



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 7O1L / pdb_00007o1l
Title : Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme
alpha-H462A mutant
Authors : Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on : 2021-03-29
Resolution : 2.38 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

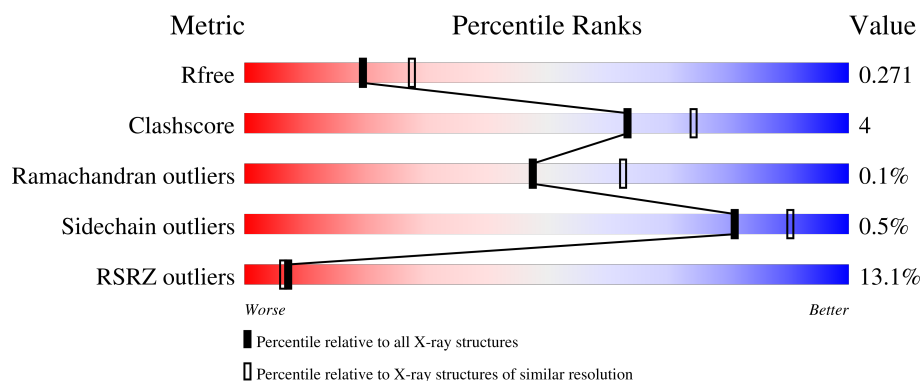
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	
2	A	736	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8301 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	402	Total	C	N	O	S	0	2	0
			2948	1843	521	569	15			

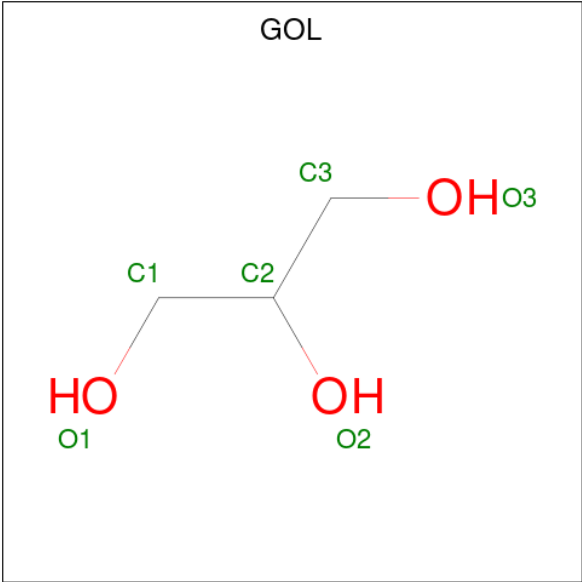
- Molecule 2 is a protein called 3-hydroxyacyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	727	Total	C	N	O	S	0	0	0
			5112	3225	887	980	20			

There are 17 discrepancies between the modelled and reference sequences:

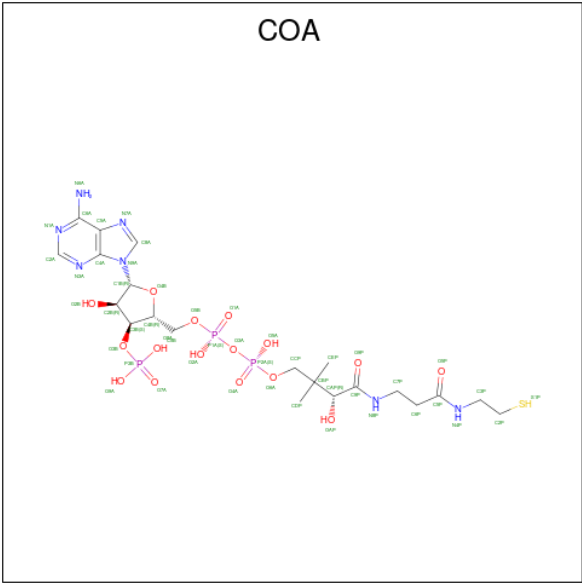
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP O53872
A	-10	GLY	-	expression tag	UNP O53872
A	-9	SER	-	expression tag	UNP O53872
A	-8	SER	-	expression tag	UNP O53872
A	-7	HIS	-	expression tag	UNP O53872
A	-6	HIS	-	expression tag	UNP O53872
A	-5	HIS	-	expression tag	UNP O53872
A	-4	HIS	-	expression tag	UNP O53872
A	-4A	HIS	-	expression tag	UNP O53872
A	-4B	HIS	-	expression tag	UNP O53872
A	-4C	SER	-	expression tag	UNP O53872
A	-4D	GLN	-	expression tag	UNP O53872
A	-4E	ASP	-	expression tag	UNP O53872
A	-4F	PRO	-	expression tag	UNP O53872
A	-4G	ASN	-	expression tag	UNP O53872
A	-4H	SER	-	expression tag	UNP O53872
A	462	ALA	HIS	engineered mutation	UNP O53872

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



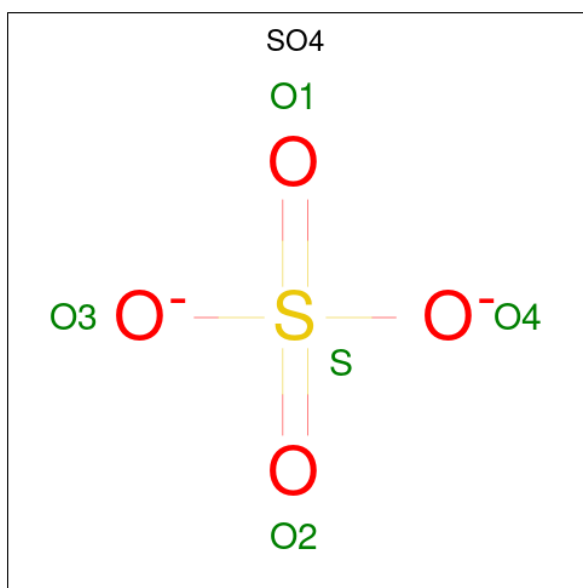
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- 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	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		

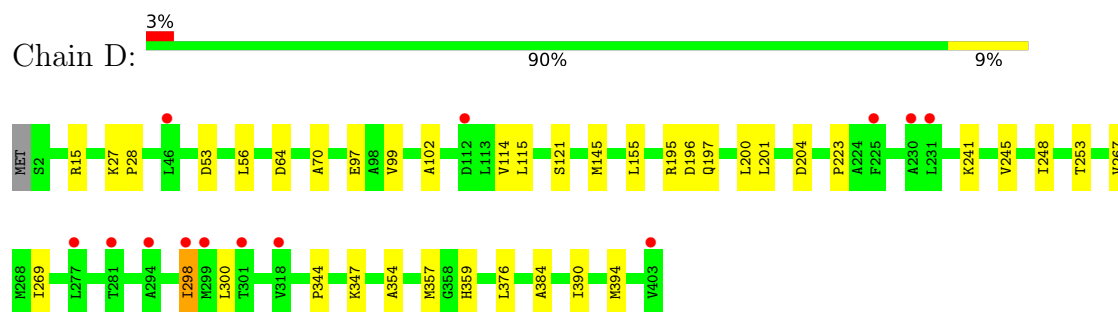
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	55	Total	O	0	0
			55	55		
6	A	75	Total	O	0	0
			75	75		

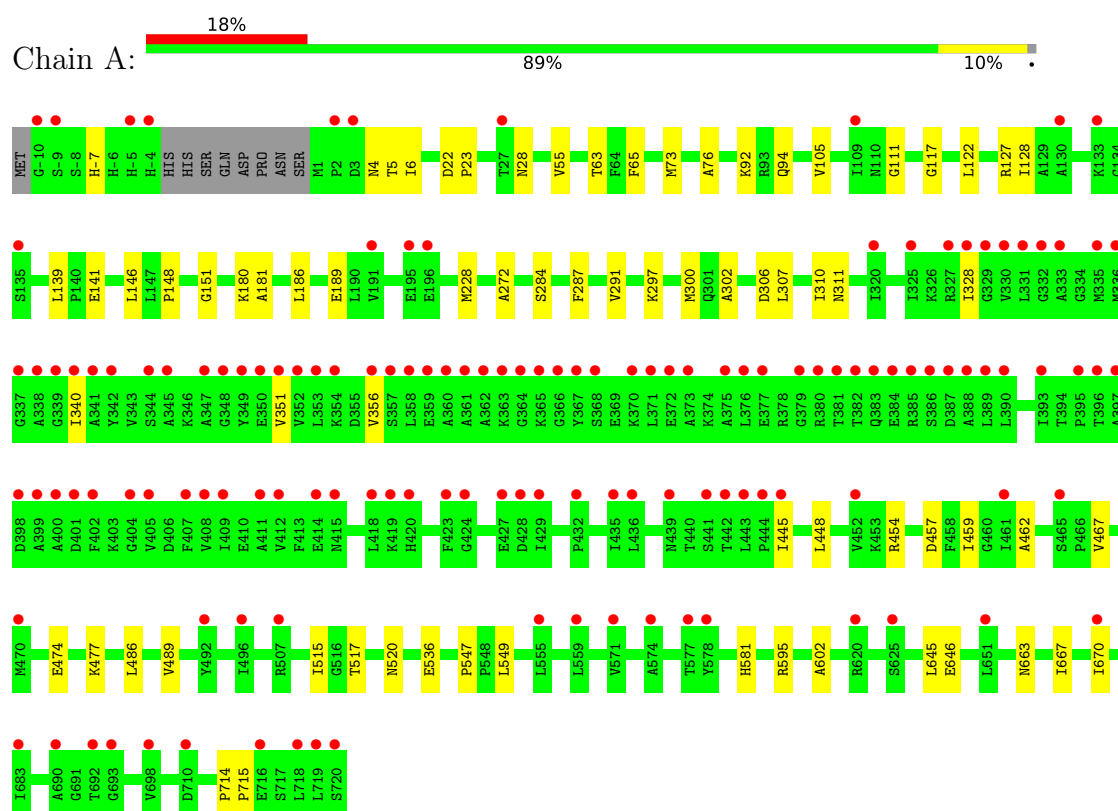
3 Residue-property plots [i](#)

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	100.75Å 207.63Å 134.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.64 – 2.38 90.64 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.2 (90.64-2.38) 99.3 (90.64-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.229 , 0.269 0.231 , 0.271	Depositor DCC
R_{free} test set	2733 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8301	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: 2CO, SO4, GOL, COA

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	0.12	0/2990	0.30	0/4055
2	A	0.11	0/5207	0.27	0/7089
All	All	0.11	0/8197	0.28	0/11144

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	2948	0	2947	23	0
2	A	5112	0	4895	41	0
3	A	6	0	8	1	0
3	D	12	0	16	2	0
4	D	48	0	32	0	0
5	A	25	0	0	0	0
5	D	20	0	0	0	0
6	A	75	0	0	1	0
6	D	55	0	0	1	0
All	All	8301	0	7898	64	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 (64) 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:517:THR:HG21	2:A:646:GLU:HG3	1.59	0.85
2:A:228:MET:HE1	2:A:272:ALA:HB1	1.76	0.67
2:A:146:LEU:HD22	2:A:291:VAL:HG22	1.83	0.60
1:D:53:ASP:HB3	1:D:114:VAL:HG13	1.83	0.59
2:A:127:ARG:NH2	6:A:904:HOH:O	2.34	0.59
1:D:145:MET:HE1	1:D:241:LYS:HD3	1.86	0.58
1:D:245:VAL:HG13	3:D:602:GOL:H2	1.87	0.57
1:D:344:PRO:HD2	1:D:347:LYS:HD3	1.88	0.56
2:A:454:ARG:NH2	2:A:457:ASP:OD2	2.38	0.56
1:D:99:VAL:HG13	1:D:269:ILE:HD11	1.88	0.55
2:A:63:THR:HA	2:A:111:GLY:HA3	1.89	0.54
2:A:76:ALA:O	2:A:297:LYS:NZ	2.37	0.54
2:A:328:ILE:HB	2:A:351:VAL:HG12	1.88	0.54
2:A:477:LYS:HE2	2:A:486:LEU:HD22	1.92	0.51
2:A:445:ILE:HD12	2:A:448:LEU:HD12	1.94	0.50
2:A:5:THR:HG22	2:A:23:PRO:HD2	1.92	0.50
1:D:56:LEU:HD12	1:D:70:ALA:HA	1.94	0.49
1:D:354:ALA:HB1	1:D:359:HIS:HB2	1.95	0.49
1:D:390:ILE:HB	1:D:394:MET:HB2	1.95	0.48
2:A:462:ALA:HB3	2:A:474:GLU:HB3	1.96	0.48
1:D:28:PRO:HG3	1:D:121[A]:SER:HB3	1.95	0.48
1:D:223:PRO:HA	1:D:253:THR:HG22	1.95	0.48
2:A:520:ASN:HB3	2:A:581:HIS:CE1	2.50	0.47
2:A:122:LEU:HA	2:A:127:ARG:HE	1.80	0.47
2:A:181:ALA:HB1	2:A:186:LEU:HB2	1.97	0.47
2:A:92:LYS:NZ	2:A:284:SER:OG	2.29	0.46
2:A:645:LEU:HD22	2:A:715:PRO:HD3	1.97	0.46
2:A:-7:HIS:O	2:A:94:GLN:NE2	2.42	0.46
1:D:298:ILE:H	1:D:298:ILE:HG13	1.57	0.46
1:D:155:LEU:HD13	1:D:248:ILE:HG12	1.98	0.46
2:A:515:ILE:HB	2:A:670:ILE:HG23	1.98	0.45
2:A:306:ASP:O	2:A:310:ILE:HG12	2.16	0.45
2:A:55:VAL:HB	2:A:105:VAL:HG22	1.98	0.45
2:A:459:ILE:HG21	2:A:489:VAL:HG21	1.99	0.45
1:D:195:ARG:HH12	3:D:601:GOL:H31	1.81	0.45
2:A:128:ILE:HG23	2:A:189:GLU:HG3	1.99	0.45
1:D:28:PRO:HG3	1:D:121[B]:SER:HB2	1.99	0.44
2:A:22:ASP:H	2:A:28:ASN:ND2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:VAL:HG22	1:D:267[A]:VAL:HG21	2.00	0.44
2:A:595:ARG:HG2	2:A:602:ALA:HB1	1.99	0.43
1:D:298:ILE:O	1:D:300:LEU:N	2.51	0.43
2:A:73:MET:HB2	2:A:300:MET:HE1	2.00	0.43
1:D:28:PRO:HD2	1:D:64:ASP:HB3	1.99	0.43
1:D:201:LEU:HD11	1:D:204:ASP:HB3	2.01	0.43
2:A:4:ASN:ND2	2:A:6:ILE:O	2.45	0.43
2:A:536:GLU:CD	2:A:547:PRO:HB2	2.43	0.43
1:D:102:ALA:HB3	1:D:269:ILE:HD12	2.01	0.43
2:A:92:LYS:HD3	2:A:151:GLY:N	2.34	0.43
2:A:663:ASN:O	2:A:667:ILE:HG12	2.19	0.42
1:D:376:LEU:HD21	1:D:384:ALA:HB2	2.01	0.42
2:A:76:ALA:HB3	2:A:291:VAL:HG12	2.02	0.42
2:A:141:GLU:HG2	3:A:801:GOL:H32	2.02	0.42
2:A:180:LYS:HE3	2:A:180:LYS:HB2	1.82	0.42
1:D:196:ASP:OD1	1:D:200:LEU:N	2.53	0.41
1:D:15:ARG:NH2	1:D:357:MET:HE2	2.36	0.41
2:A:340:ILE:HA	2:A:467:VAL:HG11	2.02	0.41
2:A:65:PHE:HB3	2:A:117:GLY:CA	2.51	0.41
2:A:714:PRO:HA	2:A:715:PRO:HD3	1.98	0.41
2:A:139:LEU:HB3	2:A:148:PRO:HG3	2.03	0.41
1:D:27:LYS:HG2	6:D:715:HOH:O	2.20	0.41
2:A:536:GLU:CD	2:A:549:LEU:HB2	2.46	0.41
2:A:287:PHE:O	2:A:291:VAL:HG23	2.21	0.41
2:A:302:ALA:HA	2:A:306:ASP:HB2	2.03	0.40
2:A:307:LEU:O	2:A:311:ASN:ND2	2.51	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	Percentiles	
1	D	401/403 (100%)	385 (96%)	16 (4%)	0	100	100
2	A	723/736 (98%)	688 (95%)	34 (5%)	1 (0%)	48	62
All	All	1124/1139 (99%)	1073 (96%)	50 (4%)	1 (0%)	48	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	356	VAL

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	303/309 (98%)	299 (99%)	4 (1%)	61	78
2	A	480/565 (85%)	480 (100%)	0	100	100
All	All	783/874 (90%)	779 (100%)	4 (0%)	81	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	97	GLU
1	D	115	LEU
1	D	197	GLN
1	D	298	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	43	HIS
1	D	197	GLN
2	A	28	ASN
2	A	75	GLN
2	A	248	ASN
2	A	455	GLN

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Mol	Chain	Res	Type
2	A	681	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	2CO	D	92	1	3,7,8	0.79	0	1,7,9	1.26	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	2CO	D	92	1	-	0/1/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	$\# Z > 2$
4	COA	D	603	-	47,50,50	0.49	0	69,75,75	0.87	1 (1%)
5	SO4	A	806	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	D	606	-	4,4,4	0.24	0	6,6,6	0.09	0
3	GOL	D	602	-	5,5,5	0.94	0	5,5,5	1.07	0
3	GOL	D	601	-	5,5,5	0.96	0	5,5,5	1.07	0
5	SO4	D	605	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	A	803	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	A	805	-	4,4,4	0.24	0	6,6,6	0.08	0
3	GOL	A	801	-	5,5,5	0.94	0	5,5,5	1.04	0
5	SO4	A	802	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	A	804	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	D	604	-	4,4,4	0.25	0	6,6,6	0.08	0
5	SO4	D	607	-	4,4,4	0.24	0	6,6,6	0.10	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
3	GOL	D	602	-	-	0/4/4/4	-
4	COA	D	603	-	-	10/48/64/64	0/3/3/3
3	GOL	A	801	-	-	2/4/4/4	-
3	GOL	D	601	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603	COA	P3B-O3B-C3B	-5.49	108.78	123.43

There are no chirality outliers.

All (12) torsion outliers are listed below:

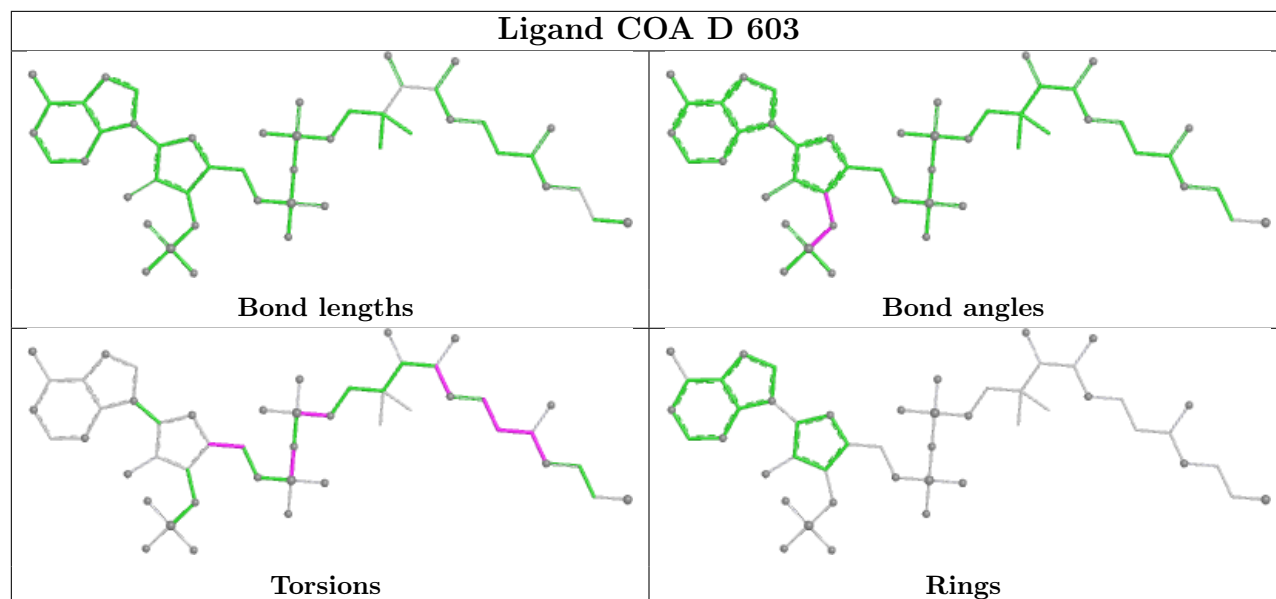
Mol	Chain	Res	Type	Atoms
3	A	801	GOL	O1-C1-C2-C3
4	D	603	COA	O4B-C4B-C5B-O5B
4	D	603	COA	CAP-C9P-N8P-C7P
4	D	603	COA	O9P-C9P-N8P-C7P
3	A	801	GOL	O1-C1-C2-O2
4	D	603	COA	C3B-C4B-C5B-O5B
4	D	603	COA	P2A-O3A-P1A-O5B
4	D	603	COA	C5P-C6P-C7P-N8P
4	D	603	COA	O5P-C5P-N4P-C3P
4	D	603	COA	CCP-O6A-P2A-O4A
4	D	603	COA	C6P-C5P-N4P-C3P
4	D	603	COA	O5P-C5P-C6P-C7P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	GOL	1	0
3	D	601	GOL	1	0
3	A	801	GOL	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, 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	401/403 (99%)	0.44	13 (3%)	50	50	25, 55, 81, 127	2 (0%)
2	A	727/736 (98%)	1.03	135 (18%)	3	3	37, 71, 137, 197	0
All	All	1128/1139 (99%)	0.82	148 (13%)	7	6	25, 64, 129, 197	2 (0%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	362	ALA	6.2
2	A	719	LEU	5.2
2	A	385	ARG	4.9
2	A	402	PHE	4.7
2	A	720	SER	4.6
2	A	-10	GLY	4.5
2	A	352	VAL	4.3
2	A	401	ASP	4.3
2	A	396	THR	4.3
2	A	357	SER	4.3
2	A	423	PHE	4.3
2	A	-9	SER	4.2
2	A	382	THR	4.1
2	A	388	ALA	4.1
2	A	358	LEU	4.1
2	A	445	ILE	4.1
2	A	389	LEU	3.9
2	A	366	GLY	3.8
2	A	328	ILE	3.8
2	A	555	LEU	3.8
2	A	716	GLU	3.7
2	A	345	ALA	3.7
2	A	393	ILE	3.7
2	A	325	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
2	A	360	ALA	3.6
2	A	400	ALA	3.6
2	A	-4	HIS	3.5
2	A	412	VAL	3.4
2	A	372	GLU	3.4
2	A	432	PRO	3.4
2	A	353	LEU	3.3
2	A	361	ALA	3.3
2	A	356	VAL	3.3
2	A	670	ILE	3.3
2	A	690	ALA	3.3
1	D	231	LEU	3.3
2	A	415	ASN	3.2
2	A	399	ALA	3.2
2	A	379	GLY	3.2
2	A	441	SER	3.2
2	A	337	GLY	3.2
2	A	698	VAL	3.2
2	A	336	MET	3.2
2	A	3	ASP	3.2
2	A	351	VAL	3.2
2	A	405	VAL	3.2
2	A	409	ILE	3.2
2	A	363	LYS	3.1
2	A	428	ASP	3.1
2	A	443	LEU	3.1
2	A	342	TYR	3.1
1	D	112	ASP	3.1
2	A	404	GLY	3.1
2	A	373	ALA	3.1
2	A	332	GLY	3.0
2	A	320	ILE	3.0
2	A	133	LYS	3.0
2	A	348	GLY	3.0
2	A	347	ALA	3.0
2	A	350	GLU	3.0
2	A	496	ILE	2.9
2	A	364	GLY	2.9
2	A	390	LEU	2.9
2	A	398	ASP	2.9
2	A	327	ARG	2.8
2	A	135	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	383	GLN	2.8
2	A	559	LEU	2.8
2	A	407	PHE	2.8
2	A	27	THR	2.8
2	A	109	ILE	2.8
2	A	381	THR	2.8
2	A	395	PRO	2.8
2	A	349	TYR	2.8
2	A	439	ASN	2.7
2	A	367	TYR	2.7
2	A	130	ALA	2.7
2	A	341	ALA	2.7
2	A	368	SER	2.7
2	A	436	LEU	2.7
2	A	365	LYS	2.6
2	A	578	TYR	2.6
2	A	444	PRO	2.6
2	A	344	SER	2.6
2	A	419	LYS	2.6
1	D	299	MET	2.6
2	A	386	SER	2.6
2	A	470	MET	2.6
2	A	424	GLY	2.6
2	A	408	VAL	2.5
2	A	340	ILE	2.5
2	A	435	ILE	2.5
2	A	442	THR	2.5
2	A	577	THR	2.5
2	A	387	ASP	2.4
2	A	359	GLU	2.4
2	A	331	LEU	2.4
1	D	281	THR	2.4
1	D	294	ALA	2.4
2	A	452	VAL	2.4
2	A	371	LEU	2.4
2	A	651	LEU	2.4
2	A	380	ARG	2.4
2	A	420	HIS	2.4
2	A	427	GLU	2.4
2	A	683	ILE	2.3
2	A	-5	HIS	2.3
2	A	418	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	195	GLU	2.3
2	A	693	GLY	2.3
2	A	492	TYR	2.3
1	D	230	ALA	2.3
2	A	574	ALA	2.3
2	A	330	VAL	2.3
2	A	335	MET	2.2
2	A	338	ALA	2.2
2	A	465	SER	2.2
2	A	571	VAL	2.2
2	A	377	GLU	2.2
2	A	333	ALA	2.2
2	A	191	VAL	2.2
1	D	225	PHE	2.2
2	A	384	GLU	2.2
2	A	414	GLU	2.2
2	A	397	ALA	2.2
2	A	411	ALA	2.2
2	A	692	THR	2.2
2	A	376	LEU	2.2
1	D	301	THR	2.2
2	A	620	ARG	2.1
2	A	718	LEU	2.1
1	D	403	VAL	2.1
2	A	375	ALA	2.1
1	D	46	LEU	2.1
2	A	2	PRO	2.1
1	D	298	ILE	2.1
2	A	429	ILE	2.1
1	D	318	VAL	2.1
2	A	625	SER	2.1
2	A	196	GLU	2.1
1	D	277	LEU	2.1
2	A	710	ASP	2.1
2	A	507	ARG	2.1
2	A	461	ILE	2.0
2	A	329	GLY	2.0
2	A	339	GLY	2.0
2	A	354	LYS	2.0
2	A	370	LYS	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	2CO	D	92	8/9	0.90	0.12	39,42,71,80	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

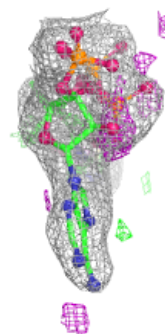
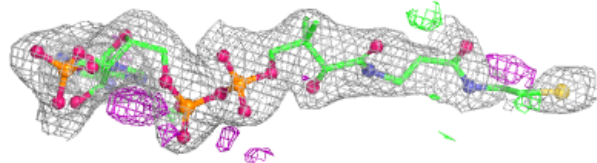
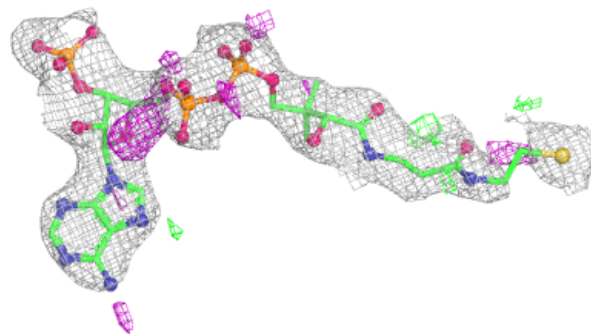
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	803	5/5	0.59	0.12	106,108,124,134	0
5	SO4	A	806	5/5	0.74	0.10	98,99,116,130	0
3	GOL	A	801	6/6	0.76	0.20	73,76,82,83	0
5	SO4	D	607	5/5	0.79	0.10	98,104,115,131	0
5	SO4	D	605	5/5	0.80	0.08	115,117,128,131	0
3	GOL	D	602	6/6	0.83	0.13	65,71,74,79	0
5	SO4	A	805	5/5	0.85	0.08	96,101,106,118	0
3	GOL	D	601	6/6	0.85	0.13	56,66,77,78	0
4	COA	D	603	48/48	0.86	0.11	53,72,100,127	0
5	SO4	A	804	5/5	0.86	0.10	72,76,79,81	0
5	SO4	D	606	5/5	0.87	0.09	95,106,109,111	0
5	SO4	A	802	5/5	0.93	0.07	71,77,90,94	0
5	SO4	D	604	5/5	0.96	0.11	67,68,73,76	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 603:

$2mF_o-DF_c$ (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.