



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:04 AM UTC

PDB ID : 7O1I / pdb_00007o1i
Title : Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme
alpha-E141A mutant
Authors : Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on : 2021-03-29
Resolution : 2.30 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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)
Xtriage (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

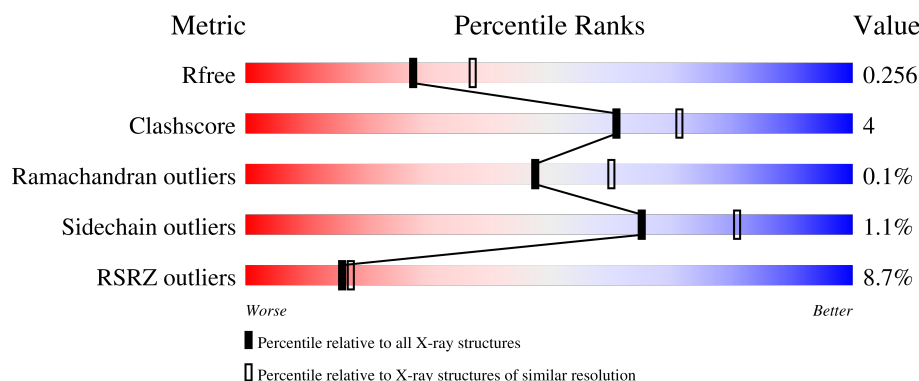
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	D	403	5% 91% 9%
2	A	736	11% 87% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8303 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 Putative acyltransferase Rv0859.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	401	Total	C	N	O	S	0	0	0
			2931	1835	522	559	15			

- Molecule 2 is a protein called 3-hydroxyacyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	726	Total	C	N	O	S	0	0	0
			5218	3312	895	991	20			

There are 17 discrepancies between the modelled and reference sequences:

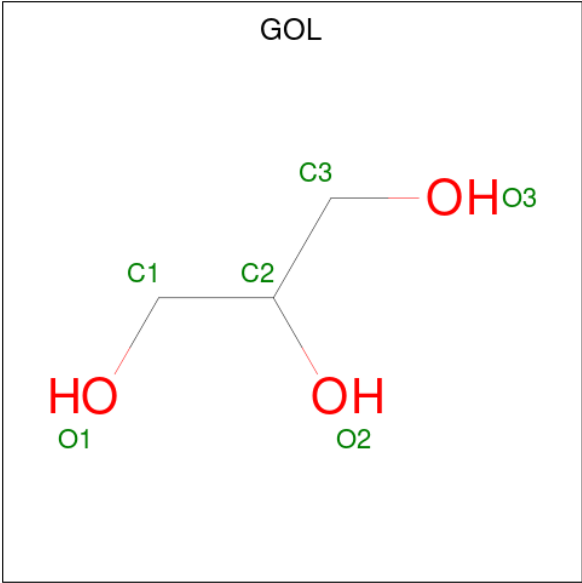
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP O53872
A	-10	GLY	-	expression tag	UNP O53872
A	-9	SER	-	expression tag	UNP O53872
A	-8	SER	-	expression tag	UNP O53872
A	-7	HIS	-	expression tag	UNP O53872
A	-6	HIS	-	expression tag	UNP O53872
A	-5	HIS	-	expression tag	UNP O53872
A	-5A	HIS	-	expression tag	UNP O53872
A	-5B	HIS	-	expression tag	UNP O53872
A	-5C	HIS	-	expression tag	UNP O53872
A	-5D	SER	-	expression tag	UNP O53872
A	-5E	GLN	-	expression tag	UNP O53872
A	-5F	ASP	-	expression tag	UNP O53872
A	-5G	PRO	-	expression tag	UNP O53872
A	-5H	ASN	-	expression tag	UNP O53872
A	-5I	SER	-	expression tag	UNP O53872
A	141	ALA	GLU	engineered mutation	UNP O53872

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



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

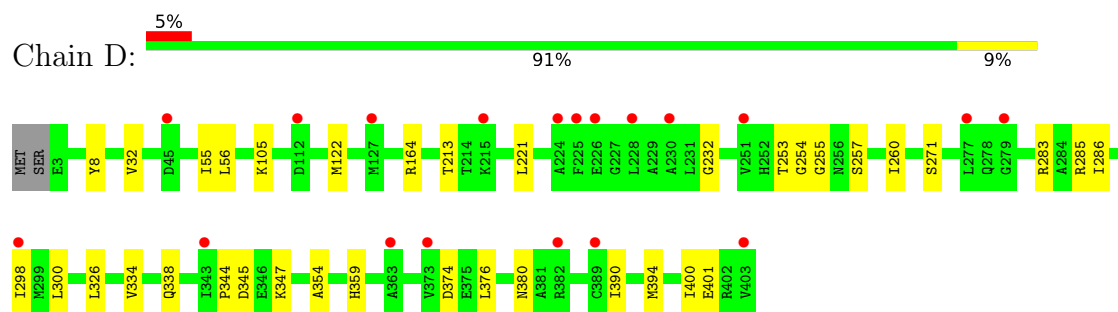
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	22	Total	O	0	0
			22	22		
6	A	22	Total	O	0	0
			22	22		

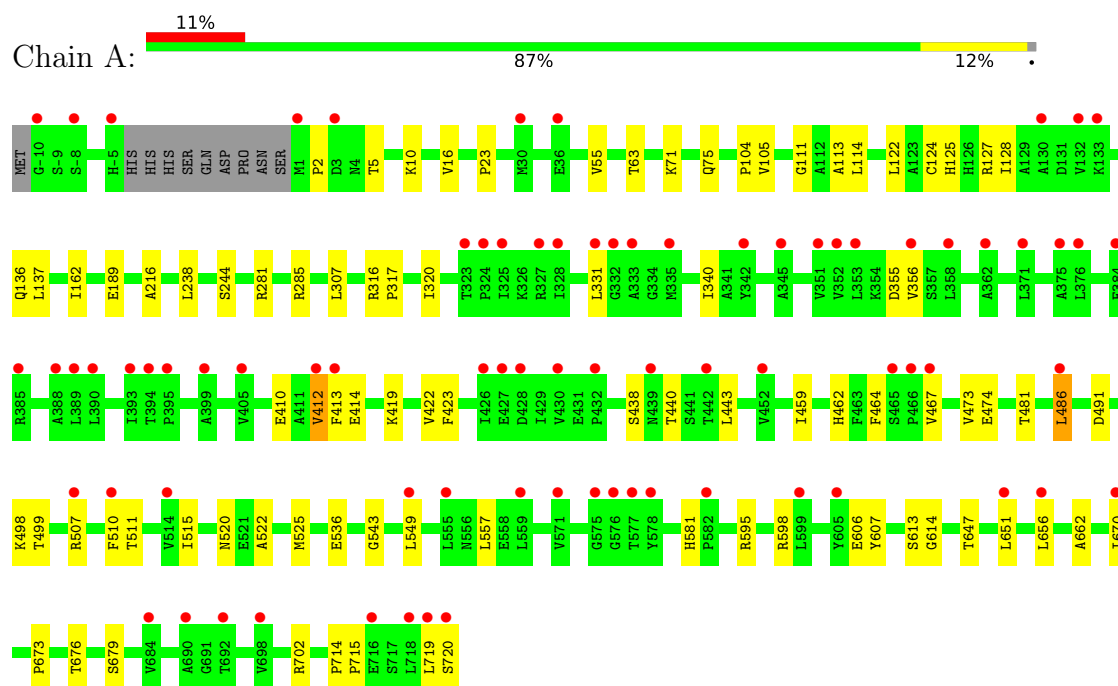
3 Residue-property plots [i](#)

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: Putative acyltransferase Rv0859



• Molecule 2: 3-hydroxyacyl-CoA dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.02Å 205.87Å 133.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.04 – 2.30 48.04 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.04-2.30) 99.5 (48.04-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.237 , 0.260 0.234 , 0.256	Depositor DCC
R_{free} test set	2092 reflections (3.35%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8303	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, CSO, GOL, 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	D	0.10	0/2968	0.28	0/4023
2	A	0.10	0/5318	0.26	0/7228
All	All	0.10	0/8286	0.27	0/11251

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

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	D	2931	0	2941	20	0
2	A	5218	0	5129	50	0
3	D	48	0	32	3	0
4	A	6	0	8	0	0
4	D	6	0	8	0	0
5	A	25	0	0	0	0
5	D	25	0	0	0	0
6	A	22	0	0	1	0
6	D	22	0	0	0	0
All	All	8303	0	8118	69	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 4.

All (69) 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:A:114:LEU:HD11	2:A:136:GLN:HB2	1.72	0.70
2:A:515:ILE:HG13	2:A:670:ILE:HD12	1.76	0.66
1:D:338:GLN:NE2	1:D:345:ASP:OD1	2.28	0.65
2:A:462:HIS:HB3	2:A:474:GLU:HB3	1.79	0.64
1:D:285:ARG:NH1	1:D:401:GLU:OE1	2.30	0.63
2:A:55:VAL:HB	2:A:105:VAL:HG12	1.79	0.63
2:A:127:ARG:NH2	6:A:903:HOH:O	2.34	0.61
2:A:113:ALA:HB3	2:A:137:LEU:HD23	1.84	0.60
1:D:283:ARG:NH2	1:D:374:ASP:OD1	2.34	0.60
2:A:410:GLU:HG3	2:A:438:SER:HA	1.84	0.60
2:A:719:LEU:HD12	2:A:719:LEU:H	1.67	0.59
1:D:213:THR:HG21	3:D:501:COA:H61A	1.70	0.57
2:A:702:ARG:HH22	2:A:720:SER:HB3	1.71	0.56
2:A:63:THR:HA	2:A:111:GLY:HA3	1.87	0.56
2:A:5:THR:HG22	2:A:23:PRO:HD2	1.87	0.56
1:D:257:SER:HB2	3:D:501:COA:H131	1.87	0.55
2:A:510:PHE:HE1	2:A:647:THR:HG22	1.72	0.55
2:A:355:ASP:OD1	2:A:356:VAL:N	2.33	0.54
2:A:595:ARG:HH22	2:A:606:GLU:HG2	1.72	0.54
2:A:316:ARG:NH2	2:A:320:ILE:O	2.41	0.54
2:A:412:VAL:HG12	2:A:413:PHE:H	1.72	0.53
2:A:316:ARG:NH1	2:A:491:ASP:OD1	2.42	0.52
1:D:286:ILE:HD13	1:D:400:ILE:HG22	1.92	0.52
2:A:598:ARG:HG2	2:A:607:TYR:CZ	2.46	0.51
1:D:253:THR:HG23	1:D:255:GLY:H	1.75	0.51
1:D:122:MET:HE2	1:D:260:ILE:HG23	1.93	0.51
2:A:440:THR:HG21	2:A:443:LEU:HB2	1.93	0.48
2:A:473:VAL:HG23	2:A:498:LYS:HD2	1.94	0.48
1:D:354:ALA:HB1	1:D:359:HIS:HB2	1.95	0.48
2:A:307:LEU:HD11	2:A:499:THR:HG21	1.95	0.48
2:A:520:ASN:HB3	2:A:581:HIS:CE1	2.49	0.48
1:D:344:PRO:HD2	1:D:347:LYS:HD2	1.95	0.47
2:A:702:ARG:NH2	2:A:720:SER:HB3	2.29	0.47
2:A:613:SER:OG	2:A:614:GLY:N	2.48	0.46
2:A:511:THR:HA	2:A:670:ILE:HD11	1.97	0.46
2:A:673:PRO:HB2	2:A:676:THR:HG23	1.98	0.46
1:D:8:TYR:OH	1:D:271:SER:O	2.34	0.46
1:D:326:LEU:HD23	1:D:334:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:543:GLY:HA3	2:A:673:PRO:HB3	1.98	0.46
2:A:656:LEU:HD13	2:A:662:ALA:HB2	1.97	0.45
2:A:647:THR:HG21	2:A:679:SER:OG	2.17	0.45
1:D:298:ILE:O	1:D:300:LEU:N	2.43	0.45
2:A:522:ALA:HA	2:A:525:MET:HE2	1.99	0.44
2:A:162:ILE:HD12	2:A:238:LEU:HD21	1.98	0.44
2:A:419:LYS:HA	2:A:422:VAL:HG22	1.98	0.44
1:D:164:ARG:NH1	1:D:221:LEU:O	2.42	0.44
2:A:105:VAL:HG23	2:A:124:CYS:HA	2.00	0.43
2:A:317:PRO:HD3	2:A:486:LEU:HD11	2.01	0.43
1:D:253:THR:OG1	1:D:254:GLY:N	2.48	0.43
2:A:459:ILE:HD13	2:A:481:THR:HG21	2.01	0.43
1:D:232:GLY:HA2	2:A:244:SER:HB2	2.01	0.42
2:A:464:PHE:HZ	2:A:511:THR:HG21	1.84	0.42
1:D:55:ILE:HD11	1:D:105:LYS:HD2	2.02	0.42
2:A:281:ARG:O	2:A:285:ARG:HG3	2.20	0.42
2:A:128:ILE:HG23	2:A:189:GLU:HG3	2.01	0.42
2:A:10:LYS:HB2	2:A:16:VAL:HG22	2.01	0.41
2:A:71:LYS:O	2:A:75:GLN:NE2	2.44	0.41
1:D:32:VAL:HG11	1:D:56:LEU:HD11	2.01	0.41
2:A:714:PRO:HA	2:A:715:PRO:HD3	1.98	0.41
1:D:254:GLY:HA2	3:D:501:COA:H143	2.01	0.41
2:A:105:VAL:HG22	2:A:125:HIS:ND1	2.36	0.41
1:D:390:ILE:HB	1:D:394:MET:HB2	2.02	0.41
2:A:510:PHE:CE1	2:A:656:LEU:HD11	2.56	0.41
2:A:536:GLU:CD	2:A:549:LEU:HB2	2.45	0.41
2:A:414:GLU:HG3	2:A:443:LEU:HG	2.01	0.41
2:A:122:LEU:HA	2:A:127:ARG:HE	1.86	0.40
2:A:104:PRO:HG3	2:A:216:ALA:HB1	2.02	0.40
2:A:651:LEU:HD23	2:A:656:LEU:HB2	2.03	0.40
2:A:410:GLU:HG2	2:A:423:PHE:CZ	2.57	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	D	398/403 (99%)	386 (97%)	12 (3%)	0	100	100
2	A	722/736 (98%)	697 (96%)	24 (3%)	1 (0%)	48	60
All	All	1120/1139 (98%)	1083 (97%)	36 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	2	PRO

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	D	299/309 (97%)	297 (99%)	2 (1%)	76	87
2	A	511/565 (90%)	504 (99%)	7 (1%)	59	76
All	All	810/874 (93%)	801 (99%)	9 (1%)	65	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	376	LEU
1	D	380	ASN
2	A	331	LEU
2	A	340	ILE
2	A	412	VAL
2	A	467	VAL
2	A	486	LEU
2	A	507	ARG
2	A	557	LEU

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

Mol	Chain	Res	Type
2	A	136	GLN
2	A	248	ASN
2	A	520	ASN
2	A	629	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CSO	D	92	1	3,6,7	0.57	0	1,6,8	0.20	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	CSO	D	92	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	92	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	D	507	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	A	806	-	4,4,4	0.28	0	6,6,6	0.26	0
5	SO4	A	805	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	A	802	-	4,4,4	0.24	0	6,6,6	0.09	0
3	COA	D	501	-	47,50,50	0.54	0	69,75,75	0.89	1 (1%)
4	GOL	D	502	-	5,5,5	0.99	0	5,5,5	1.03	0
5	SO4	D	504	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	A	803	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	D	505	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	D	506	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	A	804	-	4,4,4	0.23	0	6,6,6	0.07	0
4	GOL	A	801	-	5,5,5	0.95	0	5,5,5	1.06	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
4	GOL	D	502	-	-	0/4/4/4	-
3	COA	D	501	-	-	18/48/64/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	801	-	-	1/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	COA	P3B-O3B-C3B	-5.86	107.80	123.43

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	COA	C5B-O5B-P1A-O2A
3	D	501	COA	C5B-O5B-P1A-O3A
3	D	501	COA	CDP-CBP-CCP-O6A
3	D	501	COA	CEP-CBP-CCP-O6A
3	D	501	COA	CAP-CBP-CCP-O6A
3	D	501	COA	C9P-CAP-CBP-CCP
3	D	501	COA	O9P-C9P-CAP-OAP
3	D	501	COA	C5B-O5B-P1A-O1A
3	D	501	COA	N8P-C9P-CAP-CBP
3	D	501	COA	C4B-C5B-O5B-P1A
3	D	501	COA	N8P-C9P-CAP-OAP
3	D	501	COA	C9P-CAP-CBP-CDP
3	D	501	COA	C9P-CAP-CBP-CEP
3	D	501	COA	P1A-O3A-P2A-O4A
3	D	501	COA	O9P-C9P-CAP-CBP
4	A	801	GOL	O2-C2-C3-O3
3	D	501	COA	C5P-C6P-C7P-N8P
3	D	501	COA	S1P-C2P-C3P-N4P
3	D	501	COA	P1A-O3A-P2A-O5A

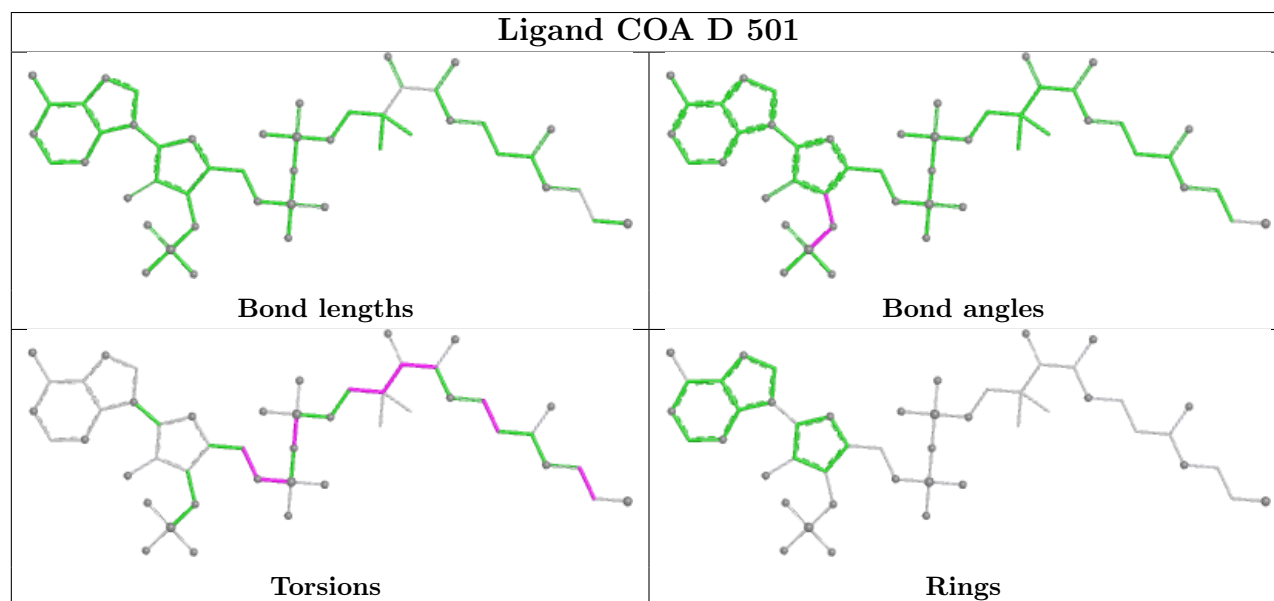
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	COA	3	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, 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	D	400/403 (99%)	0.76	19 (4%) 35 37	58, 84, 113, 142	0
2	A	726/736 (98%)	0.94	79 (10%) 10 12	61, 97, 140, 172	0
All	All	1126/1139 (98%)	0.87	98 (8%) 16 17	58, 92, 134, 172	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	719	LEU	5.0
2	A	690	ALA	4.1
1	D	228	LEU	4.1
2	A	412	VAL	4.0
2	A	651	LEU	3.9
2	A	388	ALA	3.7
2	A	577	THR	3.6
2	A	376	LEU	3.3
2	A	698	VAL	3.3
2	A	3	ASP	3.2
2	A	720	SER	3.2
2	A	385	ARG	3.2
2	A	426	ILE	3.1
1	D	403	VAL	3.1
2	A	413	PHE	3.0
2	A	323	THR	3.0
2	A	467	VAL	2.9
2	A	559	LEU	2.9
2	A	328	ILE	2.9
2	A	510	PHE	2.9
2	A	507	ARG	2.8
2	A	353	LEU	2.8
2	A	399	ALA	2.8
1	D	225	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	358	LEU	2.8
2	A	582	PRO	2.8
2	A	427	GLU	2.8
1	D	389	CYS	2.7
2	A	351	VAL	2.7
2	A	571	VAL	2.7
1	D	277	LEU	2.7
2	A	335	MET	2.7
2	A	371	LEU	2.7
1	D	45	ASP	2.6
2	A	352	VAL	2.6
2	A	324	PRO	2.6
2	A	333	ALA	2.6
2	A	578	TYR	2.6
2	A	656	LEU	2.6
2	A	405	VAL	2.6
2	A	393	ILE	2.6
2	A	-10	GLY	2.6
2	A	670	ILE	2.6
2	A	331	LEU	2.5
2	A	389	LEU	2.5
1	D	226	GLU	2.5
2	A	384	GLU	2.5
2	A	684	VAL	2.5
1	D	215	LYS	2.5
2	A	130	ALA	2.5
2	A	132	VAL	2.4
2	A	362	ALA	2.4
2	A	-8	SER	2.4
1	D	298	ILE	2.4
2	A	599	LEU	2.4
2	A	356	VAL	2.4
2	A	-5	HIS	2.3
2	A	332	GLY	2.3
1	D	373	VAL	2.3
2	A	342	TYR	2.3
2	A	442	THR	2.3
2	A	465	SER	2.3
2	A	375	ALA	2.3
2	A	692	THR	2.3
2	A	390	LEU	2.2
2	A	452	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	395	PRO	2.2
2	A	1	MET	2.2
1	D	224	ALA	2.2
2	A	36	GLU	2.2
2	A	514	VAL	2.2
1	D	230	ALA	2.2
2	A	549	LEU	2.2
2	A	718	LEU	2.2
1	D	382	ARG	2.2
2	A	432	PRO	2.2
2	A	576	GLY	2.2
2	A	394	THR	2.2
2	A	325	ILE	2.2
2	A	428	ASP	2.2
2	A	439	ASN	2.2
2	A	716	GLU	2.2
2	A	486	LEU	2.1
1	D	127	MET	2.1
2	A	30	MET	2.1
2	A	133	LYS	2.1
1	D	279	GLY	2.1
1	D	251	VAL	2.1
2	A	430	VAL	2.1
1	D	343	ILE	2.1
2	A	555	LEU	2.1
1	D	112	ASP	2.1
2	A	575	GLY	2.1
1	D	363	ALA	2.0
2	A	345	ALA	2.0
2	A	605	TYR	2.0
2	A	327	ARG	2.0
2	A	466	PRO	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, 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	CSO	D	92	7/8	0.82	0.18	61,70,94,106	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

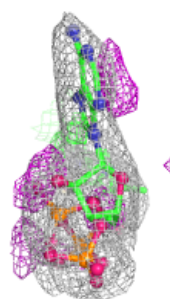
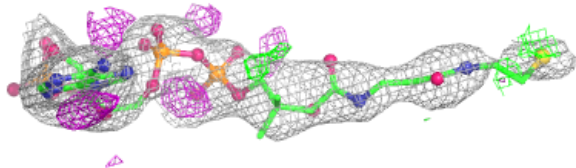
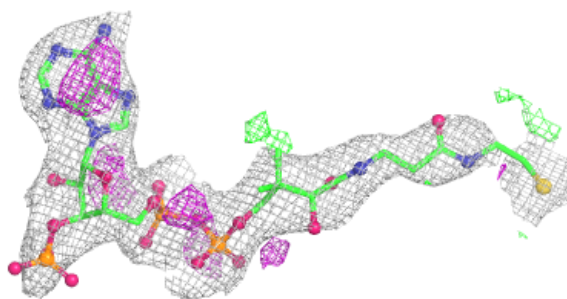
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	805	5/5	0.40	0.10	179,179,185,189	0
5	SO4	D	506	5/5	0.61	0.12	178,178,178,184	0
5	SO4	D	505	5/5	0.70	0.08	136,139,143,150	0
5	SO4	D	504	5/5	0.78	0.11	129,130,130,146	0
5	SO4	A	806	5/5	0.79	0.21	125,134,142,263	0
5	SO4	D	503	5/5	0.80	0.12	93,94,106,110	0
5	SO4	A	803	5/5	0.80	0.12	112,112,113,115	0
5	SO4	D	507	5/5	0.81	0.10	147,148,148,155	0
4	GOL	D	502	6/6	0.84	0.22	81,90,94,95	0
3	COA	D	501	48/48	0.84	0.14	88,112,158,190	0
5	SO4	A	802	5/5	0.84	0.12	101,105,109,112	0
4	GOL	A	801	6/6	0.86	0.16	112,115,124,125	0
5	SO4	A	804	5/5	0.88	0.08	117,117,123,130	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around COA D 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.