



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:09 PM UTC

PDB ID : 7O4T / pdb_00007o4t
Title : Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme with Coenzyme A bound at the hydratase, thiolase active sites and possible additional binding site (CoA(ECH/HAD))
Authors : Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on : 2021-04-07
Resolution : 2.10 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

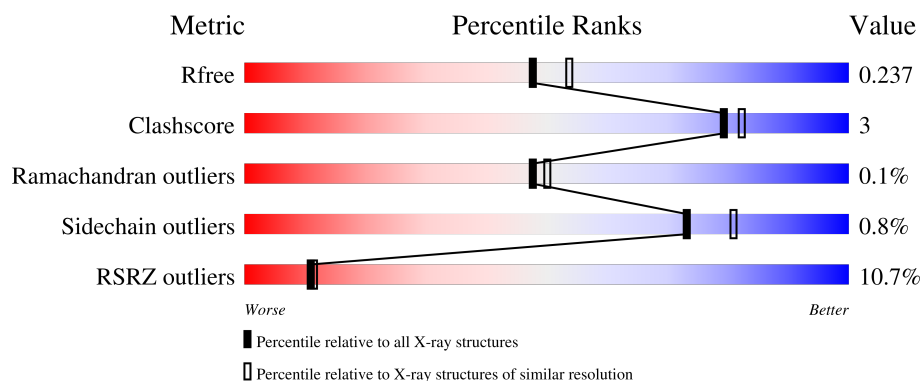
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	9% 93% 6%
1	B	736	16% 91% 8%
2	C	403	7% 91% 9%
2	D	403	8% 91% 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17555 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	1	0
			5424	3430	936	1037	21			
1	B	729	Total	C	N	O	S	0	1	0
			5405	3420	931	1033	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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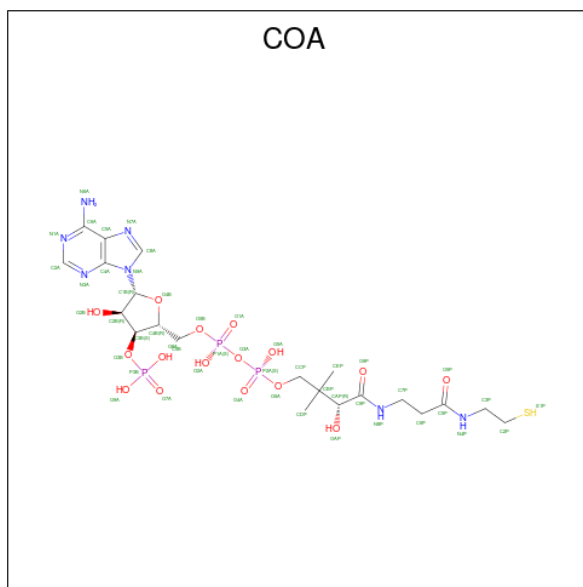
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression 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	2	0
			2974	1857	526	576	15			
2	D	403	Total	C	N	O	S	0	3	0
			2984	1864	528	577	15			

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



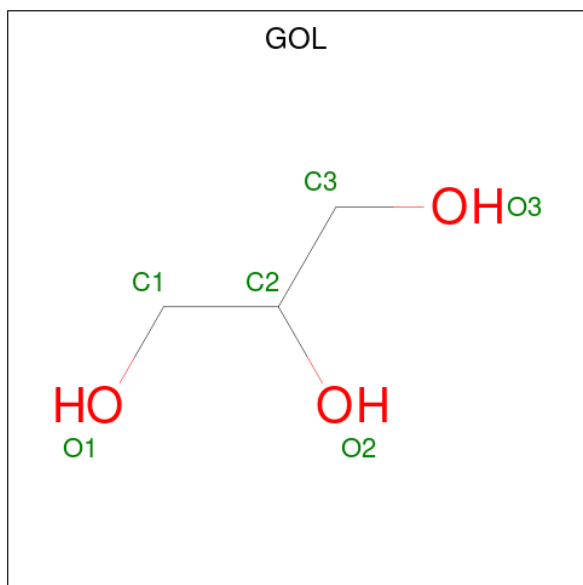
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		
3	A	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		
3	B	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		

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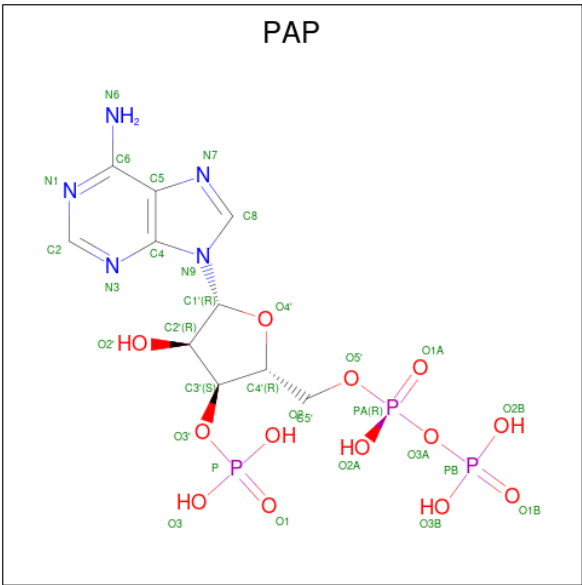
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



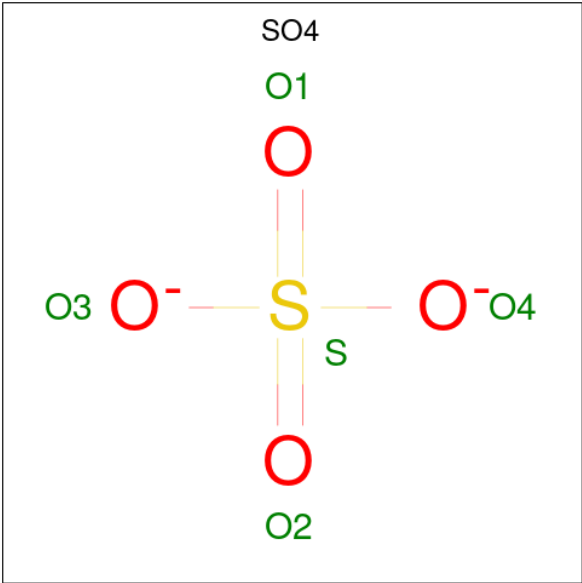
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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



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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

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

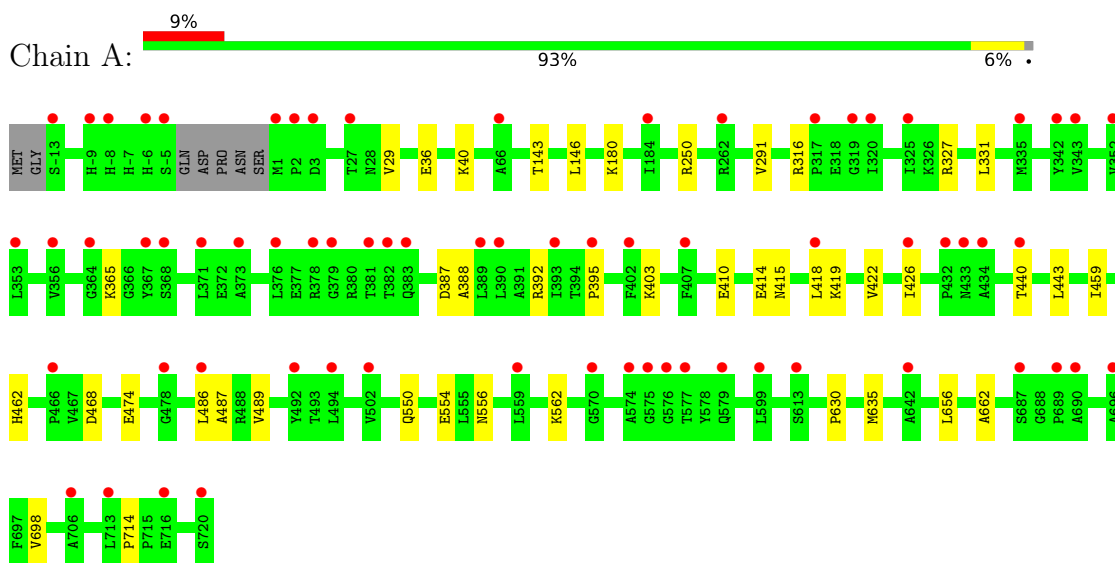
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	60	Total	O	0	0
			60	60		
7	B	73	Total	O	0	0
			73	73		
7	C	73	Total	O	0	0
			73	73		
7	D	59	Total	O	0	0
			59	59		

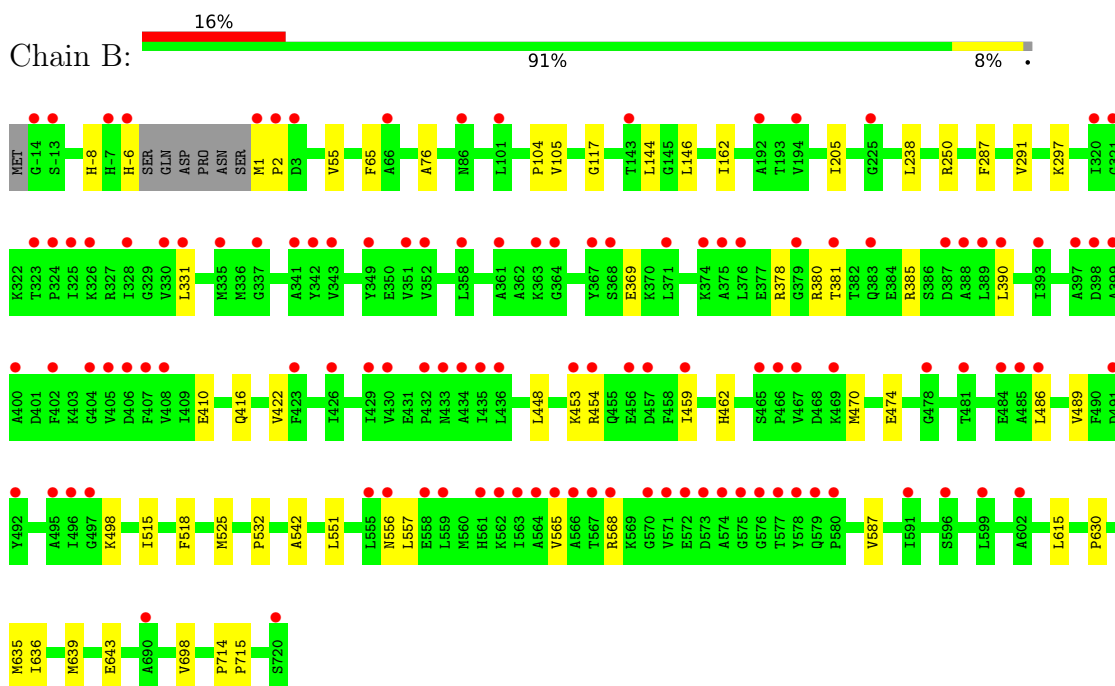
3 Residue-property plots [i](#)

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.

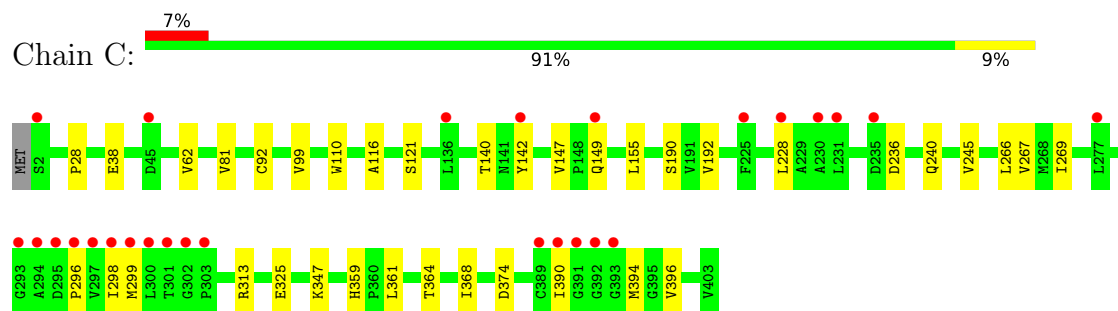
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase



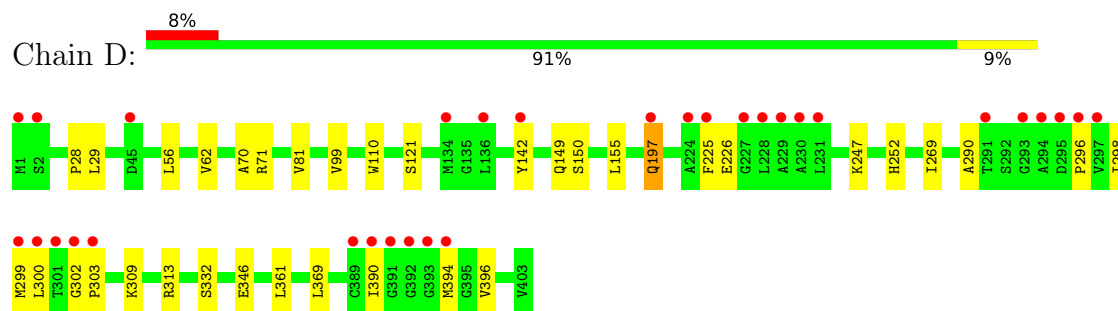
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase



- 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	247.54Å 136.25Å 117.80Å 90.00° 110.50° 90.00°	Depositor
Resolution (Å)	58.74 – 2.10 58.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (58.74-2.10) 99.6 (58.74-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.206 , 0.234 0.209 , 0.237	Depositor DCC
R_{free} test set	10661 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	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	0.96	EDS
Total number of atoms	17555	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: PAP, GOL, SO4, 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	A	0.09	0/5530	0.26	0/7487
1	B	0.10	0/5510	0.27	0/7460
2	C	0.11	0/3025	0.32	0/4096
2	D	0.10	0/3035	0.30	0/4110
All	All	0.10	0/17100	0.28	0/23153

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	5424	0	5444	19	0
1	B	5405	0	5429	33	0
2	C	2974	0	2989	22	0
2	D	2984	0	3003	24	0
3	A	96	0	64	1	0
3	B	96	0	64	1	0
3	C	48	0	32	2	0
3	D	48	0	32	0	0
4	A	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	0	0
5	A	31	0	11	0	0
5	B	31	0	11	0	0
6	A	30	0	0	0	0
6	B	40	0	0	0	0
6	C	35	0	0	0	0
6	D	30	0	0	0	0
7	A	60	0	0	0	0
7	B	73	0	0	0	0
7	C	73	0	0	1	0
7	D	59	0	0	1	0
All	All	17555	0	17103	91	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 3.

All (91) 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:A:143:THR:HG23	3:A:802:COA:H142	1.76	0.67
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.78	0.66
2:D:197[A]:GLN:OE1	7:D:601:HOH:O	2.15	0.63
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.84	0.60
2:C:81:VAL:HG11	2:D:296:PRO:HD3	1.84	0.59
2:D:252:HIS:HE1	2:D:332:SER:H	1.50	0.59
1:B:525:MET:HE1	1:B:639:MET:HE2	1.85	0.56
2:C:313:ARG:HD3	2:D:110:TRP:CD1	2.41	0.56
1:B:565:VAL:HG13	1:B:568:ARG:HH21	1.70	0.56
1:B:250:ARG:NH1	2:C:142:TYR:O	2.41	0.54
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.89	0.54
1:A:414:GLU:O	1:A:562:LYS:NZ	2.37	0.54
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.43	0.54
1:B:146:LEU:HD22	1:B:291:VAL:HG22	1.90	0.53
2:D:390:ILE:HB	2:D:394:MET:HB2	1.91	0.53
2:C:62:VAL:HG12	2:D:62[A]:VAL:HG22	1.89	0.53
2:C:99:VAL:HG13	2:C:269:ILE:HD11	1.91	0.52
1:B:378:ARG:HB2	1:B:380:ARG:HD2	1.91	0.52
2:C:140:THR:HG21	2:D:29:LEU:HD23	1.93	0.51
2:C:347:LYS:NZ	7:C:601:HOH:O	2.42	0.51
2:D:28:PRO:HG3	2:D:121[A]:SER:HB3	1.92	0.51
1:B:698:VAL:HG13	1:B:714:PRO:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ILE:HD11	1:B:486:LEU:HD12	1.94	0.50
1:A:459:ILE:HG21	1:A:489:VAL:HG21	1.94	0.50
2:D:290:ALA:HB1	2:D:309:LYS:HE2	1.95	0.49
2:D:302:GLY:N	2:D:303:PRO:HD2	2.27	0.48
1:B:416:GLN:HG3	1:B:448:LEU:HD23	1.94	0.48
1:B:518:PHE:HB2	1:B:643:GLU:CD	2.39	0.48
2:C:296:PRO:HD3	2:D:81:VAL:HG21	1.95	0.48
1:A:250:ARG:NH1	2:D:142:TYR:O	2.47	0.48
1:A:630:PRO:HG2	1:A:635:MET:HE2	1.95	0.47
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.96	0.47
2:D:149:GLN:HG3	2:D:299:MET:SD	2.55	0.47
1:B:381:THR:HA	1:B:385:ARG:HH21	1.79	0.47
2:C:190:SER:OG	2:C:374:ASP:OD2	2.22	0.47
1:A:698:VAL:HG13	1:A:714:PRO:HG3	1.95	0.47
1:B:369:GLU:HG2	1:B:390:LEU:HD13	1.96	0.47
3:C:501:COA:H8A	3:C:501:COA:H52A	1.96	0.47
1:B:76:ALA:O	1:B:297:LYS:NZ	2.40	0.46
1:A:410:GLU:OE2	1:A:419:LYS:NZ	2.44	0.46
1:B:453:LYS:HG3	1:B:454:ARG:HG3	1.98	0.46
2:D:252:HIS:CE1	2:D:332:SER:H	2.32	0.46
1:B:557:LEU:HD23	1:B:587:VAL:HA	1.97	0.46
2:D:390:ILE:HD11	2:D:396:VAL:HG23	1.98	0.46
1:B:470:MET:O	1:B:498:LYS:NZ	2.41	0.46
2:D:99:VAL:HG11	2:D:369:LEU:HD22	1.98	0.46
1:B:65:PHE:HB3	1:B:117:GLY:HA2	1.99	0.45
1:A:327:ARG:NH1	1:A:403:LYS:O	2.50	0.44
2:C:28:PRO:HG3	2:C:121:SER:HB3	1.99	0.44
1:A:440:THR:HG21	1:A:443:LEU:HB2	2.00	0.44
1:B:532:PRO:HB2	1:B:615:LEU:HD13	1.98	0.44
1:B:144:LEU:HD12	3:B:801:COA:H31	1.99	0.44
2:C:38:GLU:HG2	2:C:192:VAL:HG21	1.99	0.44
2:C:116:ALA:O	2:C:267:VAL:N	2.44	0.44
1:A:146:LEU:HD22	1:A:291:VAL:HG22	1.99	0.43
1:B:331:LEU:HD13	1:B:422:VAL:HG12	2.00	0.43
2:D:28:PRO:HG3	2:D:121[B]:SER:HB2	1.99	0.43
1:A:415:ASN:HB3	1:A:418:LEU:HB3	2.00	0.43
2:C:390:ILE:HB	2:C:394:MET:HB2	2.00	0.43
1:A:36:GLU:HG3	1:A:40:LYS:HE3	2.01	0.43
1:A:388:ALA:O	1:A:392:ARG:HG3	2.19	0.43
1:B:459:ILE:HG21	1:B:489:VAL:HG21	2.01	0.43
1:B:515:ILE:HD11	1:B:551:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LYS:HD2	1:A:395:PRO:HD3	2.00	0.42
2:D:150:SER:HB2	2:D:225:PHE:CG	2.54	0.42
1:B:714:PRO:HA	1:B:715:PRO:HD3	1.95	0.42
2:C:325:GLU:HG2	2:C:368:ILE:HB	2.02	0.42
2:C:149:GLN:HG3	2:C:299:MET:SD	2.60	0.42
1:B:65:PHE:HB3	1:B:117:GLY:CA	2.50	0.42
2:C:236:ASP:O	2:C:240:GLN:HG3	2.20	0.42
1:B:331:LEU:HB2	1:B:410:GLU:HA	2.01	0.41
1:B:542:ALA:HB2	1:B:636:ILE:HG23	2.02	0.41
2:D:56:LEU:HD12	2:D:70:ALA:HA	2.02	0.41
1:A:656:LEU:HD13	1:A:662:ALA:HB2	2.01	0.41
1:B:55:VAL:HB	1:B:105:VAL:HG22	2.03	0.41
2:C:155:LEU:HD23	2:C:298:ILE:HG13	2.02	0.41
2:C:359:HIS:ND1	2:C:364:THR:OG1	2.49	0.41
2:C:390:ILE:HD11	2:C:396:VAL:HG23	2.01	0.41
1:A:331:LEU:HD13	1:A:422:VAL:HG12	2.03	0.41
2:D:155:LEU:HD23	2:D:298:ILE:HG13	2.02	0.41
2:C:266:LEU:HD23	2:C:266:LEU:HA	1.89	0.41
1:B:287:PHE:CE2	1:B:291:VAL:HG21	2.56	0.41
1:B:162:ILE:HD12	1:B:238:LEU:HD21	2.03	0.41
2:C:92:CYS:HG	3:C:501:COA:HS1	1.64	0.41
1:B:104:PRO:HG2	1:B:205:ILE:HG23	2.02	0.40
1:B:630:PRO:HG2	1:B:635:MET:HE2	2.02	0.40
2:D:298:ILE:O	2:D:300:LEU:N	2.46	0.40
1:A:316:ARG:NH2	1:A:487:ALA:HB1	2.37	0.40
1:A:550:GLN:O	1:A:554:GLU:HG2	2.22	0.40
1:B:-8:HIS:C	1:B:-6:HIS:H	2.30	0.40
2:D:71:ARG:HH22	2:D:81:VAL:HG22	1.85	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	726/736 (99%)	709 (98%)	16 (2%)	1 (0%)	48	50
1	B	726/736 (99%)	707 (97%)	19 (3%)	0	100	100
2	C	402/403 (100%)	394 (98%)	7 (2%)	1 (0%)	43	44
2	D	404/403 (100%)	392 (97%)	11 (3%)	1 (0%)	43	44
All	All	2258/2278 (99%)	2202 (98%)	53 (2%)	3 (0%)	48	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	361	LEU
2	D	361	LEU
1	A	556	ASN

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	557/566 (98%)	551 (99%)	6 (1%)	65	74
1	B	554/566 (98%)	553 (100%)	1 (0%)	87	93
2	C	310/310 (100%)	307 (99%)	3 (1%)	68	76
2	D	311/310 (100%)	306 (98%)	5 (2%)	55	64
All	All	1732/1752 (99%)	1717 (99%)	15 (1%)	73	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	180	LYS
1	A	387	ASP
1	A	426	ILE
1	A	468	ASP
1	A	486	LEU
1	B	556	ASN
2	C	147	VAL

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Mol	Chain	Res	Type
2	C	228	LEU
2	C	245	VAL
2	D	197[A]	GLN
2	D	197[B]	GLN
2	D	226	GLU
2	D	247	LYS
2	D	346	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	294	GLN
1	A	416	GLN
1	A	550	GLN
1	B	550	GLN
2	D	43	HIS

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 oligosaccharides 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	$\# Z > 2$
6	SO4	A	808	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	B	808	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	A	806	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	D	502	-	4,4,4	0.23	0	6,6,6	0.07	0
3	COA	C	501	-	47,50,50	0.49	0	69,75,75	0.90	2 (2%)
4	GOL	B	802	-	5,5,5	0.93	0	5,5,5	1.09	0
6	SO4	C	502	-	4,4,4	0.25	0	6,6,6	0.08	0
5	PAP	A	805	-	32,33,33	1.35	4 (12%)	50,52,52	1.70	8 (16%)
6	SO4	D	506	-	4,4,4	0.24	0	6,6,6	0.06	0
5	PAP	B	804	-	32,33,33	1.36	4 (12%)	50,52,52	1.69	8 (16%)
4	GOL	A	804	-	5,5,5	0.94	0	5,5,5	1.06	0
6	SO4	C	506	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	C	505	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	A	811	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	B	812	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	C	508	-	4,4,4	0.24	0	6,6,6	0.07	0
3	COA	A	802	-	47,50,50	0.60	1 (2%)	69,75,75	0.81	2 (2%)
6	SO4	B	805	-	4,4,4	0.24	0	6,6,6	0.06	0
6	SO4	D	505	-	4,4,4	0.23	0	6,6,6	0.07	0
3	COA	D	501	-	47,50,50	0.53	0	69,75,75	0.81	1 (1%)
6	SO4	C	503	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	B	806	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	A	809	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	B	809	-	4,4,4	0.23	0	6,6,6	0.08	0
3	COA	B	803	-	47,50,50	0.54	0	69,75,75	0.92	2 (2%)
3	COA	A	801	-	47,50,50	0.51	0	69,75,75	0.84	1 (1%)
6	SO4	A	807	-	4,4,4	0.24	0	6,6,6	0.09	0
6	SO4	B	807	-	4,4,4	0.24	0	6,6,6	0.06	0
6	SO4	B	811	-	4,4,4	0.24	0	6,6,6	0.06	0
6	SO4	C	504	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	D	504	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	D	507	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	A	810	-	4,4,4	0.24	0	6,6,6	0.07	0
4	GOL	A	803	-	5,5,5	0.97	0	5,5,5	1.05	0
6	SO4	B	810	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	C	507	-	4,4,4	0.23	0	6,6,6	0.07	0
3	COA	B	801	-	47,50,50	0.50	0	69,75,75	0.83	1 (1%)

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	COA	A	801	-	-	4/48/64/64	0/3/3/3
3	COA	A	802	-	-	15/48/64/64	0/3/3/3
4	GOL	B	802	-	-	0/4/4/4	-
3	COA	D	501	-	-	6/48/64/64	0/3/3/3
5	PAP	A	805	-	-	3/21/37/37	0/3/3/3
5	PAP	B	804	-	-	7/21/37/37	0/3/3/3
4	GOL	A	804	-	-	0/4/4/4	-
3	COA	C	501	-	-	7/48/64/64	0/3/3/3
4	GOL	A	803	-	-	0/4/4/4	-
3	COA	B	801	-	-	6/48/64/64	0/3/3/3
3	COA	B	803	-	-	16/48/64/64	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	805	PAP	C5-C4	4.69	1.47	1.39
5	B	804	PAP	C5-C4	4.69	1.47	1.39
5	B	804	PAP	C5-C6	2.77	1.48	1.41
5	A	805	PAP	C5-C6	2.74	1.48	1.41
3	A	802	COA	P3B-O3B	2.47	1.63	1.59
5	B	804	PAP	C8-N7	2.46	1.36	1.31
5	A	805	PAP	C8-N7	2.43	1.36	1.31
5	A	805	PAP	C5-N7	-2.18	1.35	1.39
5	B	804	PAP	C5-N7	-2.14	1.35	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	805	PAP	C5-C4-N3	-5.81	118.72	126.72
5	B	804	PAP	C5-C4-N3	-5.63	118.97	126.72
3	C	501	COA	P3B-O3B-C3B	-5.29	109.31	123.43
3	A	801	COA	P3B-O3B-C3B	-5.01	110.05	123.43
3	B	801	COA	P3B-O3B-C3B	-4.87	110.43	123.43
3	D	501	COA	P3B-O3B-C3B	-4.81	110.60	123.43
3	B	803	COA	P3B-O3B-C3B	-4.55	111.29	123.43
5	A	805	PAP	N3-C4-N9	4.50	134.83	127.17
5	B	804	PAP	N3-C4-N9	4.31	134.50	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	805	PAP	C2-N3-C4	3.69	120.84	111.83
5	B	804	PAP	C2-N3-C4	3.63	120.69	111.83
5	B	804	PAP	C4-C5-N7	-3.59	106.47	110.58
5	A	805	PAP	C4-C5-N7	-3.55	106.53	110.58
5	A	805	PAP	N3-C2-N1	-3.22	123.70	128.58
5	B	804	PAP	N3-C2-N1	-3.20	123.74	128.58
5	B	804	PAP	C4-N9-C8	2.57	108.44	105.74
5	A	805	PAP	C4-N9-C8	2.53	108.40	105.74
5	A	805	PAP	C5-N7-C8	2.53	107.43	103.45
5	B	804	PAP	C5-N7-C8	2.53	107.42	103.45
3	B	803	COA	C4B-O4B-C1B	-2.44	104.08	109.47
3	A	802	COA	C4B-O4B-C1B	-2.29	104.42	109.47
5	B	804	PAP	C6-C5-N7	2.26	136.45	132.09
5	A	805	PAP	C6-C5-N7	2.17	136.27	132.09
3	A	802	COA	O4B-C1B-N9A	2.11	112.14	108.09
3	C	501	COA	C2B-C3B-C4B	-2.06	99.64	103.24

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	COA	N8P-C9P-CAP-OAP
3	A	802	COA	C5B-O5B-P1A-O3A
3	A	802	COA	CDP-CBP-CCP-O6A
3	A	802	COA	CEP-CBP-CCP-O6A
3	A	802	COA	CAP-CBP-CCP-O6A
3	B	801	COA	N8P-C9P-CAP-OAP
3	B	803	COA	C3B-C4B-C5B-O5B
3	B	803	COA	C5B-O5B-P1A-O3A
3	B	803	COA	OAP-CAP-CBP-CCP
3	B	803	COA	C9P-CAP-CBP-CCP
3	B	803	COA	OAP-CAP-CBP-CDP
3	B	803	COA	C9P-CAP-CBP-CDP
3	B	803	COA	C9P-CAP-CBP-CEP
3	C	501	COA	C5P-C6P-C7P-N8P
3	C	501	COA	S1P-C2P-C3P-N4P
3	D	501	COA	CAP-C9P-N8P-C7P
3	D	501	COA	C6P-C5P-N4P-C3P
3	D	501	COA	O5P-C5P-N4P-C3P
5	A	805	PAP	C5'-O5'-PA-O1A
5	A	805	PAP	O4'-C4'-C5'-O5'
5	A	805	PAP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	B	804	PAP	C5'-O5'-PA-O1A
3	C	501	COA	C6P-C5P-N4P-C3P
3	A	802	COA	C3B-C4B-C5B-O5B
3	C	501	COA	O5P-C5P-N4P-C3P
3	A	802	COA	C2B-C3B-O3B-P3B
3	D	501	COA	O9P-C9P-N8P-C7P
3	A	802	COA	O4B-C4B-C5B-O5B
3	B	803	COA	O4B-C4B-C5B-O5B
5	B	804	PAP	O4'-C4'-C5'-O5'
5	B	804	PAP	C3'-C4'-C5'-O5'
3	A	802	COA	C4B-C3B-O3B-P3B
3	C	501	COA	O4B-C4B-C5B-O5B
3	B	801	COA	O9P-C9P-CAP-OAP
3	B	803	COA	OAP-CAP-CBP-CEP
3	A	802	COA	O9P-C9P-CAP-CBP
3	A	802	COA	P2A-O3A-P1A-O5B
3	B	803	COA	P2A-O3A-P1A-O5B
5	B	804	PAP	PA-O3A-PB-O1B
3	B	801	COA	C9P-CAP-CBP-CEP
3	A	801	COA	O9P-C9P-CAP-OAP
3	B	801	COA	C9P-CAP-CBP-CCP
3	B	803	COA	C3B-O3B-P3B-O7A
3	A	802	COA	S1P-C2P-C3P-N4P
3	A	801	COA	CCP-O6A-P2A-O4A
3	A	802	COA	C5B-O5B-P1A-O1A
3	A	802	COA	CCP-O6A-P2A-O4A
3	B	801	COA	CCP-O6A-P2A-O4A
3	B	803	COA	C5B-O5B-P1A-O1A
3	B	803	COA	C5B-O5B-P1A-O2A
3	B	803	COA	CCP-O6A-P2A-O4A
3	A	802	COA	N8P-C9P-CAP-CBP
3	A	801	COA	C2P-C3P-N4P-C5P
3	B	801	COA	C2P-C3P-N4P-C5P
3	B	803	COA	C2P-C3P-N4P-C5P
3	C	501	COA	C2P-C3P-N4P-C5P
3	D	501	COA	C3B-O3B-P3B-O7A
5	B	804	PAP	PA-O3A-PB-O2B
5	B	804	PAP	PA-O3A-PB-O3B
3	D	501	COA	C4B-C5B-O5B-P1A
3	B	803	COA	P2A-O3A-P1A-O2A
3	C	501	COA	C3B-C4B-C5B-O5B
3	A	802	COA	C4B-C5B-O5B-P1A

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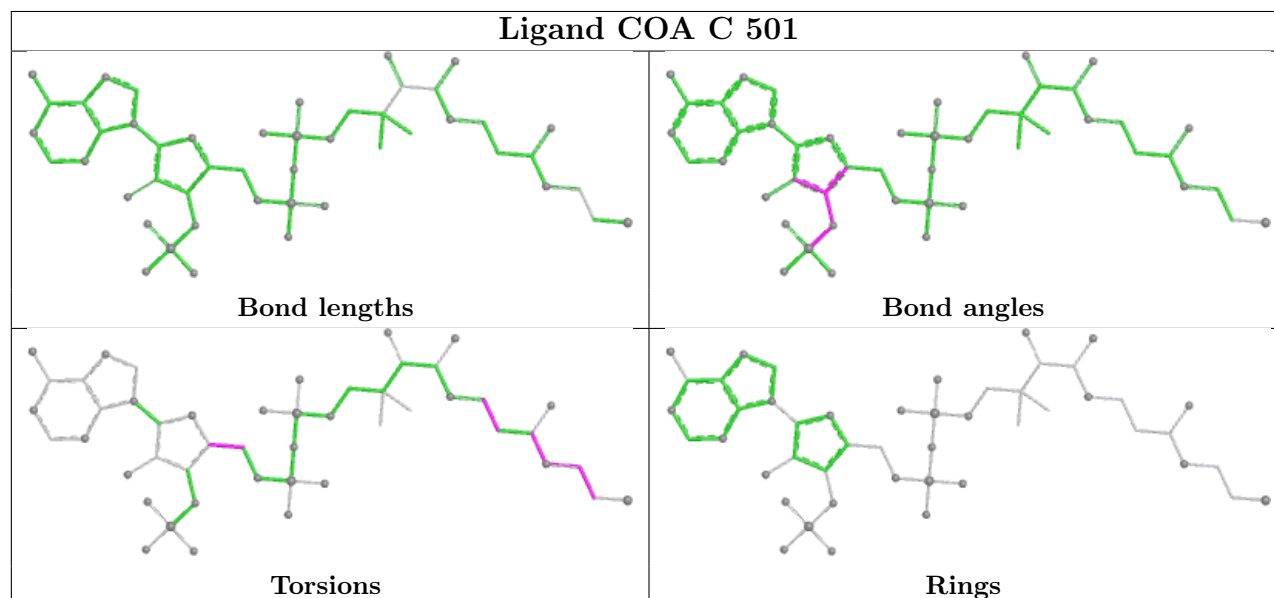
Mol	Chain	Res	Type	Atoms
5	B	804	PAP	C3'-O3'-P-O1

There are no ring outliers.

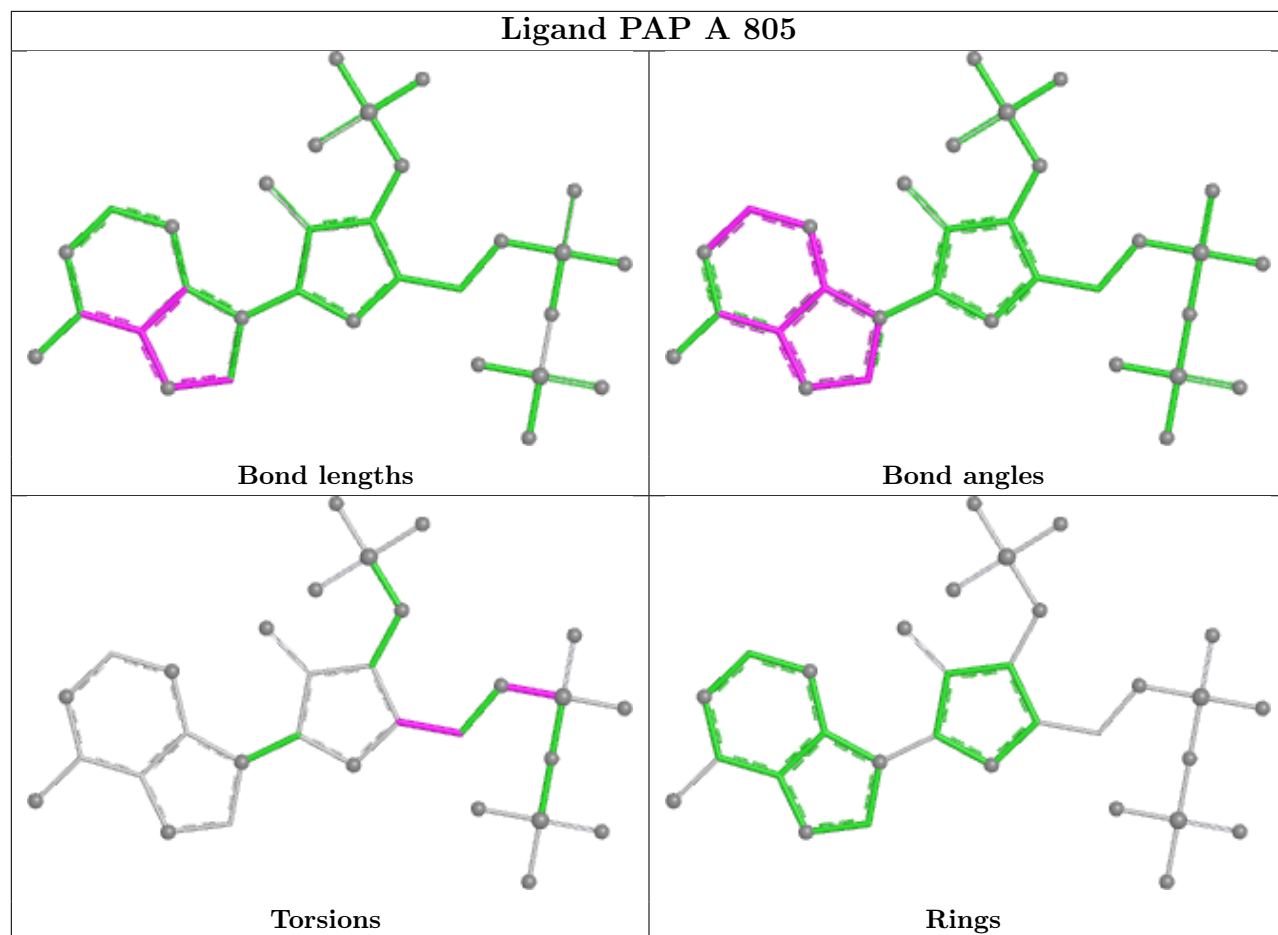
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	COA	2	0
3	A	802	COA	1	0
3	B	801	COA	1	0

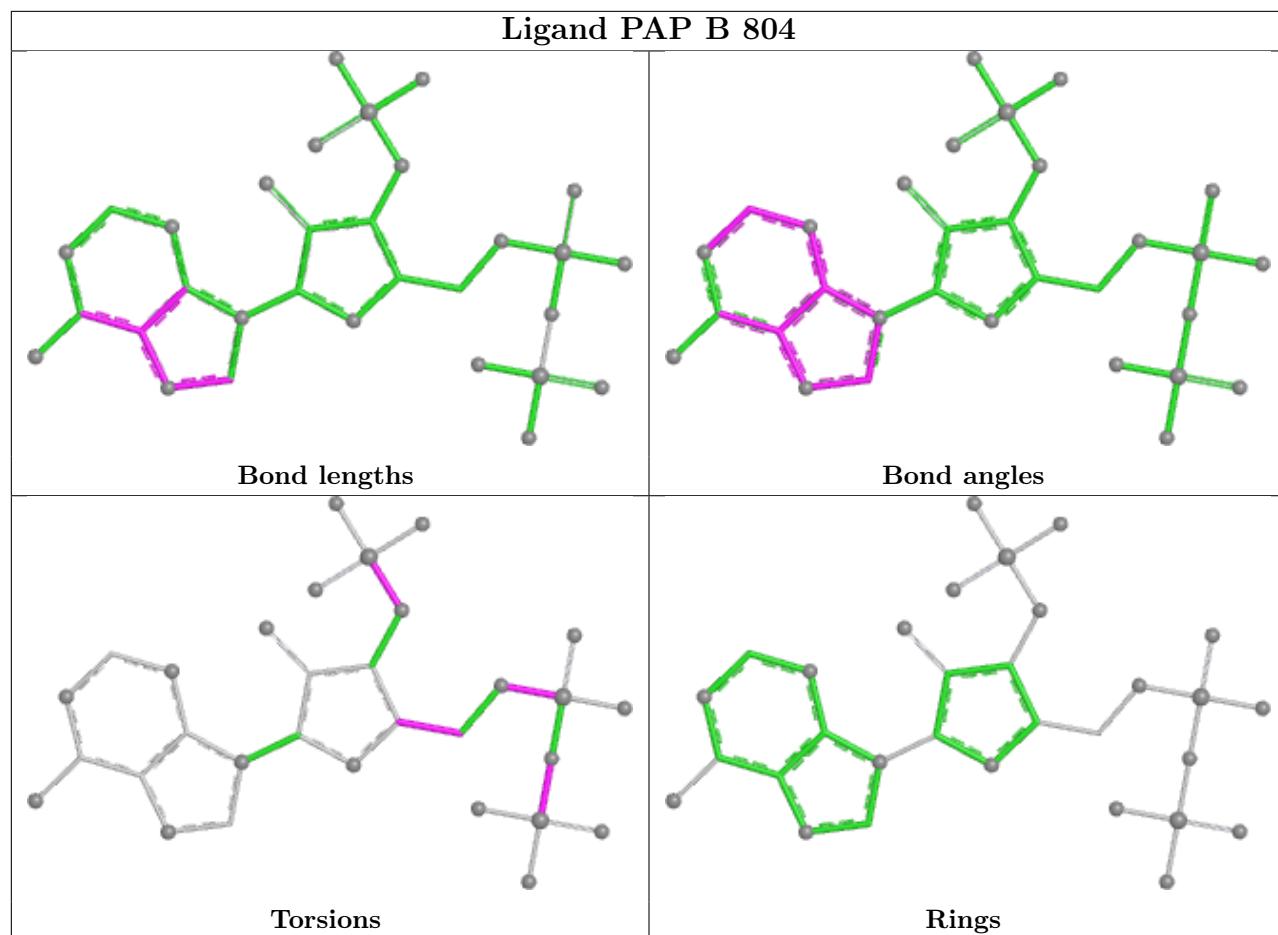
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



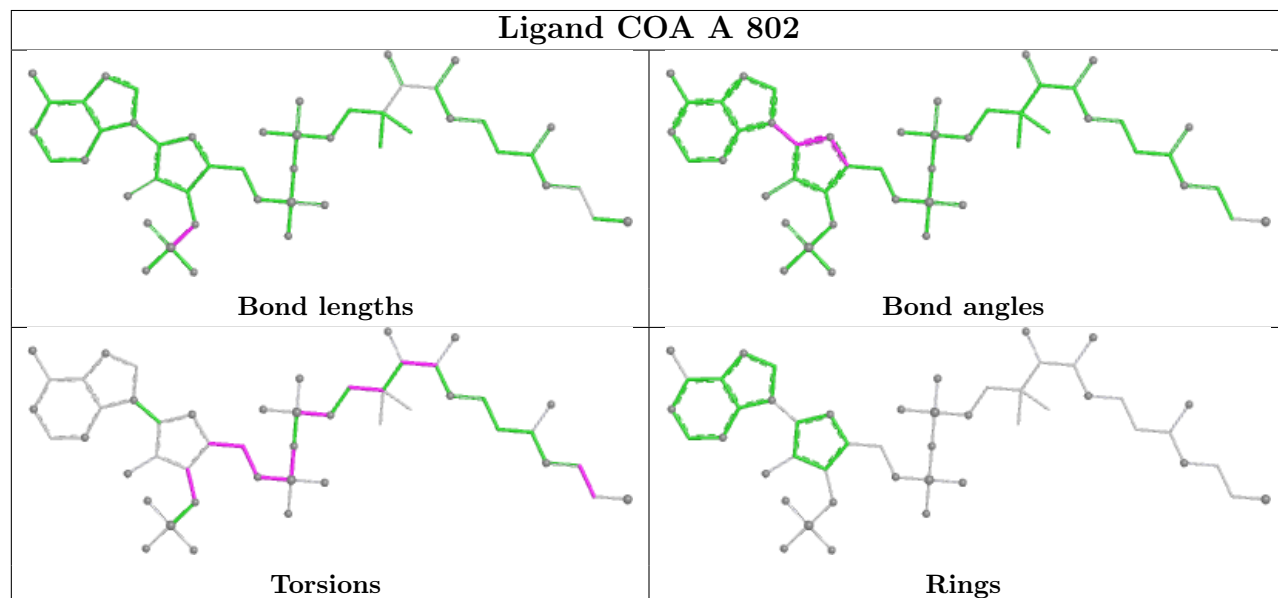
Ligand PAP A 805

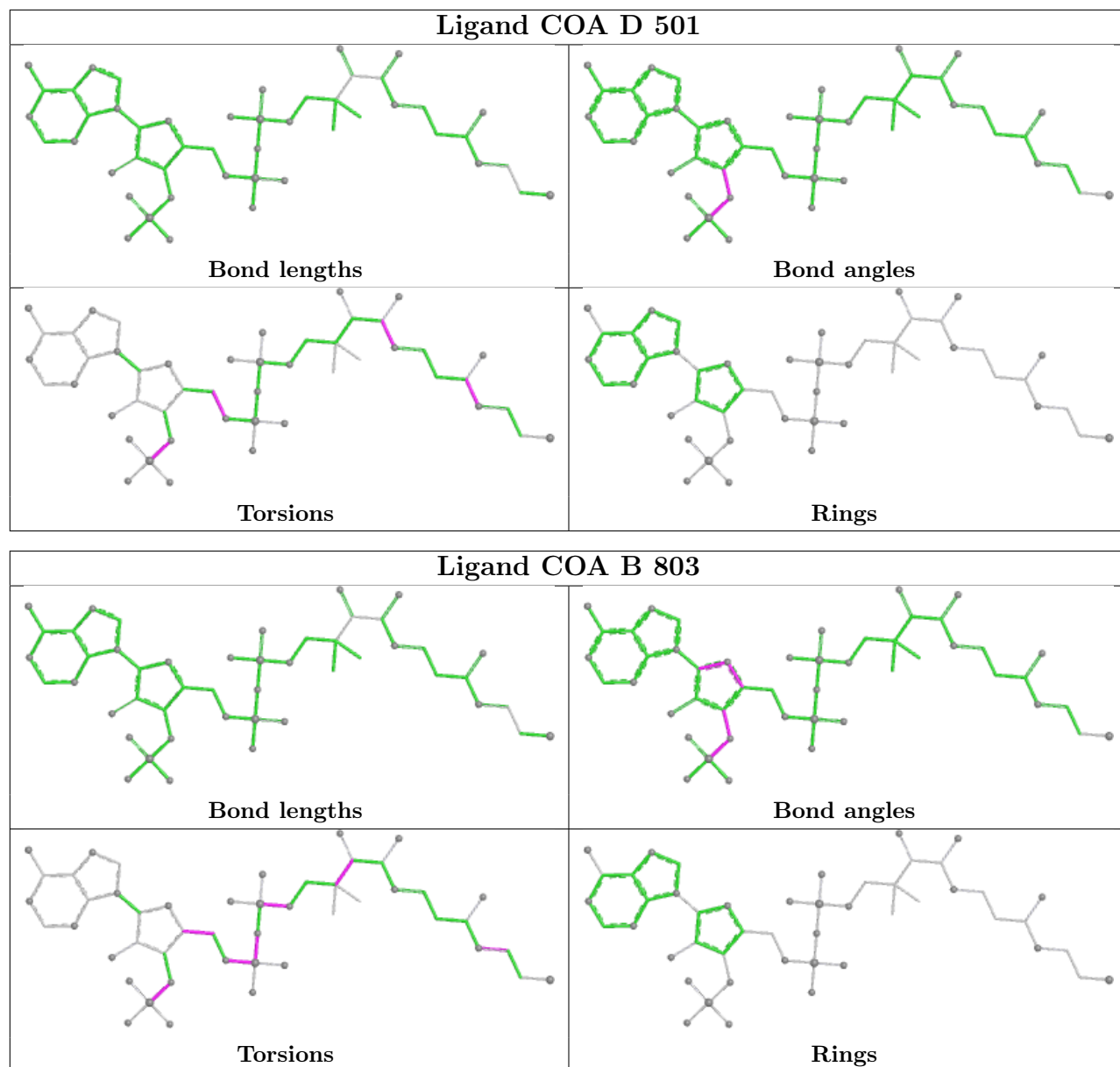


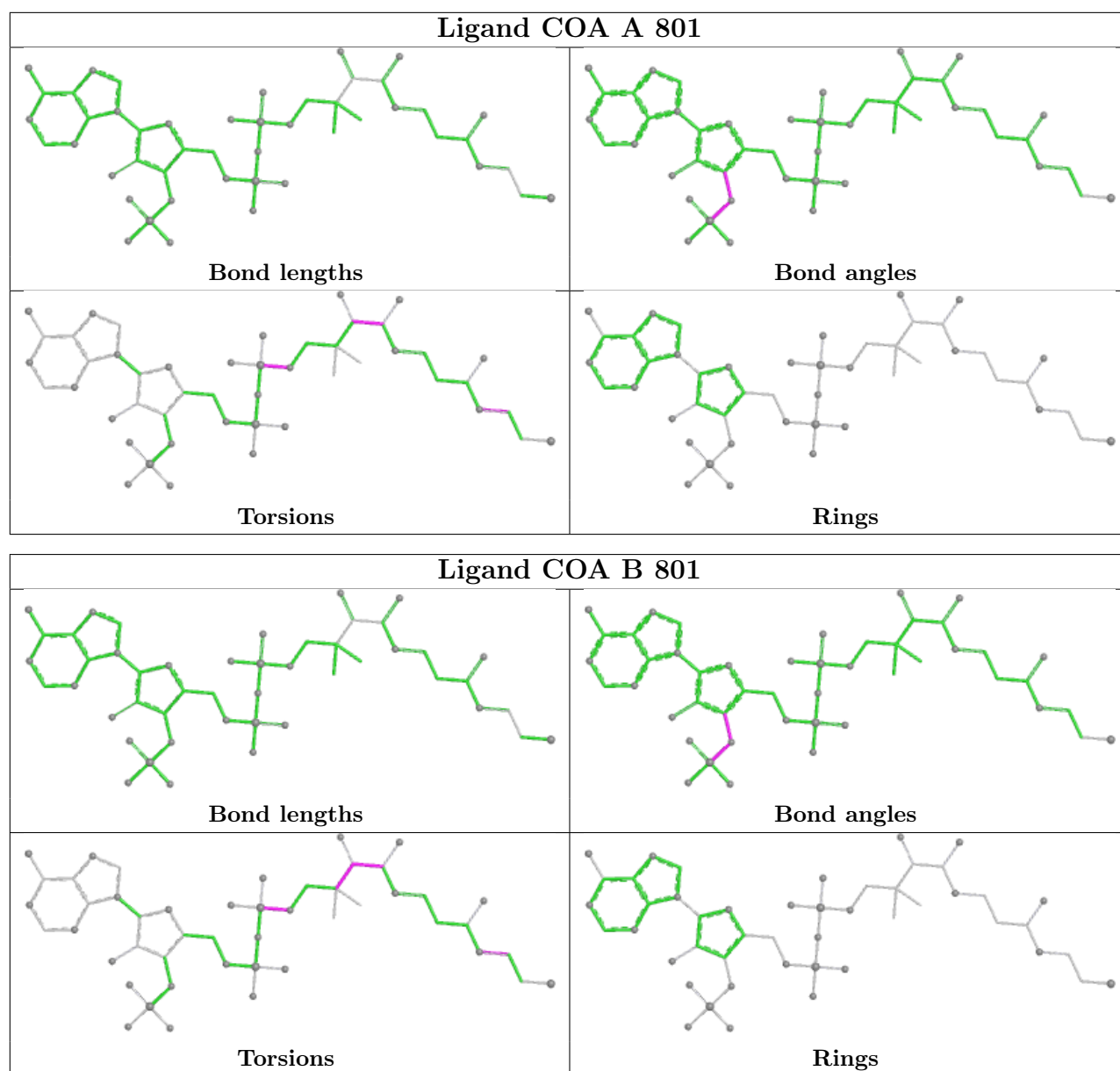
Ligand PAP B 804



Ligand COA A 802







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.83	69 (9%) 14 14	32, 68, 104, 134	1 (0%)
1	B	729/736 (99%)	0.90	116 (15%) 5 5	43, 64, 103, 155	1 (0%)
2	C	402/403 (99%)	0.35	27 (6%) 24 25	31, 52, 76, 100	2 (0%)
2	D	403/403 (100%)	0.54	31 (7%) 19 21	27, 54, 82, 98	3 (0%)
All	All	2263/2278 (99%)	0.72	243 (10%) 11 11	27, 61, 100, 155	7 (0%)

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-5	SER	8.2
2	D	1	MET	7.9
2	D	391	GLY	7.1
1	A	690	ALA	6.4
2	D	197[A]	GLN	5.7
1	B	-6	HIS	5.2
1	B	571	VAL	5.1
1	B	577	THR	4.9
2	D	301	THR	4.7
1	B	559	LEU	4.7
2	D	225	PHE	4.7
1	B	-14	GLY	4.7
2	D	228	LEU	4.6
2	D	390	ILE	4.5
1	B	402	PHE	4.5
2	D	300	LEU	4.5
2	C	300	LEU	4.4
1	B	352	VAL	4.3
1	B	720	SER	4.3
2	D	299	MET	4.2
2	D	302	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	45	ASP	4.1
1	B	349	TYR	4.1
1	B	343	VAL	4.1
1	B	567	THR	4.0
2	D	389	CYS	4.0
1	B	564	ALA	3.9
2	D	2	SER	3.9
1	B	565	VAL	3.9
1	B	574	ALA	3.7
1	A	720	SER	3.7
2	D	303	PRO	3.6
1	B	435	ILE	3.6
2	C	231	LEU	3.6
2	D	136	LEU	3.6
1	A	575	GLY	3.6
1	B	320	ILE	3.5
1	B	325	ILE	3.5
1	A	574	ALA	3.5
1	B	576	GLY	3.5
1	A	-6	HIS	3.5
1	A	356	VAL	3.5
1	A	367	TYR	3.5
2	D	142	TYR	3.5
1	B	429	ILE	3.4
1	B	432	PRO	3.4
2	D	294	ALA	3.4
1	A	-13	SER	3.4
1	A	320	ILE	3.4
1	A	689	PRO	3.4
2	D	296	PRO	3.4
1	B	324	PRO	3.4
1	A	381	THR	3.4
2	C	390	ILE	3.3
1	B	371	LEU	3.3
2	C	392	GLY	3.2
1	B	407	PHE	3.2
2	D	297	VAL	3.2
1	A	494	LEU	3.2
2	C	302	GLY	3.2
1	A	1	MET	3.1
1	B	390	LEU	3.1
2	C	228	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	3.1
1	B	376	LEU	3.1
1	B	563	ILE	3.1
1	B	492	TYR	3.0
2	D	393	GLY	3.0
1	B	2	PRO	3.0
1	A	376	LEU	3.0
1	A	579	GLN	3.0
1	A	466	PRO	3.0
2	C	299	MET	3.0
1	B	433	ASN	2.9
1	B	555	LEU	2.9
2	C	293	GLY	2.9
2	C	389	CYS	2.9
1	A	353	LEU	2.9
1	B	404	GLY	2.9
2	D	392	GLY	2.9
1	A	325	ILE	2.9
1	B	578	TYR	2.9
1	A	434	ALA	2.9
1	B	690	ALA	2.9
1	A	-9	HIS	2.9
1	B	486	LEU	2.8
1	B	323	THR	2.8
1	B	381	THR	2.8
2	D	291	THR	2.8
1	A	393	ILE	2.8
1	B	367	TYR	2.8
1	B	405	VAL	2.8
2	C	303	PRO	2.8
1	B	575	GLY	2.8
1	A	371	LEU	2.8
1	B	426	ILE	2.8
2	C	295	ASP	2.7
1	B	423	PHE	2.7
2	C	297	VAL	2.7
1	B	596	SER	2.7
2	D	293	GLY	2.7
2	C	294	ALA	2.7
1	B	436	LEU	2.7
1	B	3	ASP	2.7
1	B	497	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	383	GLN	2.7
2	C	225	PHE	2.7
2	C	230	ALA	2.7
2	D	230	ALA	2.7
1	B	398	ASP	2.7
1	B	379	GLY	2.7
1	A	383	GLN	2.6
1	A	402	PHE	2.6
1	A	440	THR	2.6
1	B	358	LEU	2.6
1	A	395	PRO	2.6
1	B	491	ASP	2.6
1	B	-7	HIS	2.6
1	B	328	ILE	2.6
1	B	558	GLU	2.6
1	B	387	ASP	2.6
1	B	434	ALA	2.6
2	D	229	ALA	2.6
1	A	317	PRO	2.5
1	A	706	ALA	2.5
1	B	591	ILE	2.5
2	C	393	GLY	2.5
1	B	192	ALA	2.5
1	B	389	LEU	2.5
1	A	319	GLY	2.5
1	B	453	LYS	2.5
1	B	-13	SER	2.5
1	B	485	ALA	2.5
1	A	599	LEU	2.5
1	B	335	MET	2.5
1	B	568	ARG	2.5
1	B	321	GLY	2.5
2	C	391	GLY	2.5
1	B	496	ILE	2.5
1	B	481	THR	2.4
1	A	66	ALA	2.4
1	A	696	ALA	2.4
1	B	397	ALA	2.4
2	D	134	MET	2.4
1	A	418	LEU	2.4
2	C	277	LEU	2.4
1	A	382	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	375	ALA	2.4
1	B	388	ALA	2.4
1	B	602	ALA	2.4
1	A	407	PHE	2.4
1	A	335	MET	2.4
1	B	454	ARG	2.4
1	B	400	ALA	2.4
1	A	576	GLY	2.4
1	B	556	ASN	2.4
1	A	343	VAL	2.4
1	B	1	MET	2.4
1	B	408	VAL	2.4
2	D	224	ALA	2.3
2	C	136	LEU	2.3
1	A	426	ILE	2.3
1	B	393	ILE	2.3
1	A	342	TYR	2.3
1	A	390	LEU	2.3
1	B	580	PRO	2.3
1	B	326	LYS	2.3
1	B	194	VAL	2.3
1	B	430	VAL	2.3
1	A	433	ASN	2.3
1	A	364	GLY	2.3
1	A	352	VAL	2.2
1	A	577	THR	2.2
1	B	143	THR	2.2
1	B	330	VAL	2.2
1	A	378	ARG	2.2
1	B	374	LYS	2.2
1	A	379	GLY	2.2
1	B	456	GLU	2.2
1	A	27	THR	2.2
1	A	184	ILE	2.2
1	B	351	VAL	2.2
1	B	562	LYS	2.2
2	C	298	ILE	2.2
1	B	573	ASP	2.2
2	D	394	MET	2.2
1	B	225	GLY	2.2
1	B	337	GLY	2.2
1	B	364	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	495	ALA	2.2
1	A	713	LEU	2.2
1	A	492	TYR	2.2
1	A	262[A]	ARG	2.2
1	A	373	ALA	2.2
2	D	231	LEU	2.2
1	A	368	SER	2.2
1	B	342	TYR	2.2
1	B	457	ASP	2.2
2	C	235	ASP	2.2
2	C	301	THR	2.2
1	B	572	GLU	2.1
2	C	296	PRO	2.1
1	A	478	GLY	2.1
1	B	561	HIS	2.1
1	A	389	LEU	2.1
1	A	559	LEU	2.1
1	A	687	SER	2.1
2	C	2	SER	2.1
2	C	142	TYR	2.1
1	A	432	PRO	2.1
1	B	579	GLN	2.1
1	B	361	ALA	2.1
1	B	399	ALA	2.1
1	B	566	ALA	2.1
1	B	331	LEU	2.1
1	B	368	SER	2.1
1	B	465	SER	2.1
1	A	-8	HIS	2.1
1	B	570	GLY	2.1
2	D	227	GLY	2.1
1	B	469	LYS	2.1
1	A	642	ALA	2.1
1	A	716	GLU	2.0
1	B	66	ALA	2.1
1	B	341	ALA	2.1
1	B	406	ASP	2.0
2	D	45	ASP	2.0
1	A	2	PRO	2.0
1	B	466	PRO	2.0
1	B	363	LYS	2.0
1	B	478	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	459	ILE	2.0
1	A	502	VAL	2.0
1	B	467	VAL	2.0
1	B	484	GLU	2.0
1	A	613	SER	2.0
1	B	86	ASN	2.0
1	A	486	LEU	2.0
1	B	101	LEU	2.0
1	B	599	LEU	2.0
2	C	149	GLN	2.0
2	D	295	ASP	2.0
1	A	570	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
6	SO4	B	810	5/5	0.60	0.12	96,100,121,121	0
5	PAP	A	805	31/31	0.63	0.13	82,152,196,212	0
3	COA	A	802	48/48	0.63	0.28	73,97,129,149	23
3	COA	B	803	48/48	0.64	0.30	75,96,118,128	23
6	SO4	B	812	5/5	0.66	0.10	118,132,145,150	0
6	SO4	A	811	5/5	0.69	0.11	112,116,131,142	0
6	SO4	A	808	5/5	0.71	0.10	105,108,128,138	0
3	COA	A	801	48/48	0.72	0.17	80,101,127,132	0
6	SO4	D	507	5/5	0.72	0.10	100,100,130,137	0
4	GOL	A	803	6/6	0.73	0.18	73,84,97,99	0
6	SO4	B	809	5/5	0.74	0.11	99,99,114,125	0

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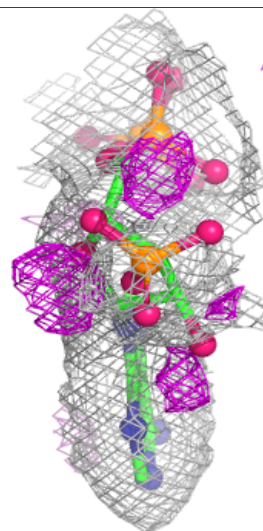
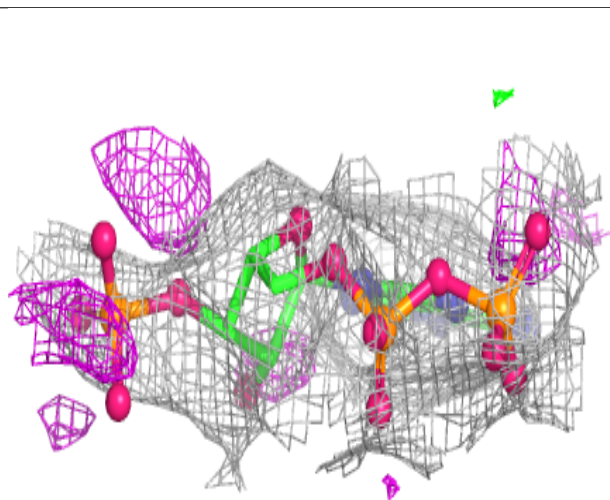
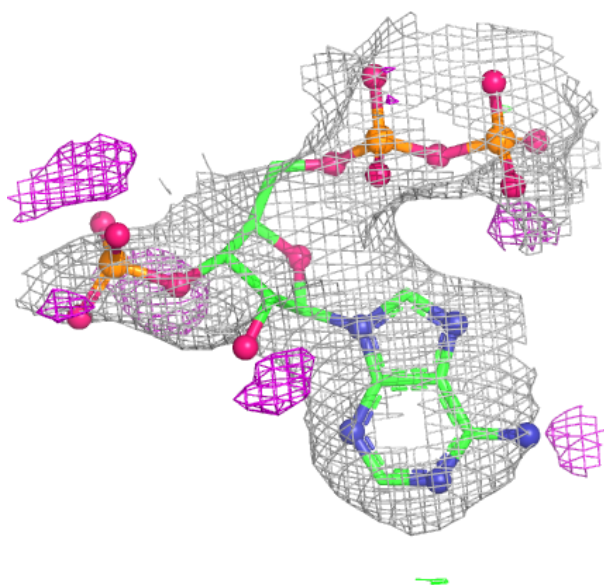
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	A	809	5/5	0.75	0.11	90,97,116,129	0
4	GOL	A	804	6/6	0.75	0.12	84,89,91,92	0
6	SO4	C	508	5/5	0.76	0.08	105,105,129,130	0
5	PAP	B	804	31/31	0.76	0.11	59,135,165,187	0
3	COA	C	501	48/48	0.77	0.15	58,90,114,126	0
6	SO4	A	810	5/5	0.77	0.08	93,98,118,122	0
4	GOL	B	802	6/6	0.78	0.16	79,84,92,98	0
3	COA	B	801	48/48	0.78	0.15	80,107,125,135	0
3	COA	D	501	48/48	0.79	0.14	72,98,128,134	0
6	SO4	C	506	5/5	0.81	0.16	57,60,70,70	5
6	SO4	B	811	5/5	0.82	0.15	63,66,71,72	5
6	SO4	B	808	5/5	0.83	0.09	92,97,115,116	0
6	SO4	A	807	5/5	0.84	0.11	67,88,91,93	0
6	SO4	D	506	5/5	0.85	0.08	87,88,99,103	0
6	SO4	C	505	5/5	0.85	0.08	85,89,100,105	0
6	SO4	C	503	5/5	0.86	0.07	91,97,109,119	0
6	SO4	C	504	5/5	0.87	0.08	80,87,93,103	0
6	SO4	C	507	5/5	0.89	0.09	74,77,84,85	0
6	SO4	D	504	5/5	0.89	0.08	81,84,97,101	0
6	SO4	B	807	5/5	0.91	0.09	59,66,72,75	5
6	SO4	D	505	5/5	0.91	0.07	82,82,85,108	0
6	SO4	C	502	5/5	0.93	0.07	63,73,76,76	0
6	SO4	B	806	5/5	0.94	0.06	81,86,89,98	0
6	SO4	D	503	5/5	0.94	0.09	67,70,72,76	5
6	SO4	B	805	5/5	0.95	0.07	58,70,75,75	0
6	SO4	D	502	5/5	0.96	0.05	73,75,78,81	0
6	SO4	A	806	5/5	0.97	0.06	66,67,73,82	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.

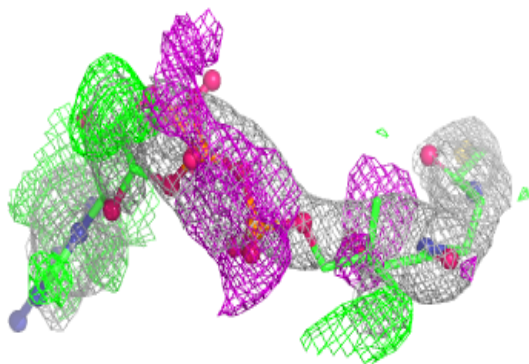
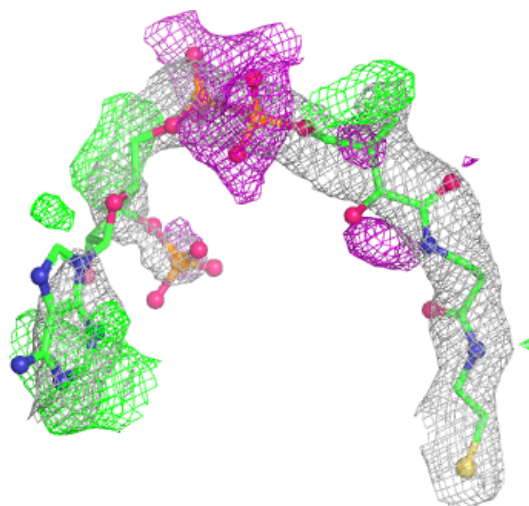
Electron density around PAP A 805:

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



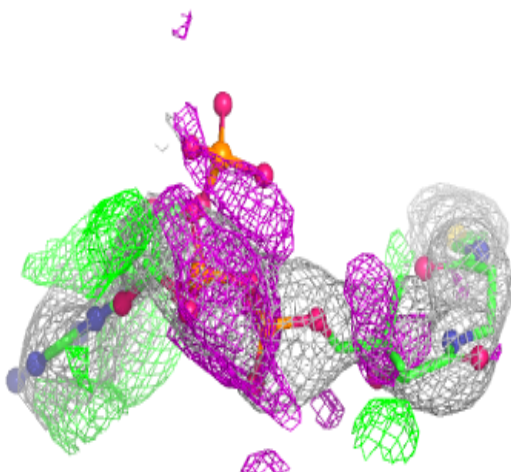
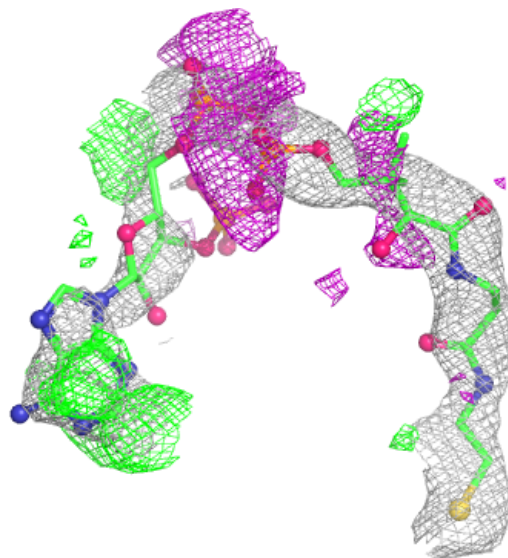
Electron density around COA A 802:

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



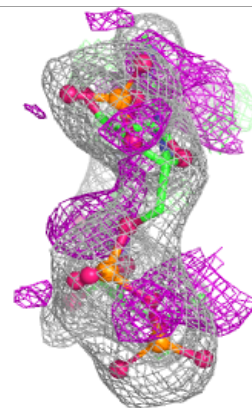
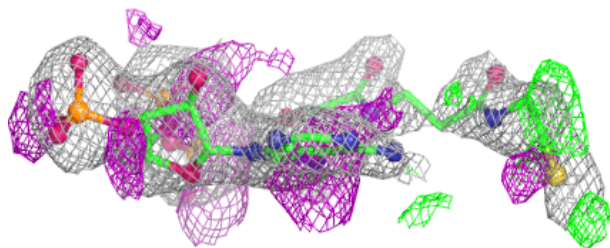
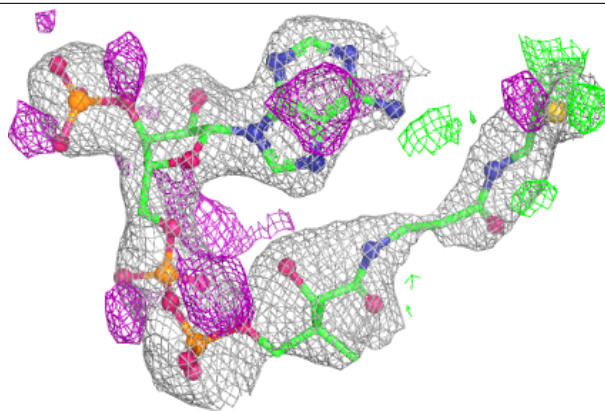
Electron density around COA B 803:

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



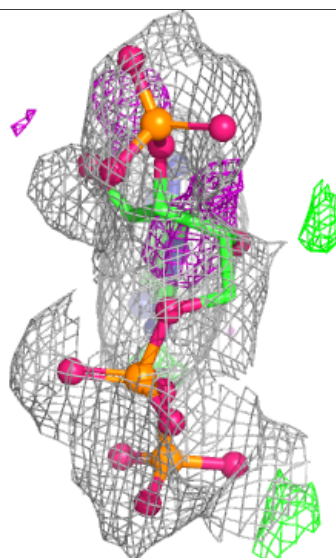
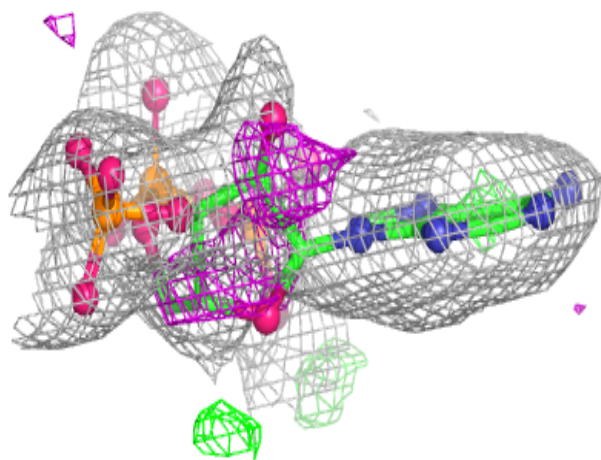
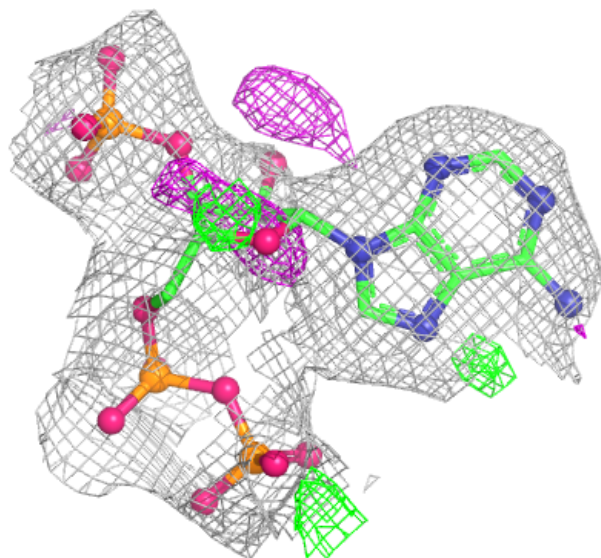
Electron density around COA A 801:

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



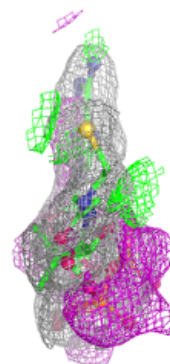
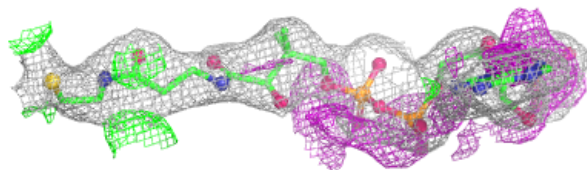
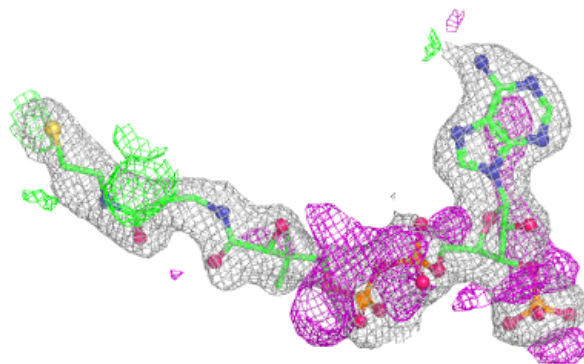
Electron density around PAP B 804:

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

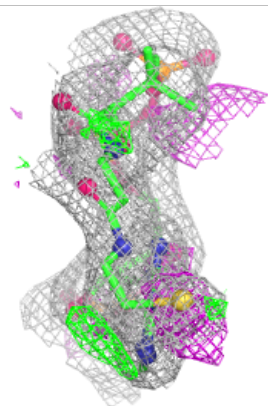
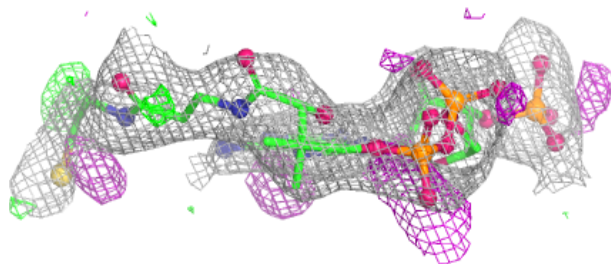
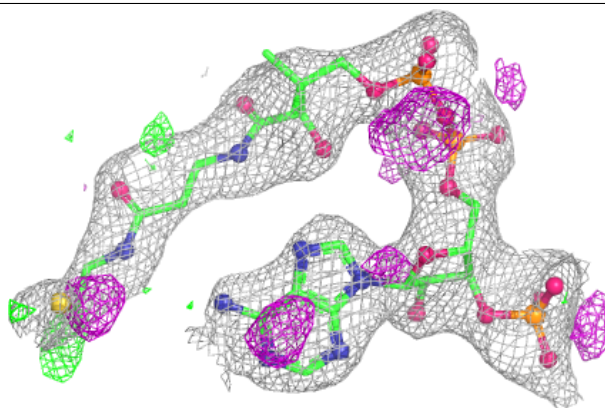


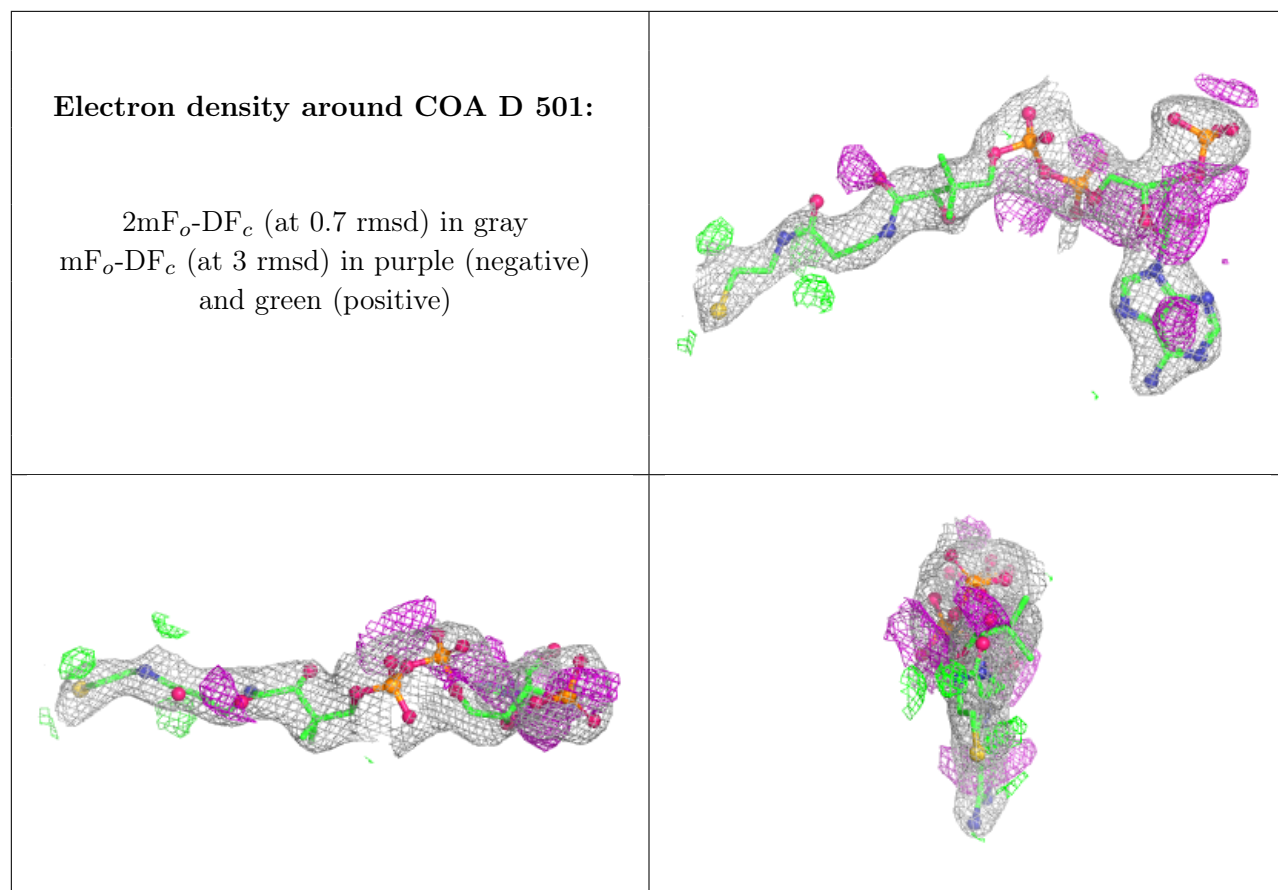
Electron density around COA C 501:

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

**Electron density around COA B 801:**

$2mF_o-DF_c$ (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.