



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:03 AM UTC

PDB ID : 7O4R / pdb_00007o4r
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 ⓘ 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

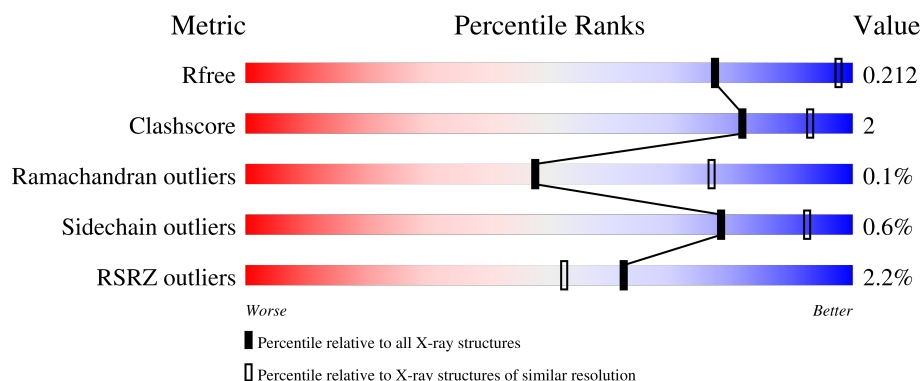
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	736	2% 93% 6%
1	B	736	2% 94% 5%
2	C	403	4% 89% 10%
2	D	403	2% 90% 8%

2 Entry composition

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	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5416	3425	933	1037	21			
1	B	728	Total	C	N	O	S	0	1	0
			5396	3414	929	1032	21			

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	UNP O53872
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
B	-15	MET	-	initiating methionine	UNP O53872
B	-14	GLY	-	expression tag	UNP O53872
B	-13	SER	-	expression tag	UNP O53872
B	-12	SER	-	expression tag	UNP O53872
B	-11	HIS	-	expression tag	UNP O53872
B	-10	HIS	-	expression tag	UNP O53872
B	-9	HIS	-	expression tag	UNP O53872
B	-8	HIS	-	expression tag	UNP O53872
B	-7	HIS	-	expression tag	UNP O53872

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

- Molecule 2 is a protein called Putative acyltransferase Rv0859.

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



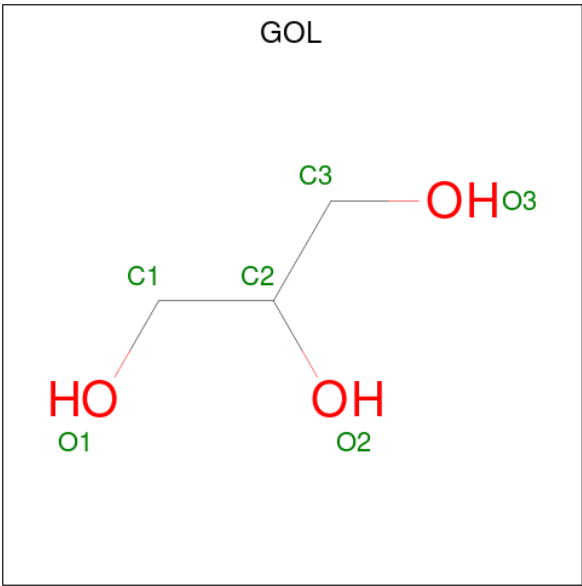
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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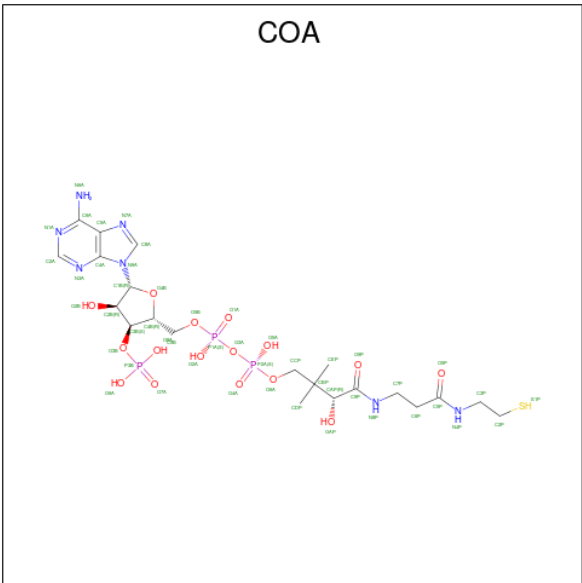
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total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

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



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

- Molecule 5 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).



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

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

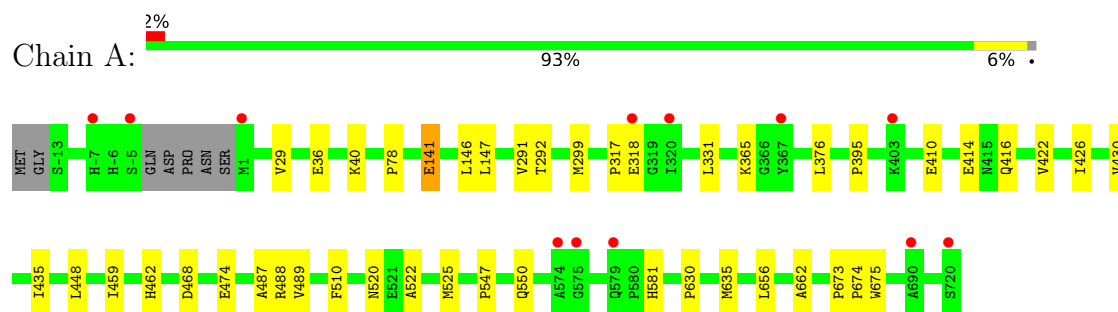
- Molecule 6 is water.

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

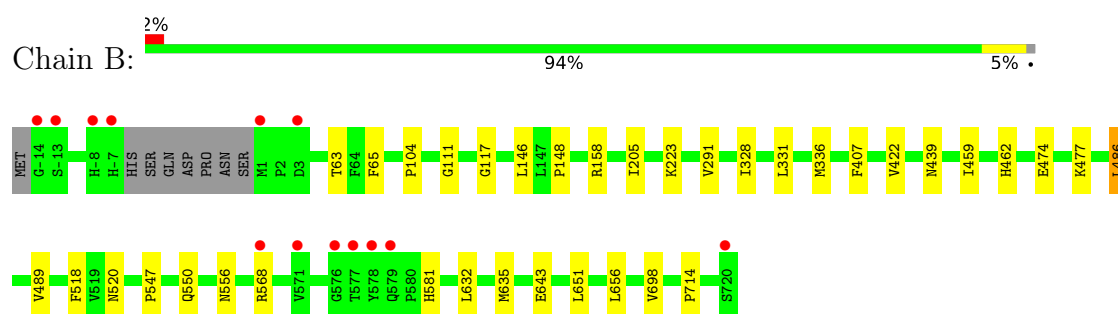
3 Residue-property plots

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.

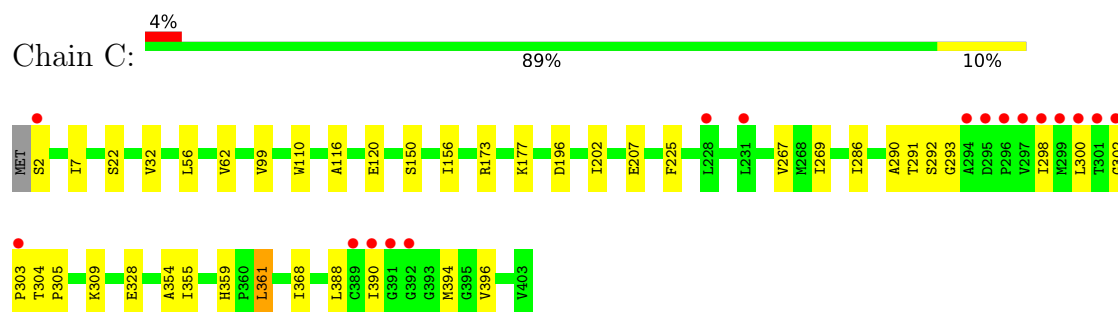
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase



• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

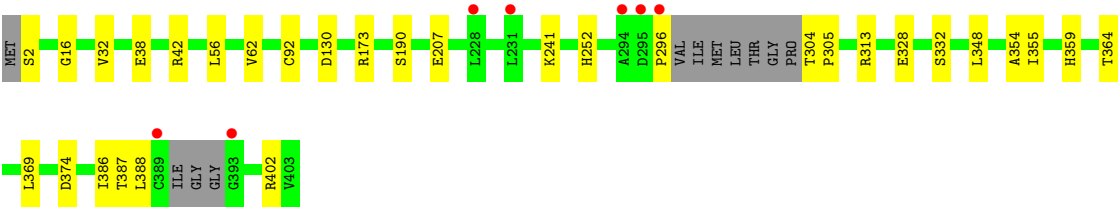


• Molecule 2: Putative acyltransferase Rv0859



• Molecule 2: Putative acyltransferase Rv0859





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	248.25Å 135.75Å 119.30Å 90.00° 110.51° 90.00°	Depositor
Resolution (Å)	48.50 – 2.79 48.50 – 2.79	Depositor EDS
% Data completeness (in resolution range)	86.8 (48.50-2.79) 86.8 (48.50-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.178 , 0.216 0.177 , 0.212	Depositor DCC
R_{free} test set	4034 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.5	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	17229	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, 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	A	0.08	0/5519	0.23	0/7473
1	B	0.08	0/5501	0.24	0/7449
2	C	0.09	0/3009	0.28	0/4075
2	D	0.08	0/2943	0.25	0/3981
All	All	0.08	0/16972	0.25	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)	H(added)	Clashes	Symm-Clashes
1	A	5416	0	5431	22	0
1	B	5396	0	5416	19	0
2	C	2964	0	2979	28	0
2	D	2901	0	2910	19	0
3	A	30	0	0	0	0
3	B	25	0	0	1	0
3	C	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	C	96	0	64	0	0
5	D	96	0	64	1	0
6	A	64	0	0	0	0
6	B	78	0	0	1	0
6	C	58	0	0	0	0
6	D	29	0	0	0	0
All	All	17229	0	16872	83	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 (83) 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:C:2:SER:N	2:D:2:SER:HG	1.88	0.71
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.80	0.63
1:B:632:LEU:HA	1:B:635:MET:HE3	1.85	0.58
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:630:PRO:HG2	1:A:635:MET:HE2	1.91	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
1:A:299:MET:HE2	1:A:675:TRP:HA	1.93	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:336:MET:HE2	1:B:439:ASN:HD21	1.82	0.45
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:22:SER:OG	2:C:207:GLU:OE2	2.34	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
1:A:522:ALA:HA	1:A:525:MET:HE3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:141:GLU:HG3	1:A:147:LEU:C	2.46	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
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:518:PHE:HB2	1:B:643:GLU:CD	2.47	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

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	725/736 (98%)	702 (97%)	23 (3%)	0	100	100
1	B	725/736 (98%)	706 (97%)	18 (2%)	1 (0%)	48	77
2	C	400/403 (99%)	386 (96%)	13 (3%)	1 (0%)	36	66
2	D	386/403 (96%)	373 (97%)	13 (3%)	0	100	100
All	All	2236/2278 (98%)	2167 (97%)	67 (3%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	361	LEU
1	B	148	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	A	556/566 (98%)	551 (99%)	5 (1%)	70	89
1	B	553/566 (98%)	551 (100%)	2 (0%)	84	94
2	C	308/310 (99%)	308 (100%)	0	100	100
2	D	302/310 (97%)	299 (99%)	3 (1%)	68	88
All	All	1719/1752 (98%)	1709 (99%)	10 (1%)	78	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	141	GLU
1	A	318	GLU
1	A	376	LEU
1	A	414	GLU
1	B	486	LEU
1	B	556	ASN
2	D	387	THR
2	D	388	LEU
2	D	402	ARG

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

Mol	Chain	Res	Type
1	A	416	GLN
1	A	681	GLN
1	B	28	ASN
1	B	633	GLN
1	B	681	GLN

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Mol	Chain	Res	Type
2	C	327	ASN
2	D	43	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	C	505	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	D	504	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	D	508	-	4,4,4	0.24	0	6,6,6	0.07	0
5	COA	C	508	-	47,50,50	0.53	0	69,75,75	0.87	1 (1%)
3	SO4	A	807	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	801	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	D	505	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	D	502	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	C	510	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	C	507	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	804	-	4,4,4	0.24	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	806	-	5,5,5	0.95	0	5,5,5	1.07	0
3	SO4	A	802	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	803	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	503	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	B	805	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	803	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	504	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	C	506	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	502	-	4,4,4	0.23	0	6,6,6	0.07	0
5	COA	D	507	-	47,50,50	0.50	0	69,75,75	0.86	2 (2%)
5	COA	C	509	-	47,50,50	0.53	0	69,75,75	0.84	1 (1%)
3	SO4	B	802	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	B	801	-	4,4,4	0.24	0	6,6,6	0.06	0
5	COA	D	506	-	47,50,50	0.51	0	69,75,75	0.84	1 (1%)
3	SO4	A	805	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	B	804	-	4,4,4	0.24	0	6,6,6	0.07	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	-	-	11/48/64/64	0/3/3/3
5	COA	C	508	-	-	13/48/64/64	0/3/3/3
5	COA	C	509	-	-	4/48/64/64	0/3/3/3
5	COA	D	506	-	-	0/48/64/64	0/3/3/3
4	GOL	A	806	-	-	2/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	508	COA	P3B-O3B-C3B	-5.21	109.51	123.43
5	D	507	COA	P3B-O3B-C3B	-5.00	110.07	123.43
5	D	506	COA	P3B-O3B-C3B	-4.79	110.64	123.43
5	C	509	COA	P3B-O3B-C3B	-4.67	110.97	123.43
5	D	507	COA	O6A-CCP-CBP	-2.51	106.52	110.55

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	806	GOL	C1-C2-C3-O3
5	C	508	COA	P1A-O3A-P2A-O6A
5	C	508	COA	CCP-O6A-P2A-O3A
5	C	508	COA	OAP-CAP-CBP-CCP
5	C	508	COA	C9P-CAP-CBP-CCP
5	C	508	COA	OAP-CAP-CBP-CDP
5	C	508	COA	C9P-CAP-CBP-CDP
5	C	508	COA	OAP-CAP-CBP-CEP
5	C	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	CDP-CBP-CCP-O6A
5	D	507	COA	CEP-CBP-CCP-O6A
5	D	507	COA	CAP-CBP-CCP-O6A
5	C	508	COA	C6P-C5P-N4P-C3P
5	C	509	COA	C6P-C5P-N4P-C3P
5	C	509	COA	O5P-C5P-N4P-C3P
5	C	508	COA	O5P-C5P-N4P-C3P
4	A	806	GOL	O2-C2-C3-O3
5	C	509	COA	C2P-C3P-N4P-C5P
5	C	508	COA	CCP-O6A-P2A-O4A
5	D	507	COA	C5B-O5B-P1A-O1A
5	D	507	COA	C5B-O5B-P1A-O3A
5	D	507	COA	O9P-C9P-CAP-OAP
5	C	508	COA	C4B-C5B-O5B-P1A
5	D	507	COA	C4B-C5B-O5B-P1A
5	C	509	COA	O4B-C4B-C5B-O5B
5	D	507	COA	C6P-C7P-N8P-C9P
5	C	508	COA	N8P-C9P-CAP-OAP
5	D	507	COA	N8P-C9P-CAP-OAP

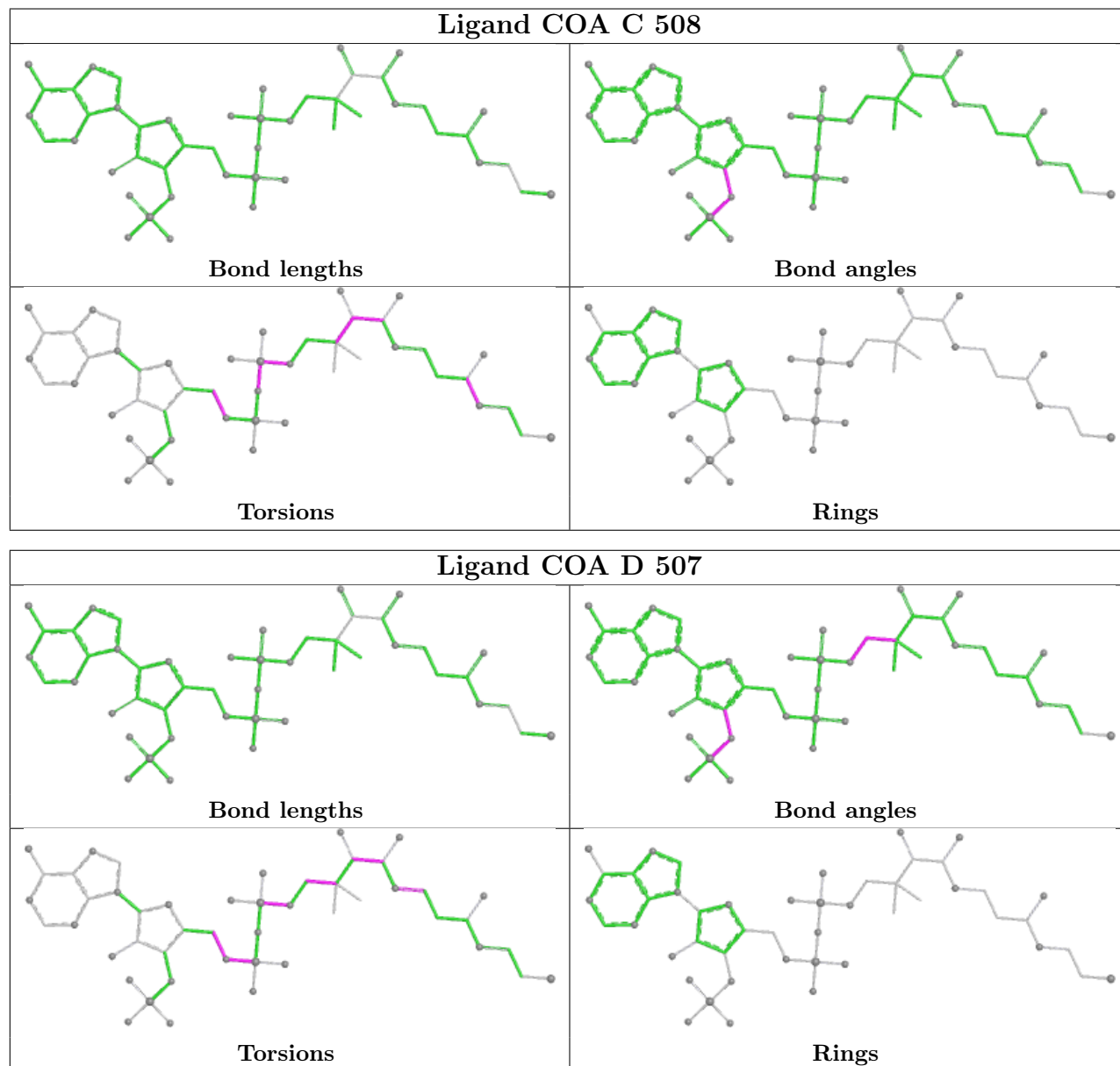
There are no ring outliers.

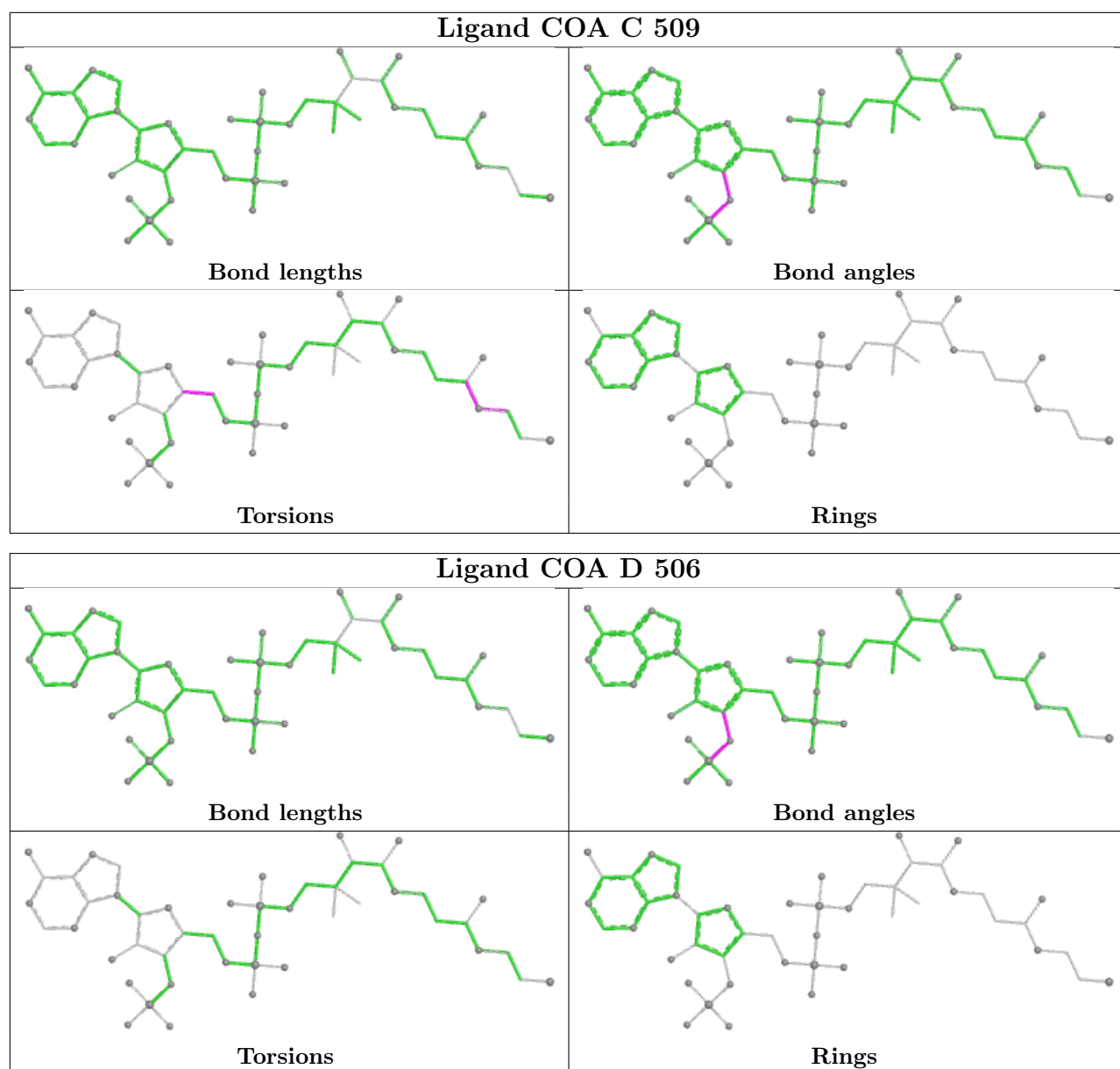
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	A	729/736 (99%)	-0.06	12 (1%) 70 61	23, 52, 93, 113	0
1	B	728/736 (98%)	-0.24	13 (1%) 67 58	22, 46, 82, 131	1 (0%)
2	C	402/403 (99%)	-0.29	17 (4%) 40 32	21, 36, 75, 120	0
2	D	392/403 (97%)	-0.41	7 (1%) 67 58	18, 37, 67, 137	1 (0%)
All	All	2251/2278 (98%)	-0.22	49 (2%) 62 52	18, 44, 87, 137	2 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	301	THR	7.2
2	C	295	ASP	5.9
2	D	228	LEU	5.5
2	D	389	CYS	5.1
2	C	296	PRO	5.1
2	C	299	MET	5.1
1	A	720	SER	5.0
2	D	296	PRO	5.0
2	C	300	LEU	5.0
1	B	-14	GLY	4.6
2	C	390	ILE	4.6
1	B	577	THR	4.5
2	C	298	ILE	4.3
2	C	294	ALA	4.1
2	C	303	PRO	4.1
2	C	392	GLY	4.1
1	A	-5	SER	4.1
2	D	295	ASP	3.8
1	A	575	GLY	3.8
2	C	389	CYS	3.7
2	D	294	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	231	LEU	3.5
2	C	391	GLY	3.4
1	B	576	GLY	3.3
2	C	228	LEU	3.1
1	A	574	ALA	3.1
2	C	2	SER	3.0
1	B	571	VAL	3.0
2	C	297	VAL	3.0
1	B	1	MET	3.0
1	B	-8	HIS	2.9
1	A	1	MET	2.9
2	C	302	GLY	2.9
1	B	578	TYR	2.9
1	B	-7	HIS	2.8
1	B	579	GLN	2.7
1	A	579	GLN	2.7
1	A	-7	HIS	2.7
1	B	720	SER	2.7
1	A	318	GLU	2.5
2	D	393	GLY	2.5
1	A	690	ALA	2.5
1	B	3	ASP	2.5
2	D	231	LEU	2.4
1	A	320	ILE	2.3
1	B	568	ARG	2.2
1	A	403	LYS	2.2
1	B	-13	SER	2.1
1	A	367	TYR	2.1

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

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

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,

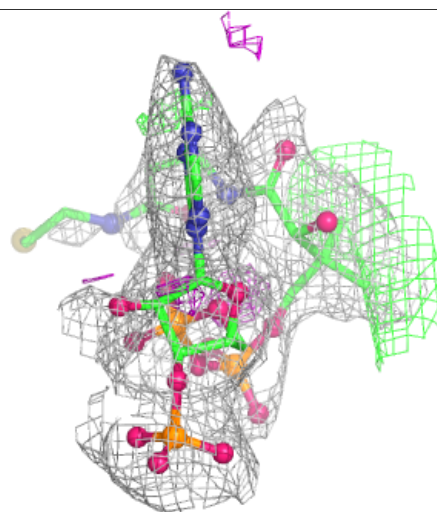
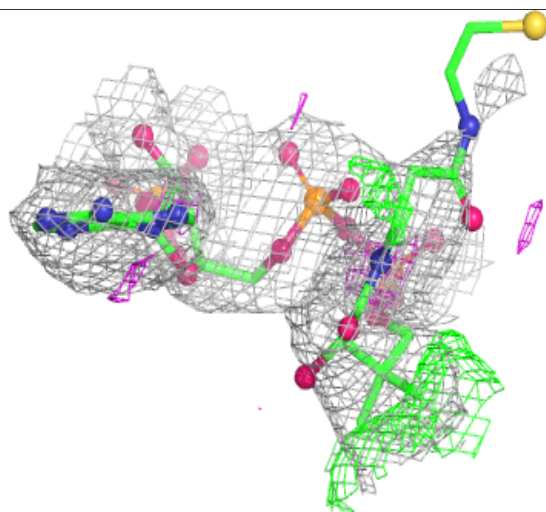
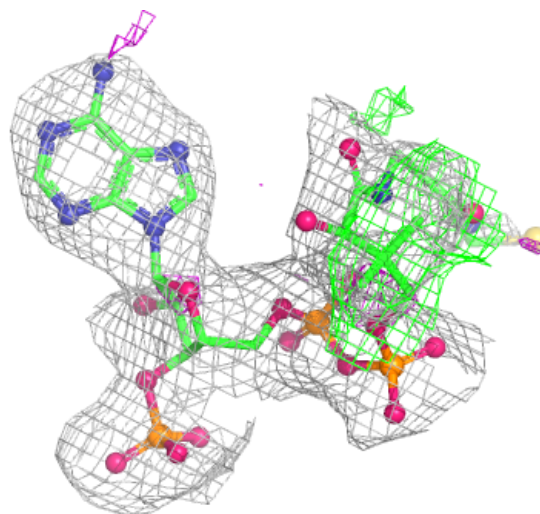
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	COA	C	508	48/48	0.74	0.15	57,113,138,141	0
5	COA	D	506	48/48	0.76	0.15	56,117,151,162	0
3	SO4	A	802	5/5	0.78	0.12	95,103,116,117	0
3	SO4	A	803	5/5	0.79	0.10	70,70,91,105	5
3	SO4	B	804	5/5	0.81	0.17	94,99,105,136	0
5	COA	C	509	48/48	0.82	0.15	46,93,131,158	0
3	SO4	A	805	5/5	0.83	0.12	35,46,58,65	5
3	SO4	D	505	5/5	0.84	0.24	82,94,107,112	1
3	SO4	D	508	5/5	0.85	0.14	73,78,98,109	0
4	GOL	A	806	6/6	0.86	0.13	52,81,95,98	0
3	SO4	B	803	5/5	0.86	0.11	53,65,85,104	5
3	SO4	C	507	5/5	0.88	0.11	56,70,89,104	0
3	SO4	B	801	5/5	0.89	0.10	55,55,63,91	0
5	COA	D	507	48/48	0.89	0.20	33,46,61,69	48
3	SO4	D	502	5/5	0.90	0.17	59,69,76,100	0
3	SO4	D	503	5/5	0.90	0.15	63,75,79,105	0
3	SO4	C	501	5/5	0.90	0.18	59,65,70,94	0
3	SO4	B	802	5/5	0.91	0.19	49,54,74,91	0
3	SO4	D	504	5/5	0.91	0.17	57,57,85,91	0
3	SO4	C	506	5/5	0.91	0.15	74,81,88,101	0
3	SO4	C	505	5/5	0.92	0.17	50,59,75,111	0
3	SO4	C	504	5/5	0.93	0.16	45,54,84,86	0
3	SO4	A	804	5/5	0.93	0.09	58,73,96,107	0
3	SO4	C	503	5/5	0.94	0.11	53,55,74,87	0
3	SO4	D	501	5/5	0.94	0.07	55,64,91,92	0
3	SO4	A	801	5/5	0.94	0.10	50,63,68,85	0
3	SO4	C	510	5/5	0.95	0.10	46,68,87,92	0
3	SO4	C	502	5/5	0.95	0.13	61,71,83,86	0
3	SO4	B	805	5/5	0.95	0.07	42,49,54,59	5
3	SO4	A	807	5/5	0.95	0.20	54,72,100,106	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.

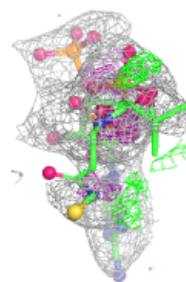
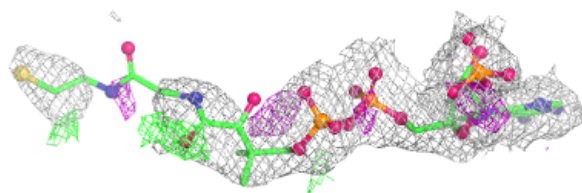
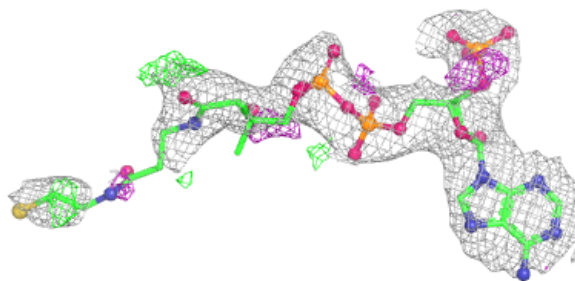
Electron density around COA C 508:

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

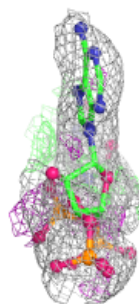
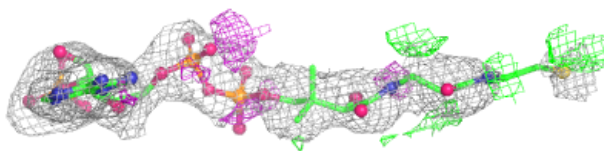
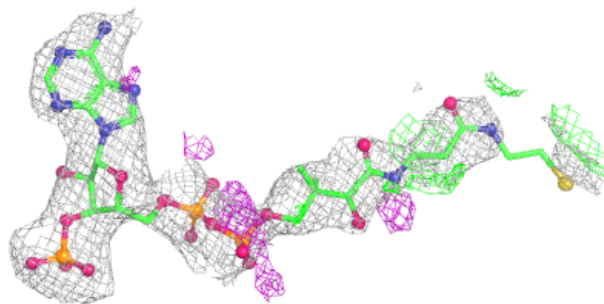


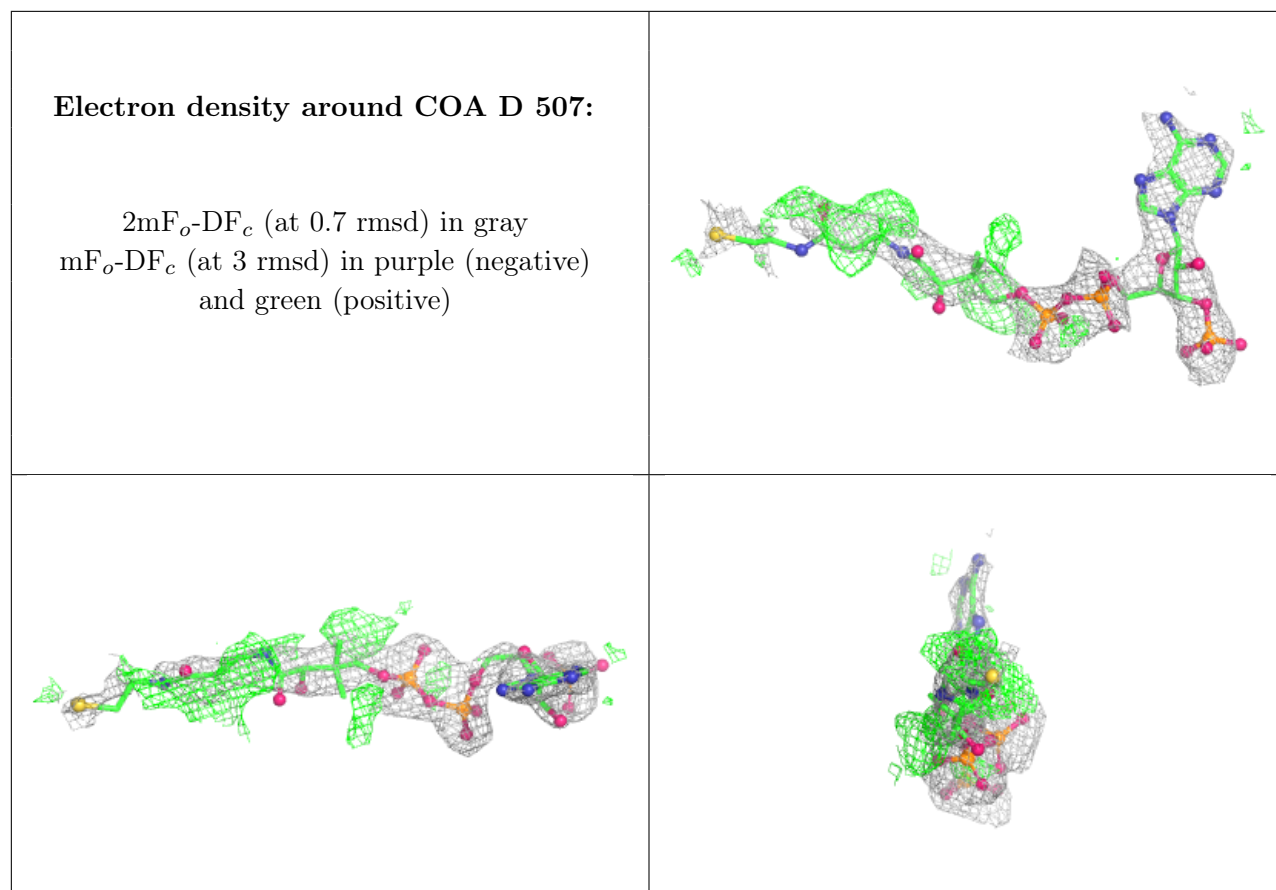
Electron density around COA D 506:

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

**Electron density around COA C 509:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.