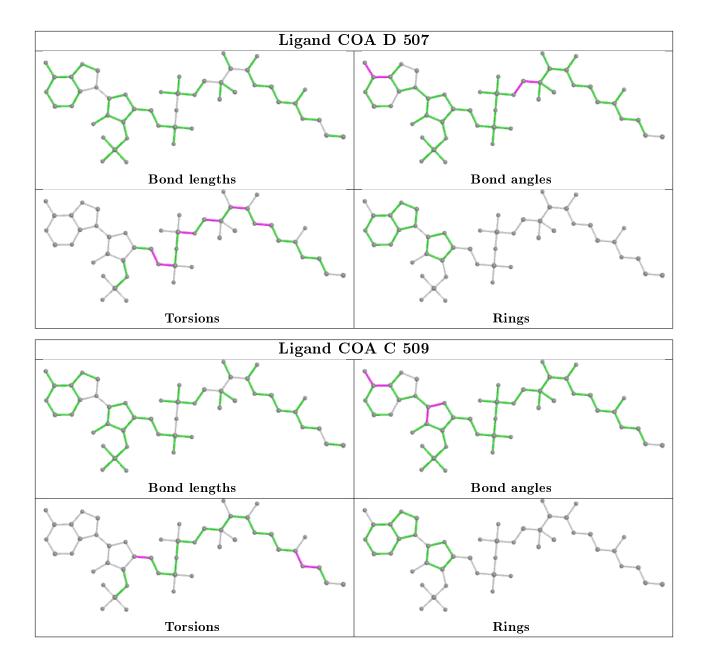
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.











## 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

