



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2021 – 02:17 pm BST

PDB ID : 7O4S
Title : Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme with Coenzyme A bound at the hydratase, thiolase active sites and additional binding site (CoA(ECH2))
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **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

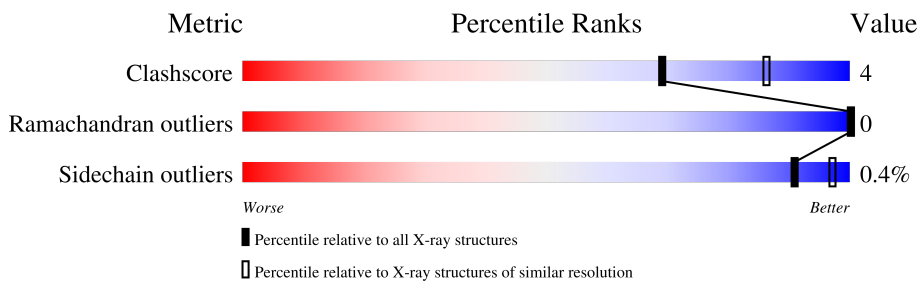
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-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))
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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	736	
1	B	736	
2	C	403	
2	D	403	

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 17341 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
			Total	C	N	O	S			
1	A	729	5417	3425	933	1038	21	0	0	0
1	B	728	5384	3407	927	1029	21	0	0	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	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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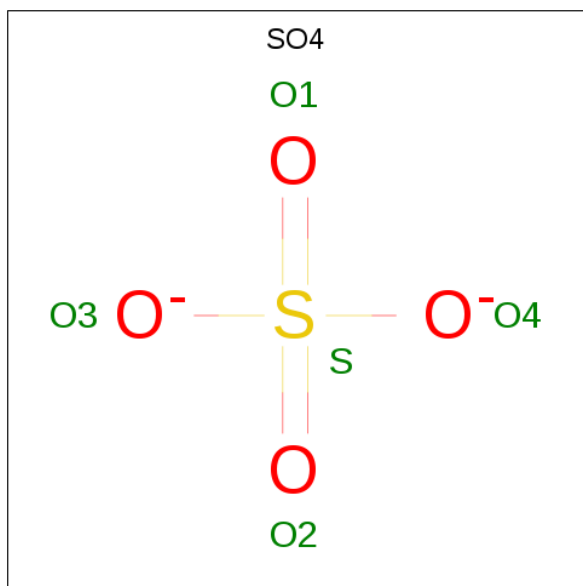
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression 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
			Total	C	N	O	S			
2	C	402	Total 2966	C 1853	N 525	O 573	S 15	0	0	0
2	D	402	Total 2963	C 1850	N 525	O 573	S 15	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

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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	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		

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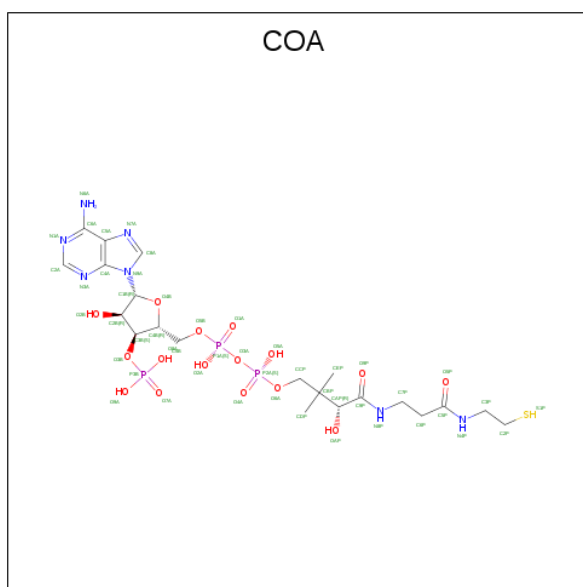
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



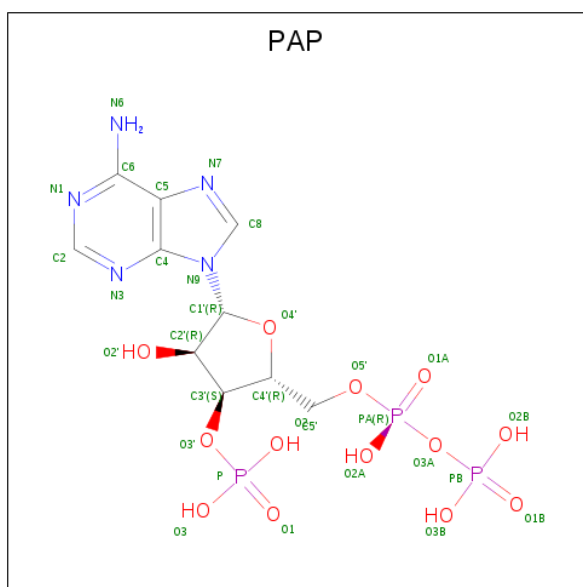
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

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



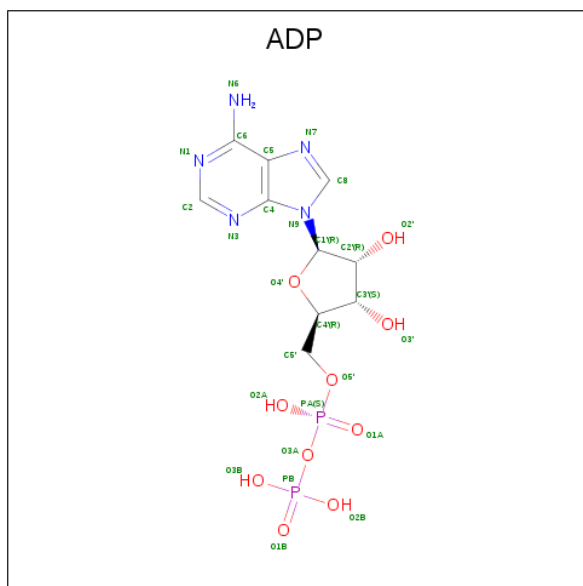
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
5	A	1	48	21	7	16	3	1	0	0
5	A	1	48	21	7	16	3	1	0	0
5	B	1	48	21	7	16	3	1	0	0
5	B	1	48	21	7	16	3	1	0	0
5	C	1	48	21	7	16	3	1	0	0
5	D	1	48	21	7	16	3	1	0	0

- Molecule 6 is 3'-PHOSPHATE-ADENOSINE-5'-DIPHOSPHATE (three-letter code: PAP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	C	1	31	10	5	13	3	0	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	D	1	27	10	5	10	2	0	0

- Molecule 8 is water.

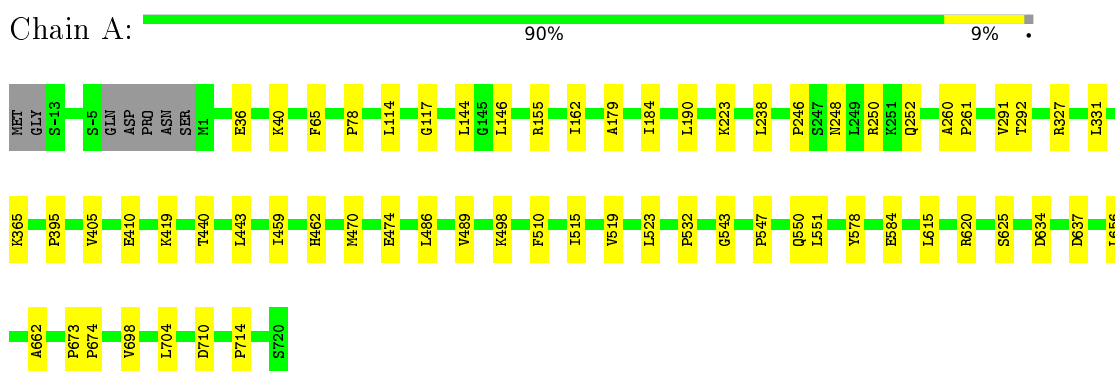
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	30	Total 30	O 30	0	0
8	B	37	Total 37	O 37	0	0
8	C	22	Total 22	O 22	0	0
8	D	22	Total 22	O 22	0	0

3 Residue-property plots [i](#)

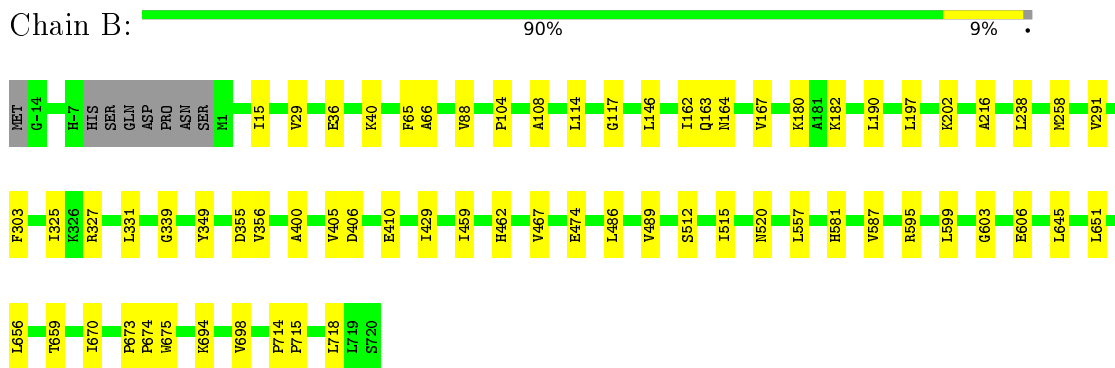
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

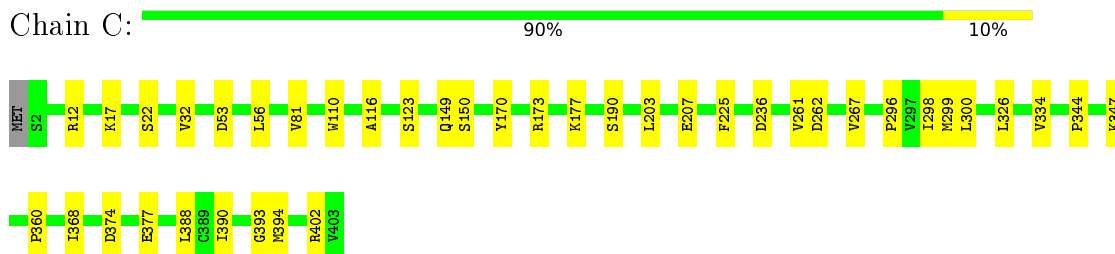
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase




- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

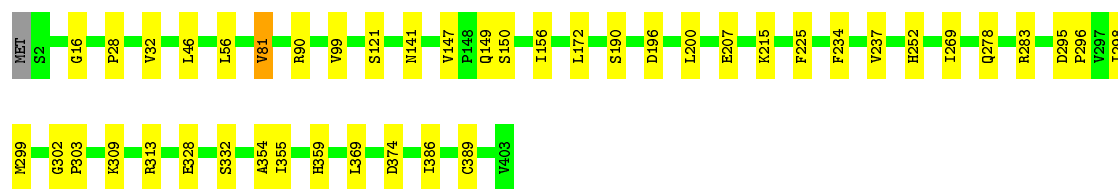


- Molecule 2: Putative acyltransferase Rv0859



- Molecule 2: Putative acyltransferase Rv0859

Chain D:  89% 11%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.41Å 136.60Å 117.91Å 90.00° 110.45° 90.00°	Depositor
Resolution (Å)	29.76 – 2.79	Depositor
% Data completeness (in resolution range)	97.5 (29.76-2.79)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.192 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	17341	wwPDB-VP
Average B, all atoms (Å ²)	67.0	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: GOL, PAP, COA, SO4, ADP

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	0.24	0/5520	0.41	0/7474
1	B	0.24	0/5486	0.40	0/7429
2	C	0.24	0/3011	0.43	0/4077
2	D	0.24	0/3008	0.43	0/4073
All	All	0.24	0/17025	0.41	0/23053

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	5417	0	5434	38	0
1	B	5384	0	5392	41	0
2	C	2966	0	2986	25	0
2	D	2963	0	2977	27	0
3	A	30	0	0	0	0
3	B	30	0	0	1	0
3	C	40	0	0	1	0
3	D	30	0	0	0	0
4	A	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	12	0	16	1	0
5	A	96	0	64	4	0
5	B	96	0	64	3	0
5	C	48	0	32	1	0
5	D	48	0	32	1	0
6	C	31	0	11	0	0
7	D	27	0	12	0	0
8	A	30	0	0	2	0
8	B	37	0	0	1	0
8	C	22	0	0	0	0
8	D	22	0	0	0	0
All	All	17341	0	17036	127	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 (127) 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)
1:B:515:ILE:HD13	1:B:670:ILE:HB	1.72	0.71
1:A:620:ARG:HG3	1:A:625:SER:HB2	1.75	0.67
5:A:809:COA:H141	5:A:809:COA:H71	1.75	0.67
2:D:252:HIS:HE1	2:D:332:SER:H	1.45	0.64
1:A:331:LEU:HB2	1:A:410:GLU:HA	1.80	0.63
1:A:698:VAL:HG13	1:A:714:PRO:HG3	1.80	0.63
2:D:147:VAL:HG13	2:D:234:PHE:HB3	1.81	0.63
2:C:190:SER:OG	2:C:374:ASP:OD2	2.15	0.63
1:A:459:ILE:HG21	1:A:489:VAL:HG21	1.80	0.62
2:C:81:VAL:HG11	2:D:296:PRO:HD3	1.83	0.60
1:A:532:PRO:HB2	1:A:615:LEU:HD13	1.83	0.60
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.84	0.59
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.85	0.59
1:B:698:VAL:HG13	1:B:714:PRO:HG3	1.84	0.59
2:C:17:LYS:HG3	2:C:207:GLU:HB3	1.84	0.58
1:A:36:GLU:HG3	1:A:40:LYS:HE3	1.86	0.58
1:A:146:LEU:HD22	1:A:291:VAL:HG22	1.86	0.57
1:A:710:ASP:H	4:A:807:GOL:H12	1.70	0.57
2:D:172:LEU:HD22	2:D:215:LYS:HG2	1.88	0.56
1:B:146:LEU:HD22	1:B:291:VAL:HG22	1.88	0.55
1:A:365:LYS:HD2	1:A:395:PRO:HD3	1.89	0.54
1:A:162:ILE:HD12	1:A:238:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:THR:HG21	1:A:443:LEU:HB2	1.90	0.53
1:B:104:PRO:HG3	1:B:216:ALA:HB1	1.91	0.53
1:B:459:ILE:HG21	1:B:489:VAL:HG21	1.89	0.53
1:A:155:ARG:NH1	8:A:901:HOH:O	2.43	0.51
2:C:53:ASP:OD2	2:D:90:ARG:NH2	2.38	0.51
2:C:296:PRO:HD3	2:D:81:VAL:HG21	1.92	0.51
2:C:344:PRO:HG2	2:C:347:LYS:HE3	1.92	0.51
1:B:88:VAL:HG12	4:B:809:GOL:H32	1.93	0.51
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.46	0.51
1:A:223:LYS:NZ	8:A:902:HOH:O	2.43	0.50
1:B:400:ALA:HA	1:B:429:ILE:HD13	1.94	0.50
2:C:298:ILE:HG22	2:C:300:LEU:H	1.77	0.50
1:B:182:LYS:HD2	1:B:190:LEU:HG	1.94	0.49
1:B:162:ILE:HD12	1:B:238:LEU:HD21	1.94	0.49
1:A:327:ARG:HD2	1:A:405:VAL:HG22	1.94	0.49
1:A:419:LYS:HE2	1:A:440:THR:HG23	1.95	0.48
2:C:368:ILE:HD11	2:C:388:LEU:HD11	1.95	0.48
1:B:459:ILE:HD11	1:B:486:LEU:HD12	1.95	0.48
2:D:190:SER:OG	2:D:374:ASP:OD2	2.20	0.48
1:B:339:GLY:HA3	1:B:467:VAL:HB	1.96	0.47
1:A:246:PRO:HG2	2:D:141:ASN:HB3	1.97	0.47
1:A:519:VAL:O	1:A:523:LEU:HG	2.14	0.47
1:A:184:ILE:O	5:A:809:COA:H31	2.14	0.47
2:C:22:SER:OG	2:C:207:GLU:OE2	2.31	0.47
2:C:32:VAL:HG11	2:C:56:LEU:HD11	1.97	0.47
2:C:299:MET:HA	2:C:393:GLY:HA2	1.96	0.47
1:B:595:ARG:HB3	1:B:603:GLY:HA2	1.98	0.46
2:C:149:GLN:OE1	5:C:508:COA:S1P	2.70	0.46
2:C:390:ILE:HB	2:C:394:MET:HB2	1.96	0.46
1:B:651:LEU:HD23	1:B:656:LEU:HB2	1.97	0.46
2:C:116:ALA:O	2:C:267:VAL:N	2.42	0.46
1:A:65:PHE:HB3	1:A:117:GLY:HA2	1.98	0.46
1:A:578:TYR:OH	1:A:584:GLU:OE2	2.27	0.45
2:C:150:SER:HB2	2:C:225:PHE:CG	2.51	0.45
1:B:595:ARG:HH22	1:B:606:GLU:HG2	1.81	0.45
2:D:149:GLN:HG2	2:D:299:MET:SD	2.55	0.45
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.98	0.45
2:C:298:ILE:O	2:C:299:MET:HG2	2.15	0.45
2:C:402:ARG:NH2	3:C:507:SO4:O4	2.50	0.45
1:A:179:ALA:HA	1:A:190:LEU:HD11	1.99	0.45
2:D:295:ASP:HB3	2:D:298:ILE:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ALA:HB1	1:B:197:LEU:HB3	1.99	0.45
2:D:32:VAL:HG11	2:D:56:LEU:HD11	1.99	0.45
1:A:656:LEU:HD13	1:A:662:ALA:HB2	1.97	0.44
2:D:328:GLU:HB3	2:D:355:ILE:HG13	2.00	0.44
1:A:114:LEU:HD12	5:A:808:COA:H141	1.99	0.44
2:C:326:LEU:HD23	2:C:334:VAL:HA	1.98	0.44
1:B:659:THR:N	3:B:804:SO4:O1	2.48	0.44
2:D:303:PRO:HD3	2:D:389:CYS:HA	1.99	0.44
2:D:156:ILE:HG12	2:D:298:ILE:HD11	2.00	0.44
1:B:645:LEU:HD22	1:B:715:PRO:HD3	1.99	0.44
1:B:36:GLU:HG3	1:B:40:LYS:HE3	2.00	0.43
1:B:164:ASN:HD22	5:B:808:COA:H61	1.83	0.43
1:B:406:ASP:OD1	1:B:406:ASP:N	2.48	0.43
2:D:369:LEU:HD12	2:D:386:ILE:HD13	2.00	0.43
1:B:325:ILE:HB	1:B:349:TYR:HE1	1.84	0.43
1:B:327:ARG:HG2	1:B:405:VAL:HG22	2.00	0.43
1:A:65:PHE:HB3	1:A:117:GLY:CA	2.48	0.43
1:A:144:LEU:HD12	5:A:808:COA:H31	2.01	0.43
1:A:250:ARG:HG2	2:D:237:VAL:HG22	2.01	0.43
1:B:355:ASP:OD1	1:B:356:VAL:N	2.42	0.43
2:C:377:GLU:HA	2:C:402:ARG:HD2	2.01	0.43
1:B:331:LEU:HB2	1:B:410:GLU:HA	2.01	0.42
1:A:248:ASN:O	1:A:252:GLN:HG2	2.19	0.42
2:D:309:LYS:HE2	2:D:313:ARG:HH22	1.85	0.42
5:D:507:COA:H62	5:D:507:COA:H31	1.78	0.42
1:A:543:GLY:HA3	1:A:673:PRO:HB3	2.02	0.42
1:B:182:LYS:NZ	8:B:902:HOH:O	2.40	0.42
1:B:557:LEU:HB3	1:B:587:VAL:HG13	2.01	0.42
2:D:196:ASP:OD1	2:D:200:LEU:N	2.53	0.42
1:B:15:ILE:HG21	1:B:202:LYS:HG2	2.01	0.42
2:C:261:VAL:HG23	2:C:360:PRO:HG3	2.00	0.42
1:A:515:ILE:HD11	1:A:551:LEU:HD21	2.01	0.42
1:A:637:ASP:HB3	1:A:704:LEU:HD11	2.02	0.42
1:B:673:PRO:HA	1:B:674:PRO:HD3	1.92	0.42
2:C:170:TYR:OH	2:C:334:VAL:HG11	2.20	0.42
1:B:303:PHE:CZ	1:B:674:PRO:HB3	2.55	0.42
2:D:252:HIS:CE1	2:D:332:SER:H	2.30	0.42
2:D:354:ALA:HB1	2:D:359:HIS:HB2	2.02	0.41
1:B:325:ILE:HB	1:B:349:TYR:CE1	2.55	0.41
1:B:714:PRO:HA	1:B:715:PRO:HD3	1.98	0.41
1:A:459:ILE:HD11	1:A:486:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLN:O	1:B:167:VAL:HG23	2.20	0.41
2:C:173:ARG:O	2:C:177:LYS:HG3	2.21	0.41
1:A:78:PRO:HA	1:A:292:THR:HB	2.03	0.41
1:A:470:MET:O	1:A:498:LYS:NZ	2.45	0.41
1:B:258:MET:HG2	1:B:675:TRP:HB3	2.01	0.41
2:D:46:LEU:HD12	2:D:278:GLN:HB3	2.03	0.41
2:D:302:GLY:N	2:D:303:PRO:HD2	2.35	0.41
1:B:520:ASN:HB3	1:B:581:HIS:CE1	2.55	0.41
1:A:510:PHE:CD1	1:A:656:LEU:HD11	2.56	0.41
1:A:547:PRO:HG2	1:A:550:GLN:HB3	2.02	0.41
1:B:512:SER:HA	1:B:515:ILE:HG22	2.03	0.41
2:D:150:SER:HB2	2:D:225:PHE:CG	2.56	0.41
1:B:694:LYS:HD3	1:B:718:LEU:O	2.21	0.41
1:B:65:PHE:HB3	1:B:117:GLY:HA2	2.02	0.40
1:A:673:PRO:HA	1:A:674:PRO:HD3	1.94	0.40
2:D:16:GLY:HA2	2:D:207:GLU:HG2	2.03	0.40
2:D:28:PRO:HG3	2:D:121:SER:HB3	2.02	0.40
1:A:260:ALA:HB3	1:A:261:PRO:HD3	2.02	0.40
2:C:123:SER:OG	2:C:262:ASP:OD2	2.31	0.40
2:C:203:LEU:HD11	2:C:207:GLU:HG3	2.03	0.40
1:B:66:ALA:O	5:B:807:COA:H61	2.22	0.40
1:B:114:LEU:HD12	5:B:807:COA:H141	2.03	0.40
1:B:599:LEU:HD12	1:B:599:LEU:HA	1.97	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	A	725/736 (98%)	701 (97%)	24 (3%)	0	100	100
1	B	724/736 (98%)	701 (97%)	23 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	400/403 (99%)	389 (97%)	11 (3%)	0	100	100
2	D	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
All	All	2249/2278 (99%)	2178 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	Percentiles	
1	A	557/566 (98%)	556 (100%)	1 (0%)	93	98
1	B	549/566 (97%)	547 (100%)	2 (0%)	91	97
2	C	309/310 (100%)	307 (99%)	2 (1%)	86	96
2	D	308/310 (99%)	306 (99%)	2 (1%)	86	96
All	All	1723/1752 (98%)	1716 (100%)	7 (0%)	91	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	634	ASP
1	B	29	VAL
1	B	180	LYS
2	C	12	ARG
2	C	236	ASP
2	D	81	VAL
2	D	283	ARG

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](#)

38 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	COA	A	808	-	41,50,50	0.59	0	52,75,75	0.75	2 (3%)
5	COA	B	808	-	41,50,50	0.59	0	52,75,75	0.81	3 (5%)
3	SO4	B	801	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	C	510	-	4,4,4	0.14	0	6,6,6	0.04	0
5	COA	C	508	-	41,50,50	0.57	0	52,75,75	0.71	1 (1%)
4	GOL	B	809	-	5,5,5	0.91	0	5,5,5	0.98	0
4	GOL	B	806	-	5,5,5	0.89	0	5,5,5	1.01	0
3	SO4	C	505	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	805	-	4,4,4	0.13	0	6,6,6	0.07	0
5	COA	A	809	-	41,50,50	0.59	0	52,75,75	0.83	2 (3%)
3	SO4	B	804	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	805	-	4,4,4	0.14	0	6,6,6	0.06	0
6	PAP	C	509	-	28,33,33	0.93	1 (3%)	35,52,52	1.20	3 (8%)
3	SO4	A	804	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	806	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.04	0
5	COA	D	507	-	41,50,50	0.59	0	52,75,75	0.69	1 (1%)
4	GOL	A	807	-	5,5,5	0.91	0	5,5,5	0.99	0
7	ADP	D	508	-	24,29,29	0.98	1 (4%)	29,45,45	1.40	4 (13%)
5	COA	B	807	-	41,50,50	0.61	0	52,75,75	0.77	1 (1%)
3	SO4	A	802	-	4,4,4	0.13	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	810	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	802	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	D	506	-	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	B	803	-	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
4	GOL	A	810	-	5,5,5	0.91	0	5,5,5	0.98	0
3	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	A	803	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	C	504	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	C	507	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	A	801	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	D	503	-	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
6	PAP	C	509	-	-	5/17/37/37	0/3/3/3
5	COA	A	808	-	-	7/44/64/64	0/3/3/3
5	COA	B	808	-	-	16/44/64/64	0/3/3/3
5	COA	D	507	-	-	9/44/64/64	0/3/3/3
4	GOL	A	810	-	-	2/4/4/4	-
4	GOL	A	807	-	-	1/4/4/4	-
5	COA	A	809	-	-	14/44/64/64	0/3/3/3
7	ADP	D	508	-	-	5/12/32/32	0/3/3/3
5	COA	B	807	-	-	17/44/64/64	0/3/3/3
5	COA	C	508	-	-	7/44/64/64	0/3/3/3
4	GOL	B	809	-	-	2/4/4/4	-
4	GOL	B	806	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	508	ADP	C5-C4	2.56	1.47	1.40
6	C	509	PAP	C5-C4	2.38	1.47	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	508	ADP	C3'-C2'-C1'	3.27	105.90	100.98
7	D	508	ADP	PA-O3A-PB	-3.15	122.03	132.83
7	D	508	ADP	N3-C2-N1	-3.08	123.86	128.68
6	C	509	PAP	C4-C5-N7	-2.82	106.46	109.40
5	B	808	COA	C7P-C6P-C5P	-2.72	107.82	112.36
6	C	509	PAP	N3-C2-N1	-2.61	124.60	128.68
6	C	509	PAP	PA-O3A-PB	-2.57	124.02	132.83
7	D	508	ADP	C4-C5-N7	-2.51	106.78	109.40
5	C	508	COA	C5A-C6A-N6A	2.31	123.86	120.35
5	B	808	COA	C5A-C6A-N6A	2.30	123.85	120.35
5	A	808	COA	O4B-C1B-C2B	-2.30	103.56	106.93
5	A	809	COA	C5A-C6A-N6A	2.30	123.84	120.35
5	D	507	COA	C5A-C6A-N6A	2.28	123.82	120.35
5	A	808	COA	C5A-C6A-N6A	2.28	123.82	120.35
5	B	807	COA	C5A-C6A-N6A	2.25	123.76	120.35
5	A	809	COA	O4B-C1B-C2B	-2.06	103.91	106.93
5	B	808	COA	C2B-C3B-C4B	-2.04	99.60	103.22

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	810	GOL	O1-C1-C2-C3
4	B	806	GOL	C1-C2-C3-O3
5	A	808	COA	N8P-C9P-CAP-OAP
5	A	809	COA	P2A-O3A-P1A-O5B
5	A	809	COA	C9P-CAP-CBP-CCP
5	A	809	COA	OAP-CAP-CBP-CDP
5	A	809	COA	C9P-CAP-CBP-CDP
5	A	809	COA	OAP-CAP-CBP-CEP
5	A	809	COA	C9P-CAP-CBP-CEP
5	A	809	COA	CAP-C9P-N8P-C7P
5	A	809	COA	O9P-C9P-N8P-C7P
5	B	807	COA	C3B-O3B-P3B-O8A
5	B	807	COA	C9P-CAP-CBP-CCP
5	B	807	COA	OAP-CAP-CBP-CDP

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Mol	Chain	Res	Type	Atoms
5	B	807	COA	C9P-CAP-CBP-CDP
5	B	807	COA	C9P-CAP-CBP-CEP
5	B	807	COA	N8P-C9P-CAP-OAP
5	B	808	COA	C4B-C5B-O5B-P1A
5	B	808	COA	C5B-O5B-P1A-O1A
5	B	808	COA	CAP-CBP-CCP-O6A
5	B	808	COA	C9P-CAP-CBP-CCP
5	B	808	COA	CAP-C9P-N8P-C7P
5	B	808	COA	C5P-C6P-C7P-N8P
5	B	808	COA	S1P-C2P-C3P-N4P
5	C	508	COA	CCP-O6A-P2A-O4A
5	C	508	COA	C5P-C6P-C7P-N8P
5	D	507	COA	C3B-O3B-P3B-O8A
5	D	507	COA	CCP-O6A-P2A-O3A
5	D	507	COA	CCP-O6A-P2A-O4A
5	D	507	COA	CAP-C9P-N8P-C7P
6	C	509	PAP	C5'-O5'-PA-O3A
6	C	509	PAP	O4'-C4'-C5'-O5'
6	C	509	PAP	C3'-C4'-C5'-O5'
7	D	508	ADP	C5'-O5'-PA-O1A
7	D	508	ADP	C5'-O5'-PA-O2A
5	C	508	COA	C6P-C5P-N4P-C3P
5	D	507	COA	C6P-C5P-N4P-C3P
5	C	508	COA	O4B-C4B-C5B-O5B
5	B	807	COA	C4B-C3B-O3B-P3B
5	C	508	COA	O5P-C5P-N4P-C3P
5	D	507	COA	O5P-C5P-N4P-C3P
5	B	808	COA	O9P-C9P-N8P-C7P
5	D	507	COA	O9P-C9P-N8P-C7P
4	A	810	GOL	O1-C1-C2-O2
4	B	806	GOL	O1-C1-C2-O2
4	B	806	GOL	O1-C1-C2-C3
4	B	809	GOL	C1-C2-C3-O3
4	B	806	GOL	O2-C2-C3-O3
5	A	809	COA	C3B-C4B-C5B-O5B
5	A	809	COA	O4B-C4B-C5B-O5B
5	A	808	COA	O9P-C9P-CAP-OAP
5	B	807	COA	O9P-C9P-CAP-OAP
5	C	508	COA	C3B-C4B-C5B-O5B
5	B	807	COA	OAP-CAP-CBP-CEP
7	D	508	ADP	O4'-C4'-C5'-O5'
5	A	809	COA	C4B-C5B-O5B-P1A

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Mol	Chain	Res	Type	Atoms
5	A	809	COA	P1A-O3A-P2A-O6A
5	B	807	COA	P1A-O3A-P2A-O6A
5	B	807	COA	C3B-O3B-P3B-O7A
6	C	509	PAP	C3'-O3'-P-O1
5	A	808	COA	C9P-CAP-CBP-CEP
5	B	808	COA	C9P-CAP-CBP-CDP
7	D	508	ADP	C5'-O5'-PA-O3A
5	B	807	COA	P2A-O3A-P1A-O1A
5	D	507	COA	CCP-O6A-P2A-O5A
6	C	509	PAP	C5'-O5'-PA-O2A
5	B	807	COA	C2P-C3P-N4P-C5P
5	A	809	COA	OAP-CAP-CBP-CCP
5	B	807	COA	OAP-CAP-CBP-CCP
5	B	808	COA	O9P-C9P-CAP-OAP
5	B	808	COA	CDP-CBP-CCP-O6A
5	B	808	COA	CEP-CBP-CCP-O6A
5	B	807	COA	C2B-C3B-O3B-P3B
5	B	808	COA	N8P-C9P-CAP-CBP
4	B	809	GOL	O2-C2-C3-O3
7	D	508	ADP	C3'-C4'-C5'-O5'
5	A	808	COA	C2P-C3P-N4P-C5P
5	B	808	COA	C9P-CAP-CBP-CEP
5	A	809	COA	C5B-O5B-P1A-O3A
5	C	508	COA	CCP-O6A-P2A-O3A
5	D	507	COA	C4B-C5B-O5B-P1A
5	A	808	COA	P2A-O3A-P1A-O2A
5	B	807	COA	P2A-O3A-P1A-O2A
5	B	808	COA	P2A-O3A-P1A-O2A
4	A	807	GOL	O1-C1-C2-C3
5	A	808	COA	CCP-O6A-P2A-O4A
5	B	807	COA	CCP-O6A-P2A-O4A
5	B	808	COA	O9P-C9P-CAP-CBP
5	A	808	COA	C9P-CAP-CBP-CCP

There are no ring outliers.

10 monomers are involved in 13 short contacts:

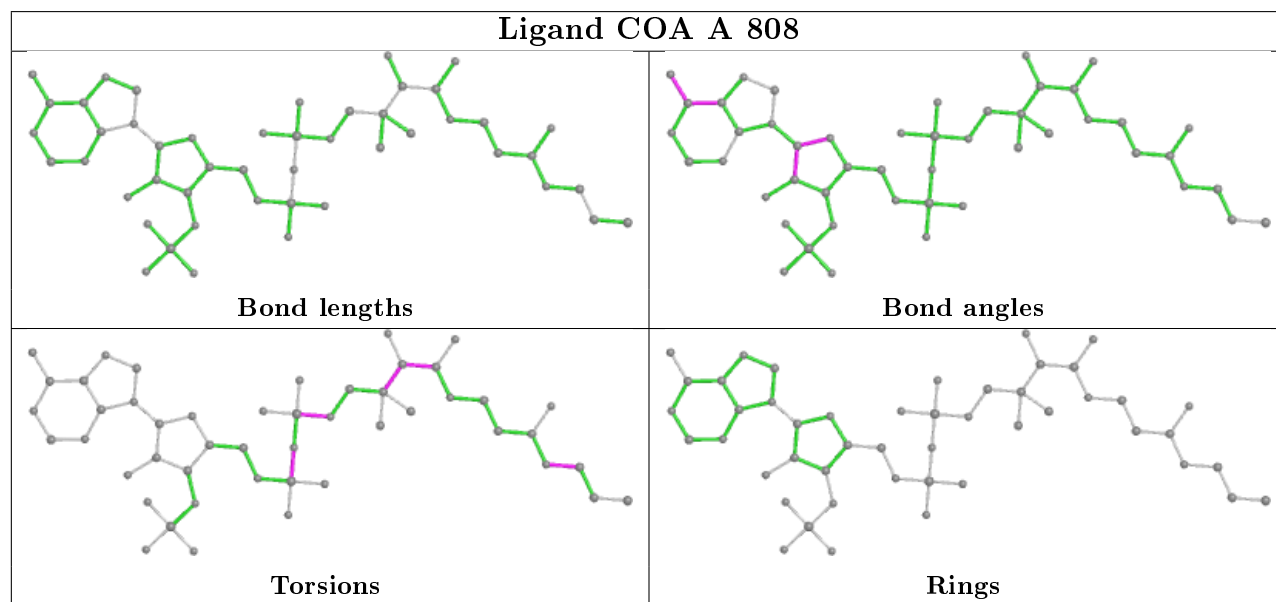
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	808	COA	2	0
5	B	808	COA	1	0
5	C	508	COA	1	0
4	B	809	GOL	1	0

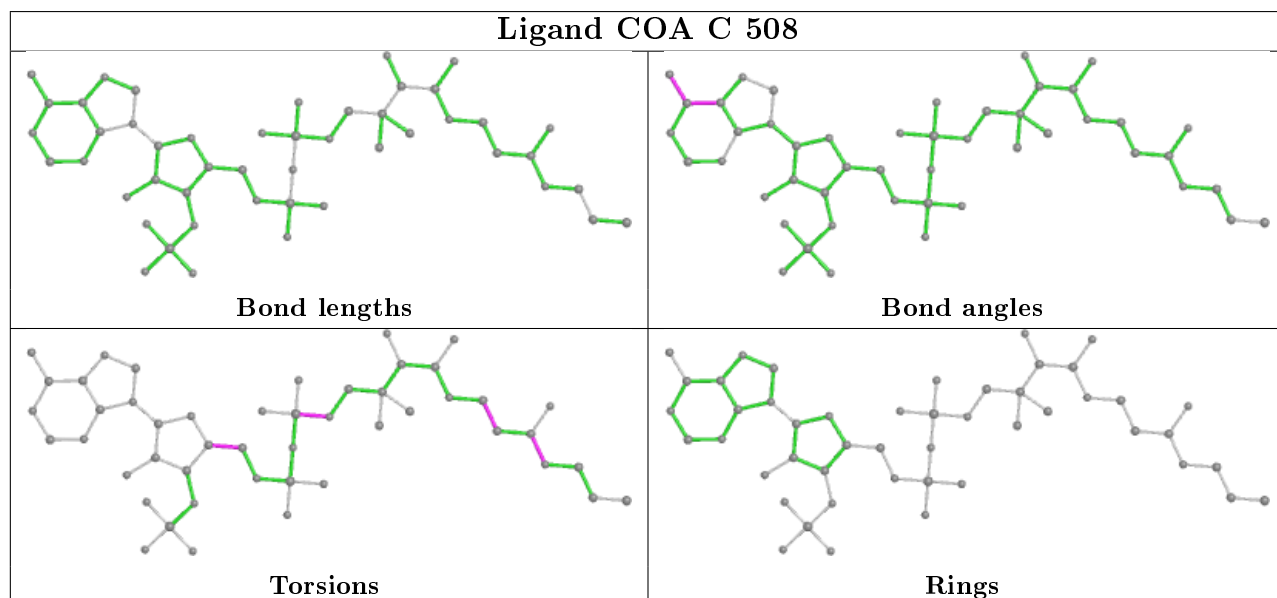
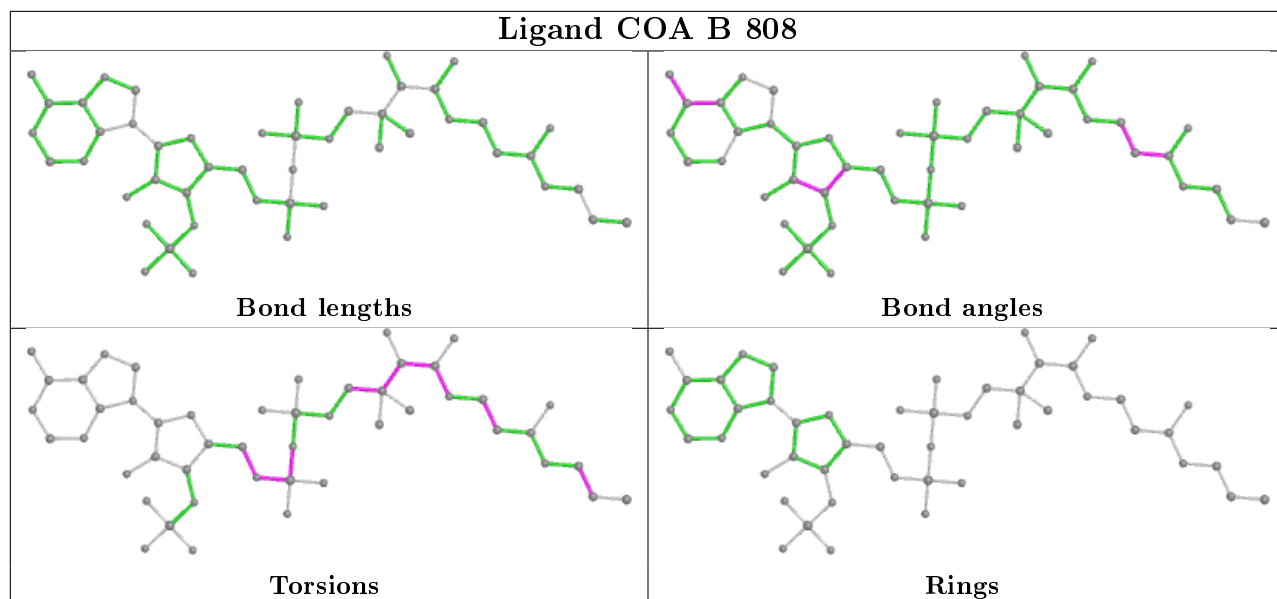
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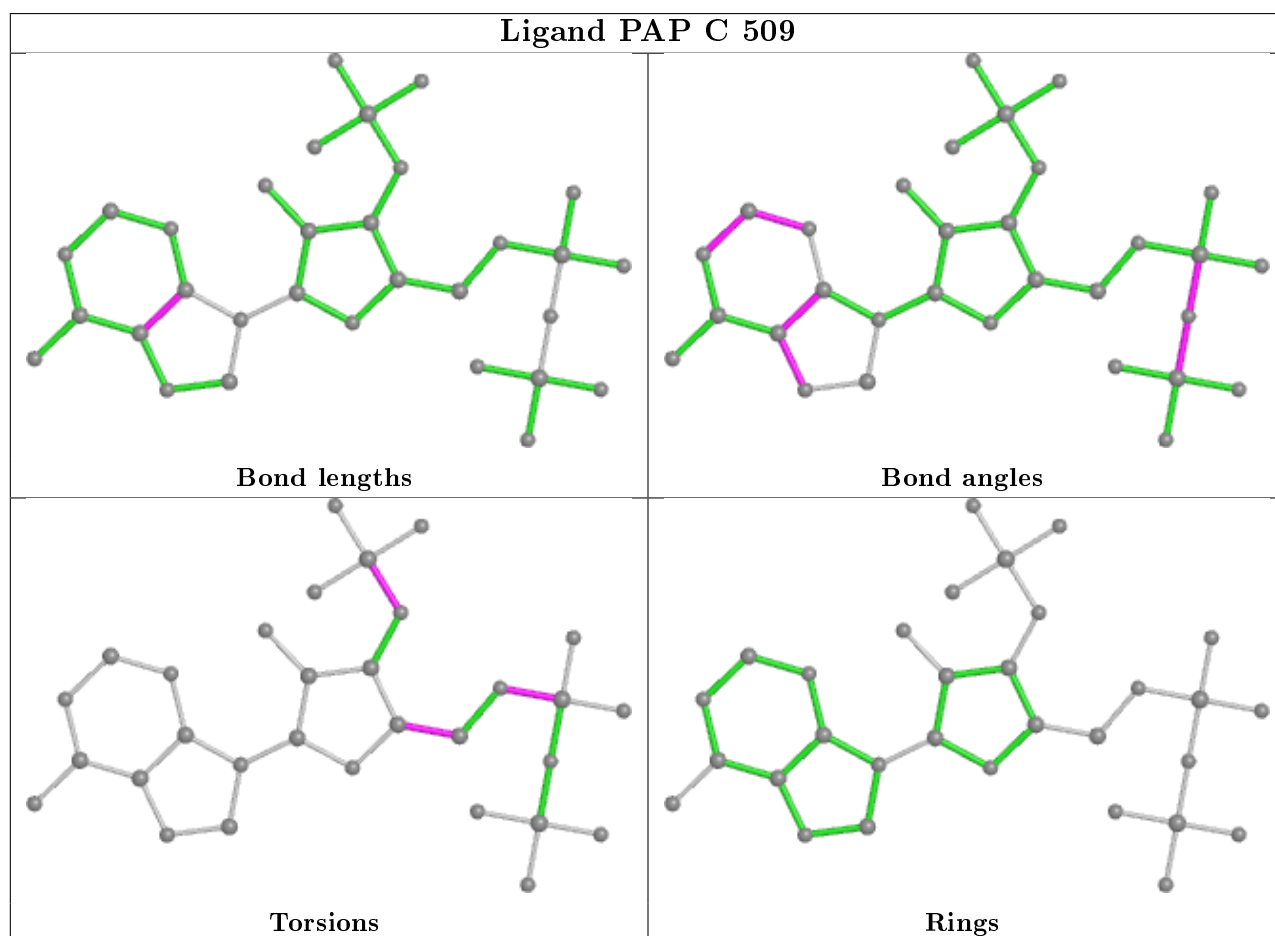
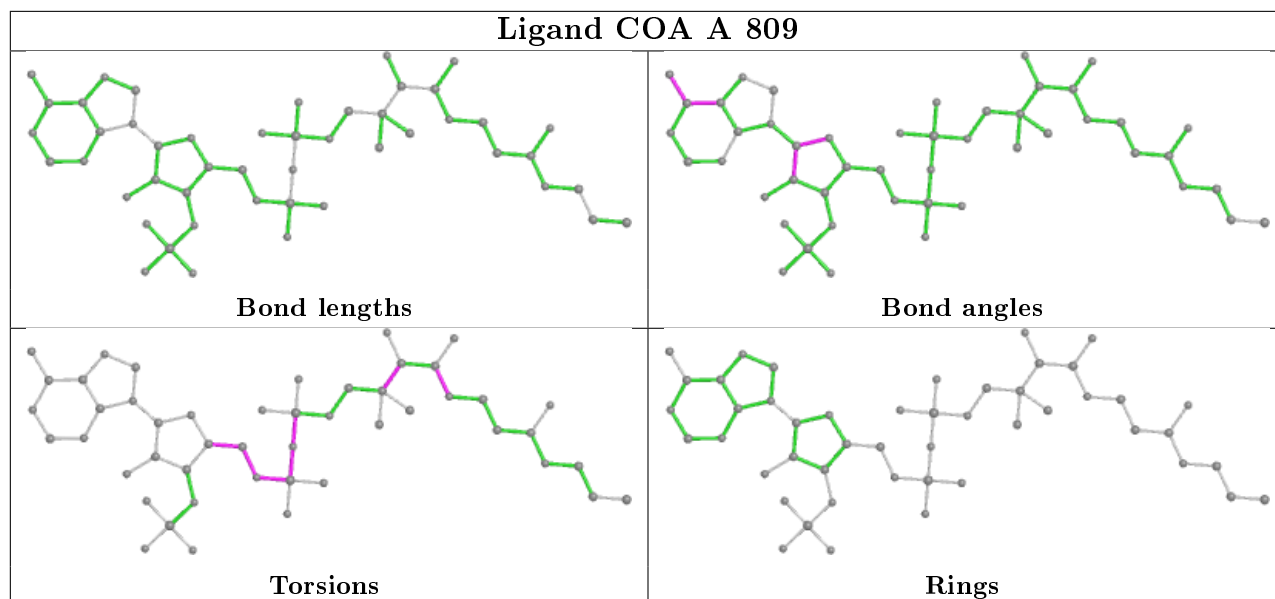
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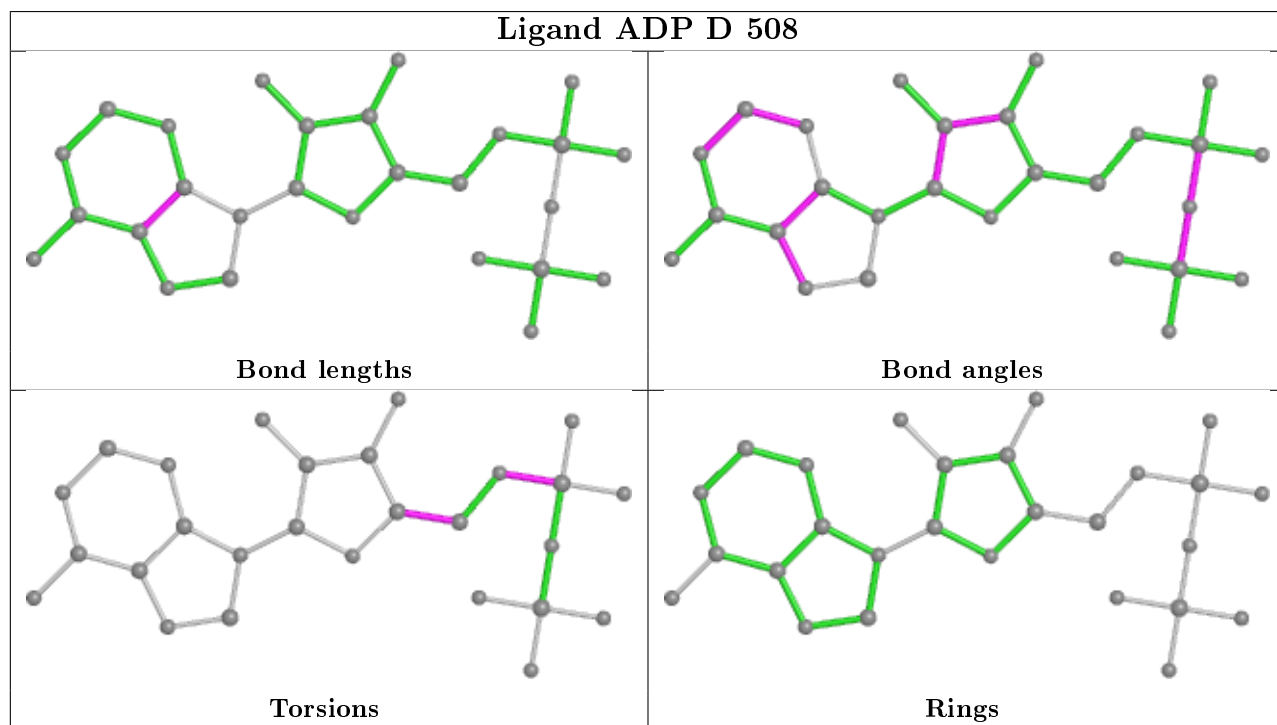
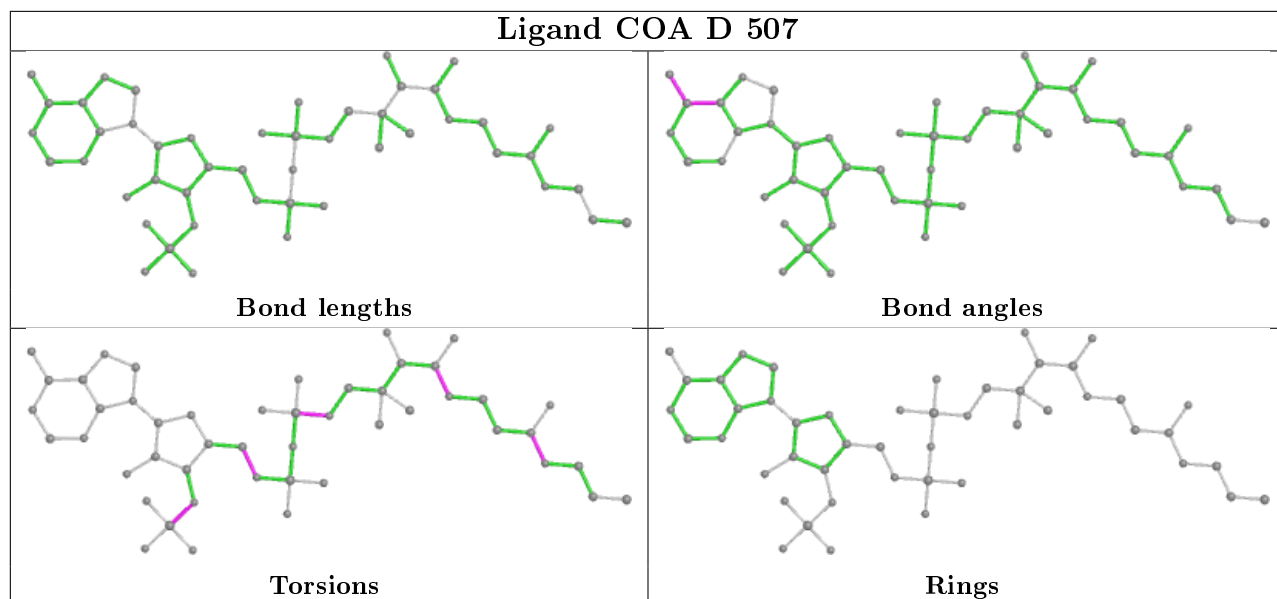
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	809	COA	2	0
3	B	804	SO4	1	0
5	D	507	COA	1	0
4	A	807	GOL	1	0
5	B	807	COA	2	0
3	C	507	SO4	1	0

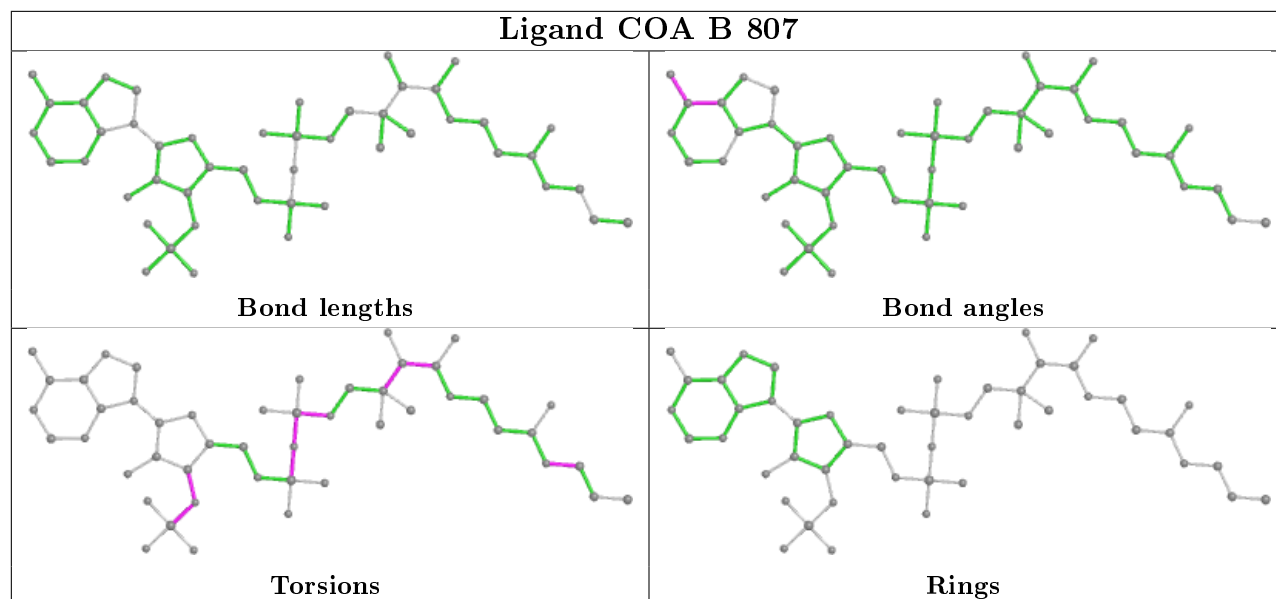
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.