



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:57 AM UTC

PDB ID : 5BZ4 / pdb_00005bz4
Title : Crystal structure of a T1-like thiolase (CoA-complex) from Mycobacterium smegmatis
Authors : Janardan, N.; Harijan, R.K.; Kiema, T.R.; Wierenga, R.K.; Murthy, M.R.N.
Deposited on : 2015-06-11
Resolution : 2.43 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

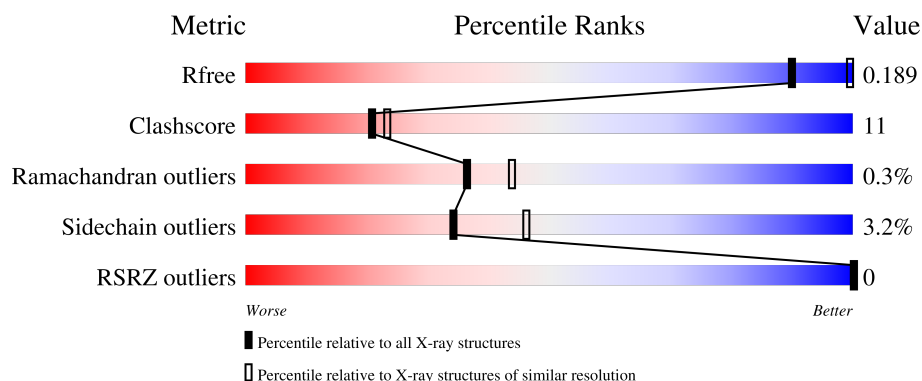
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	407	 72% 24% ..
1	B	407	 75% 22% ..
1	C	407	 76% 19% ..
1	D	407	 75% 21% ..
1	E	407	 74% 22% ..

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Mol	Chain	Length	Quality of chain
1	F	407	 76%21%..
1	G	407	 74%23%..
1	H	407	 75%21%..
1	J	407	 73%23%..
1	K	407	 75%21%..
1	L	407	 71%25%..
1	M	407	 68%29%..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36925 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 Beta-ketothiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	1	0
			2912	1802	538	556	16			
1	B	398	Total	C	N	O	S	0	0	0
			2926	1813	537	560	16			
1	C	398	Total	C	N	O	S	0	0	0
			2903	1798	529	560	16			
1	D	397	Total	C	N	O	S	0	0	0
			2923	1811	536	560	16			
1	E	396	Total	C	N	O	S	0	0	0
			2918	1805	536	561	16			
1	F	399	Total	C	N	O	S	0	0	0
			2946	1824	541	565	16			
1	G	402	Total	C	N	O	S	0	0	0
			2956	1829	544	567	16			
1	H	397	Total	C	N	O	S	0	0	0
			2929	1813	539	561	16			
1	J	396	Total	C	N	O	S	0	0	0
			2905	1798	536	555	16			
1	K	400	Total	C	N	O	S	0	0	0
			2943	1821	540	566	16			
1	L	400	Total	C	N	O	S	0	0	0
			2929	1808	541	564	16			
1	M	397	Total	C	N	O	S	0	0	0
			2921	1808	536	561	16			

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	141	Total	O	0	0
			141	141		
3	B	167	Total	O	0	0
			167	167		
3	C	147	Total	O	0	0
			147	147		
3	D	145	Total	O	0	0
			145	145		
3	E	110	Total	O	0	0
			110	110		
3	F	114	Total	O	0	0
			114	114		
3	G	121	Total	O	0	0
			121	121		

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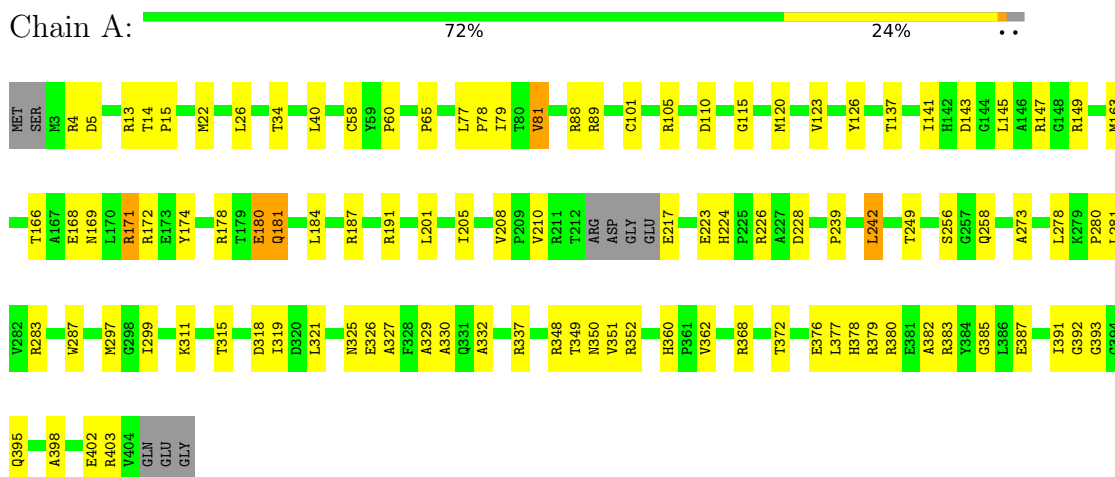
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	159	Total 159	O 159	0	0
3	J	110	Total 110	O 110	0	0
3	K	152	Total 152	O 152	0	0
3	L	106	Total 106	O 106	0	0
3	M	102	Total 102	O 102	0	0

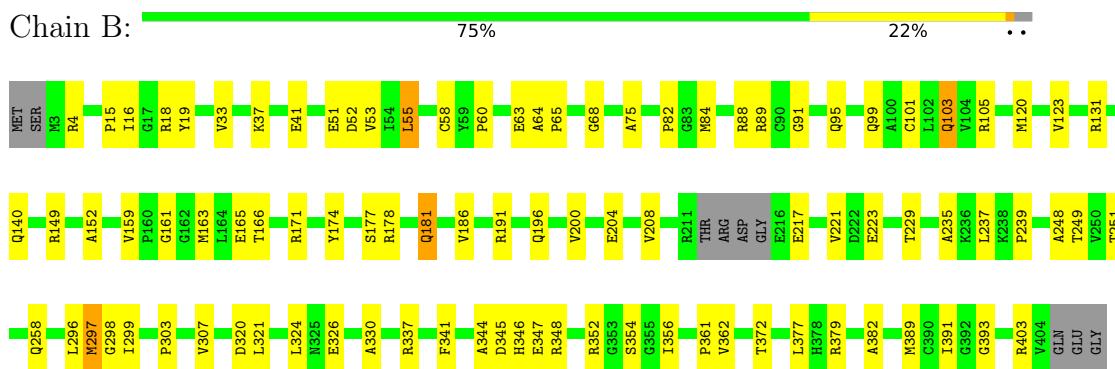
3 Residue-property plots

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.

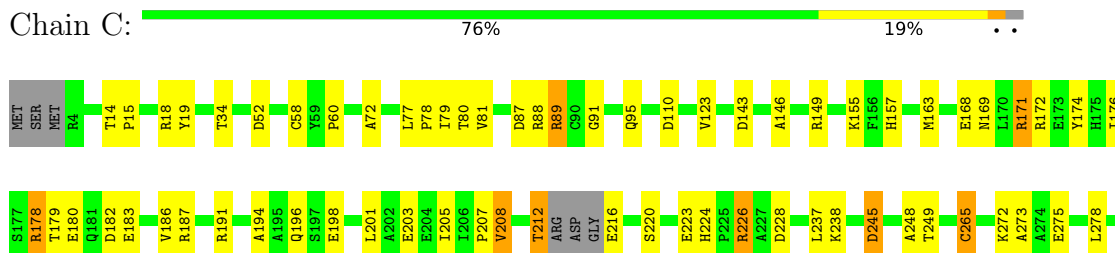
• Molecule 1: Beta-ketothiolase



• Molecule 1: Beta-ketothiolase



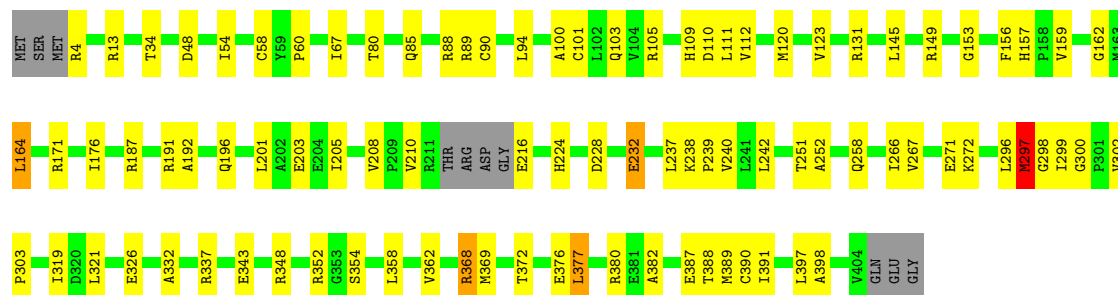
• Molecule 1: Beta-ketothiolase





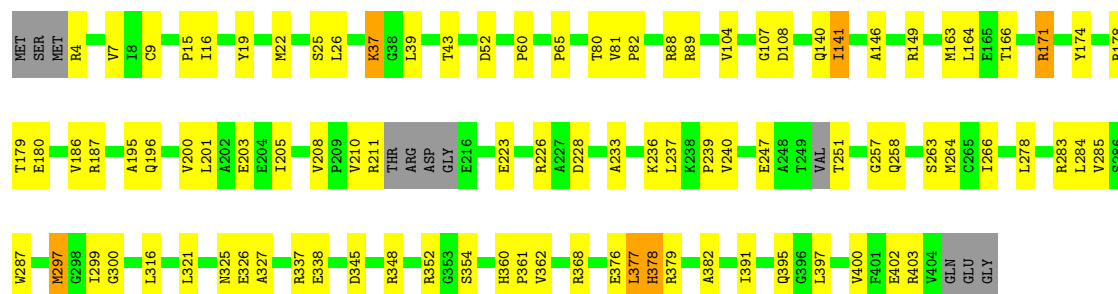
• Molecule 1: Beta-ketothiolase

Chain D: 75% 21% ..



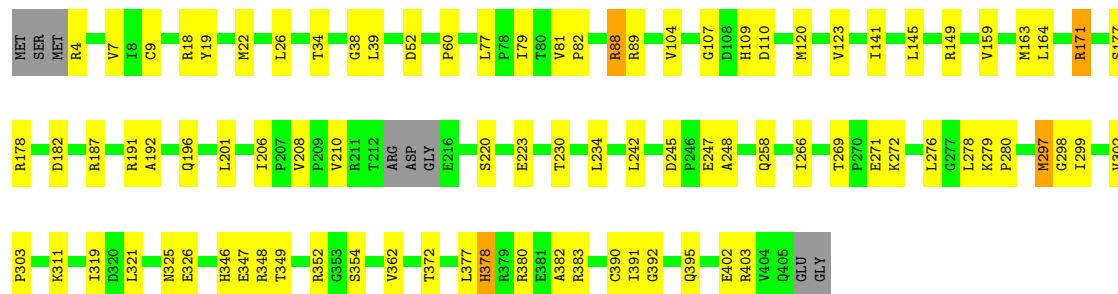
• Molecule 1: Beta-ketothiolase

Chain E: 74% 22% ..



• Molecule 1: Beta-ketothiolase

Chain F: 76% 21% ..



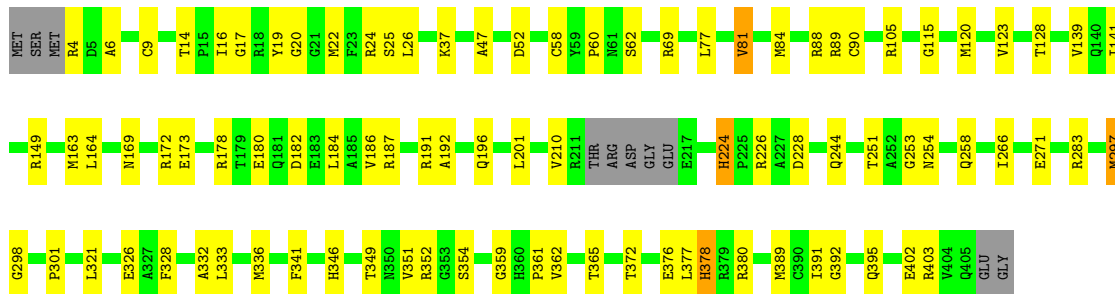
• Molecule 1: Beta-ketothiolase

Chain G: 74% 23% ..



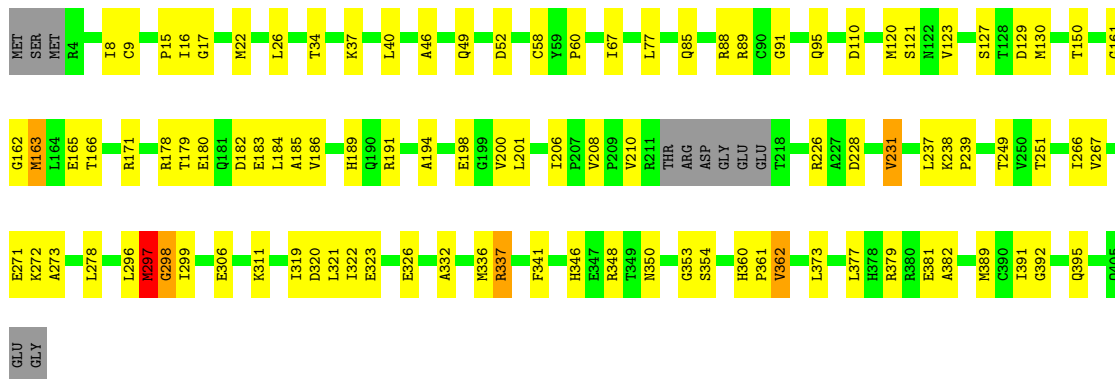
- Molecule 1: Beta-ketothiolase

Chain H: 75% 21% ..



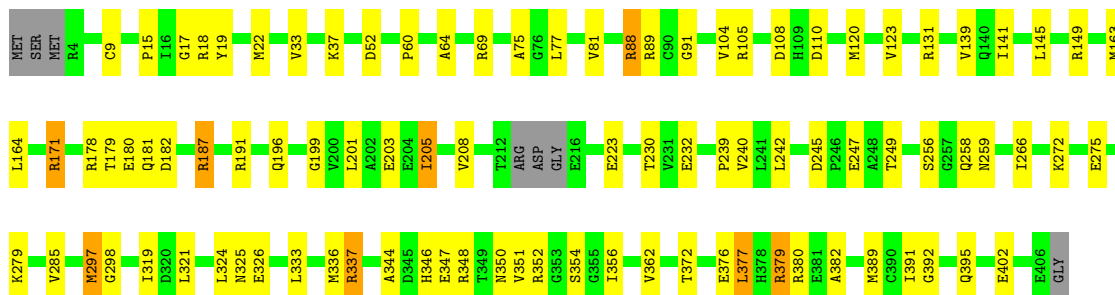
- Molecule 1: Beta-ketothiolase

Chain J:  73% 23% ..



- Molecule 1: Beta-ketothiolase

Chain K: 75% 21% .



- Molecule 1: Beta-ketothiolase

L373	A374	A227	M130	MT
R375	D228	R136	R136	SR
L376	E232	Q140	Q140	R4
R377	L237	I141	I141	D5
R380	K238	L145	L145	E10
R390	P239	A146	A146	T14
C390	D245	R149	R149	P15
I391	P246	A152	A152	L26
Q395	E247	V159	V159	K37
R403	T248	M163	M163	T43
V404	T249	L164	L164	G44
Q405	V250	M169	M169	I45
E406	T251	L170	L170	D52
GLY	N259	R171	R171	V53
	A290	R172	R172	I54
	D295	E173	E173	H57
	L296	I176	I176	C58
	M297	S177	S177	Y59
	G298	R178	R178	P60
	P300	T179	T179	A64
	V302	E180	E180	P65
	P303	Q181	Q181	R69
	A306	D182	D182	A72
	V307	E183	E183	L77
	T319	V186	V186	M94
	D320	A187	A187	R88
	L321	Q190	Q190	R89
	N325	R191	R191	Q95
	E326	A192	A192	Q99
	A330	V193	V193	V104
	R337	L201	L201	G107
	E343	A202	A202	A117
	H346	E204	E204	M120
	E347	L205	L205	S121
	R348	V208	V208	N122
	S354	P209	P209	GLY
	G355	V210	V210	V123
	G359	R211	R211	S127
	R368	THR	THR	
	N369	R213	R213	
		ASP	ASP	
		GLY	GLY	
		E216	E216	
		V224	V224	

I366	GLY	L111	MET
P361	GLU	M120	SER
V362	E217	S121	MET
		R122	R4
R368	L237	V123	V7
M369	K238	A124	I8
L370	P239	F125	C9
A371	P240	Y126	
T372	T249	S127	R13
L373			
E376	S266	M130	I16
L377		R131	
H378	I266	Q140	G20
	E271	I141	
G385		L145	R24
L386	E275	A146	S25
E387			L26
T388	R283	R149	
M389	M297	K155	T34
C390	G298		K37
I391	T299	V159	G38
G392		M163	
G393	P303	L164	R42
G394			I45
Q395	V307	M169	
Q405		R170	Q49
GLU	K311	R171	D52
GLY	T315	R172	V53
		R178	I54
D318		T179	L55
I319	D320	E180	C58
	L321		Y59
	N325	E183	P60
E326		R187	P65
	Q331	R191	A66
A332	L333	Q196	I67
		L201	G68
M336		A202	R69
R337		E203	A75
	F341	E204	
		I205	P78
D345		L206	V81
H346		P207	Q85
E347		V208	
R348		P209	R88
	V351	V210	R99
	R352	R211	C90
	G353	T18	G91
G354	G355	ARG	
		ASP	V104

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	190.08Å 190.08Å 265.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.52 – 2.43 47.52 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.52-2.43) 99.3 (47.52-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.161 , 0.188 0.160 , 0.189	Depositor DCC
R_{free} test set	10163 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36925	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7670e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA

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	0.57	0/2956	0.93	6/4015 (0.1%)
1	B	0.62	1/2970 (0.0%)	0.98	10/4029 (0.2%)
1	C	0.57	0/2946	0.96	13/4000 (0.3%)
1	D	0.58	0/2967	0.92	6/4025 (0.1%)
1	E	0.55	0/2961	0.92	3/4016 (0.1%)
1	F	0.60	3/2990 (0.1%)	0.93	7/4054 (0.2%)
1	G	0.58	0/3000	0.94	11/4071 (0.3%)
1	H	0.59	0/2973	0.92	7/4033 (0.2%)
1	J	0.55	0/2949	0.88	2/4003 (0.0%)
1	K	0.59	0/2987	0.92	8/4053 (0.2%)
1	L	0.53	0/2972	0.92	9/4030 (0.2%)
1	M	0.53	0/2964	0.91	6/4021 (0.1%)
All	All	0.57	4/35635 (0.0%)	0.93	88/48350 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	378	HIS	CG-CD2	-6.45	1.28	1.35
1	F	378	HIS	CD2-NE2	5.63	1.44	1.37
1	B	297	MET	CG-SD	-5.26	1.67	1.80
1	F	378	HIS	CE1-NE2	-5.21	1.27	1.32

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	224	HIS	CA-C-N	-8.77	110.99	119.85
1	H	224	HIS	C-N-CA	-8.77	110.99	119.85
1	A	224	HIS	CA-C-N	-7.92	111.63	119.78
1	A	224	HIS	C-N-CA	-7.92	111.63	119.78
1	B	297	MET	CB-CG-SD	7.85	136.24	112.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	GLU	Peptide

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	2912	0	2890	85	0
1	B	2926	0	2927	66	0
1	C	2903	0	2878	62	0
1	D	2923	0	2930	61	0
1	E	2918	0	2913	67	0
1	F	2946	0	2954	58	0
1	G	2956	0	2951	72	0
1	H	2929	0	2936	62	0
1	J	2905	0	2900	66	0
1	K	2943	0	2934	67	0
1	L	2929	0	2893	79	0
1	M	2921	0	2919	84	0
2	B	48	0	32	0	0
2	D	48	0	32	8	0
2	F	48	0	32	0	0
2	H	48	0	32	5	0
2	K	48	0	32	1	0
3	A	141	0	0	10	0
3	B	167	0	0	7	0
3	C	147	0	0	6	0
3	D	145	0	0	6	2
3	E	110	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	114	0	0	3	0
3	G	121	0	0	9	0
3	H	159	0	0	13	0
3	J	110	0	0	5	2
3	K	152	0	0	4	0
3	L	106	0	0	7	0
3	M	102	0	0	8	0
All	All	36925	0	35185	780	2

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 11.

The worst 5 of 780 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:H:501:COA:H71	3:H:670:HOH:O	1.60	0.98
1:L:4:ARG:NH2	1:L:104:VAL:O	1.95	0.98
1:A:166:THR:HG21	1:A:297:MET:HB3	1.51	0.92
1:L:65:PRO:HB3	1:M:89:ARG:HH21	1.37	0.90
1:L:171:ARG:HA	1:L:176:ILE:HD12	1.55	0.88

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:692:HOH:O	3:J:549:HOH:O[3_654]	1.99	0.21
3:D:603:HOH:O	3:J:502:HOH:O[3_654]	2.13	0.07

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	395/407 (97%)	384 (97%)	10 (2%)	1 (0%)	36	44
1	B	394/407 (97%)	379 (96%)	15 (4%)	0	100	100
1	C	394/407 (97%)	380 (96%)	13 (3%)	1 (0%)	36	44
1	D	393/407 (97%)	378 (96%)	14 (4%)	1 (0%)	36	44
1	E	390/407 (96%)	380 (97%)	9 (2%)	1 (0%)	36	44
1	F	395/407 (97%)	383 (97%)	10 (2%)	2 (0%)	24	29
1	G	398/407 (98%)	383 (96%)	13 (3%)	2 (0%)	24	29
1	H	393/407 (97%)	384 (98%)	8 (2%)	1 (0%)	36	44
1	J	392/407 (96%)	380 (97%)	10 (3%)	2 (0%)	24	29
1	K	396/407 (97%)	381 (96%)	14 (4%)	1 (0%)	36	44
1	L	395/407 (97%)	384 (97%)	11 (3%)	0	100	100
1	M	393/407 (97%)	382 (97%)	10 (2%)	1 (0%)	36	44
All	All	4728/4884 (97%)	4578 (97%)	137 (3%)	13 (0%)	36	44

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	VAL
1	F	362	VAL
1	J	297	MET
1	M	362	VAL
1	C	297	MET

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	293/309 (95%)	285 (97%)	8 (3%)	39	52
1	B	298/309 (96%)	292 (98%)	6 (2%)	48	62
1	C	293/309 (95%)	286 (98%)	7 (2%)	43	56
1	D	299/309 (97%)	291 (97%)	8 (3%)	39	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	298/309 (96%)	284 (95%)	14 (5%)	23	33
1	F	301/309 (97%)	293 (97%)	8 (3%)	39	52
1	G	301/309 (97%)	288 (96%)	13 (4%)	26	36
1	H	300/309 (97%)	291 (97%)	9 (3%)	36	48
1	J	295/309 (96%)	287 (97%)	8 (3%)	39	52
1	K	299/309 (97%)	289 (97%)	10 (3%)	33	45
1	L	294/309 (95%)	281 (96%)	13 (4%)	25	35
1	M	298/309 (96%)	289 (97%)	9 (3%)	36	48
All	All	3569/3708 (96%)	3456 (97%)	113 (3%)	34	46

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	226	ARG
1	M	368	ARG
1	H	365	THR
1	M	299	ILE
1	L	228	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	99	GLN
1	M	142	HIS
1	K	258	GLN
1	L	190	GLN
1	D	122	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
2	COA	H	501	-	47,50,50	1.48	6 (12%)	69,75,75	1.86	17 (24%)
2	COA	D	501	-	47,50,50	1.35	6 (12%)	69,75,75	1.96	20 (28%)
2	COA	F	501	-	47,50,50	2.61	12 (25%)	69,75,75	1.95	16 (23%)
2	COA	K	501	-	47,50,50	2.56	12 (25%)	69,75,75	2.02	20 (28%)
2	COA	B	501	-	47,50,50	2.61	12 (25%)	69,75,75	1.74	16 (23%)

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
2	COA	H	501	-	-	20/48/64/64	0/3/3/3
2	COA	D	501	-	-	13/48/64/64	0/3/3/3
2	COA	F	501	-	-	13/48/64/64	0/3/3/3
2	COA	K	501	-	-	17/48/64/64	0/3/3/3
2	COA	B	501	-	-	7/48/64/64	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	COA	O4B-C1B	8.64	1.62	1.42
2	B	501	COA	O4B-C1B	8.40	1.61	1.42
2	K	501	COA	O4B-C1B	8.35	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	COA	C2B-C1B	-7.25	1.30	1.53
2	K	501	COA	C2B-C1B	-7.22	1.30	1.53

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	501	COA	C7P-C6P-C5P	-7.71	99.55	112.39
2	H	501	COA	C5A-C4A-N3A	-6.83	117.31	126.72
2	D	501	COA	O6A-CCP-CBP	6.05	120.27	110.55
2	K	501	COA	N3A-C2A-N1A	-5.58	120.13	128.58
2	F	501	COA	N3A-C2A-N1A	-5.39	120.43	128.58

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

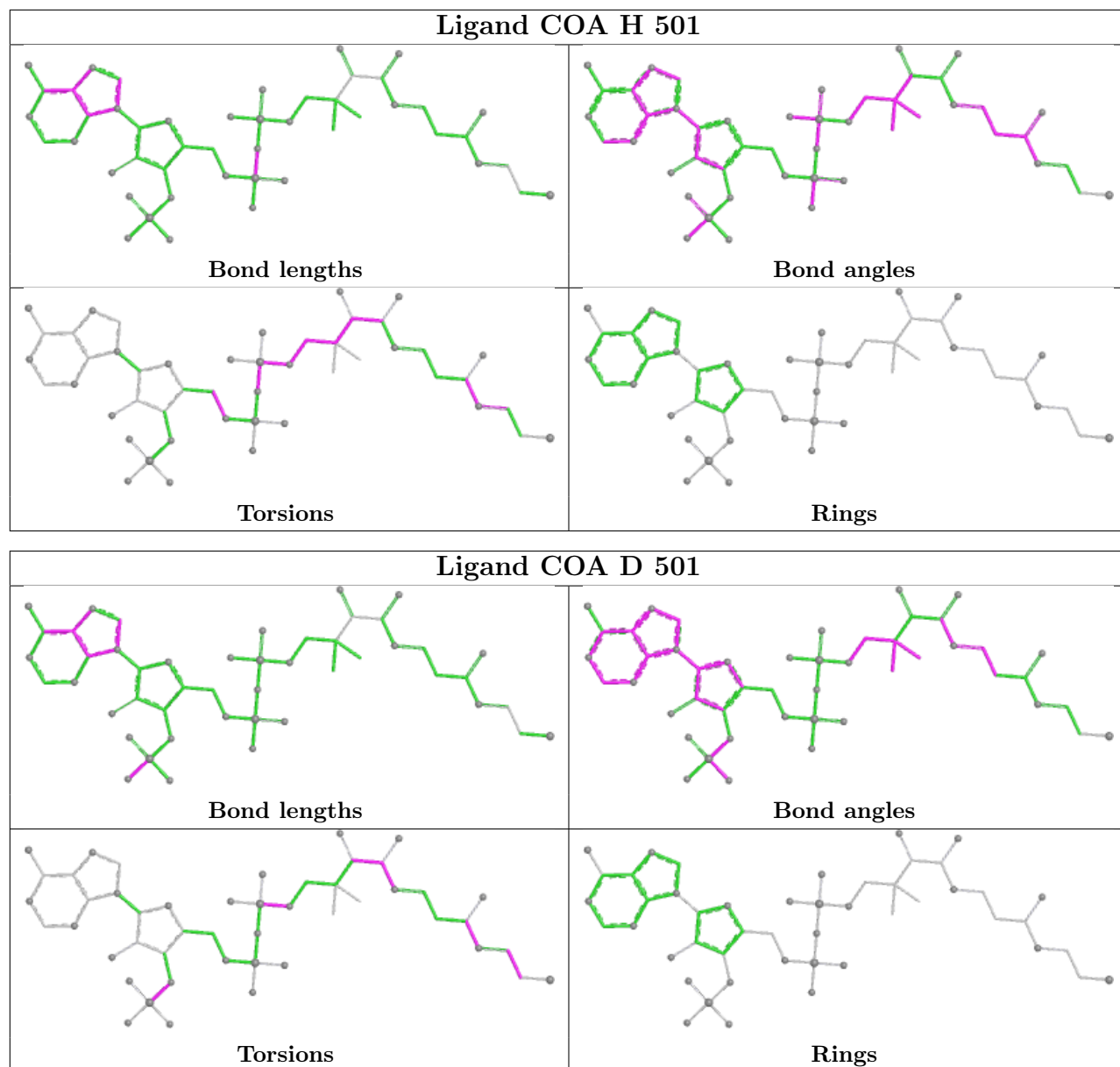
Mol	Chain	Res	Type	Atoms
2	B	501	COA	CCP-O6A-P2A-O3A
2	B	501	COA	CCP-O6A-P2A-O4A
2	B	501	COA	CCP-O6A-P2A-O5A
2	B	501	COA	CDP-CBP-CCP-O6A
2	B	501	COA	CEP-CBP-CCP-O6A

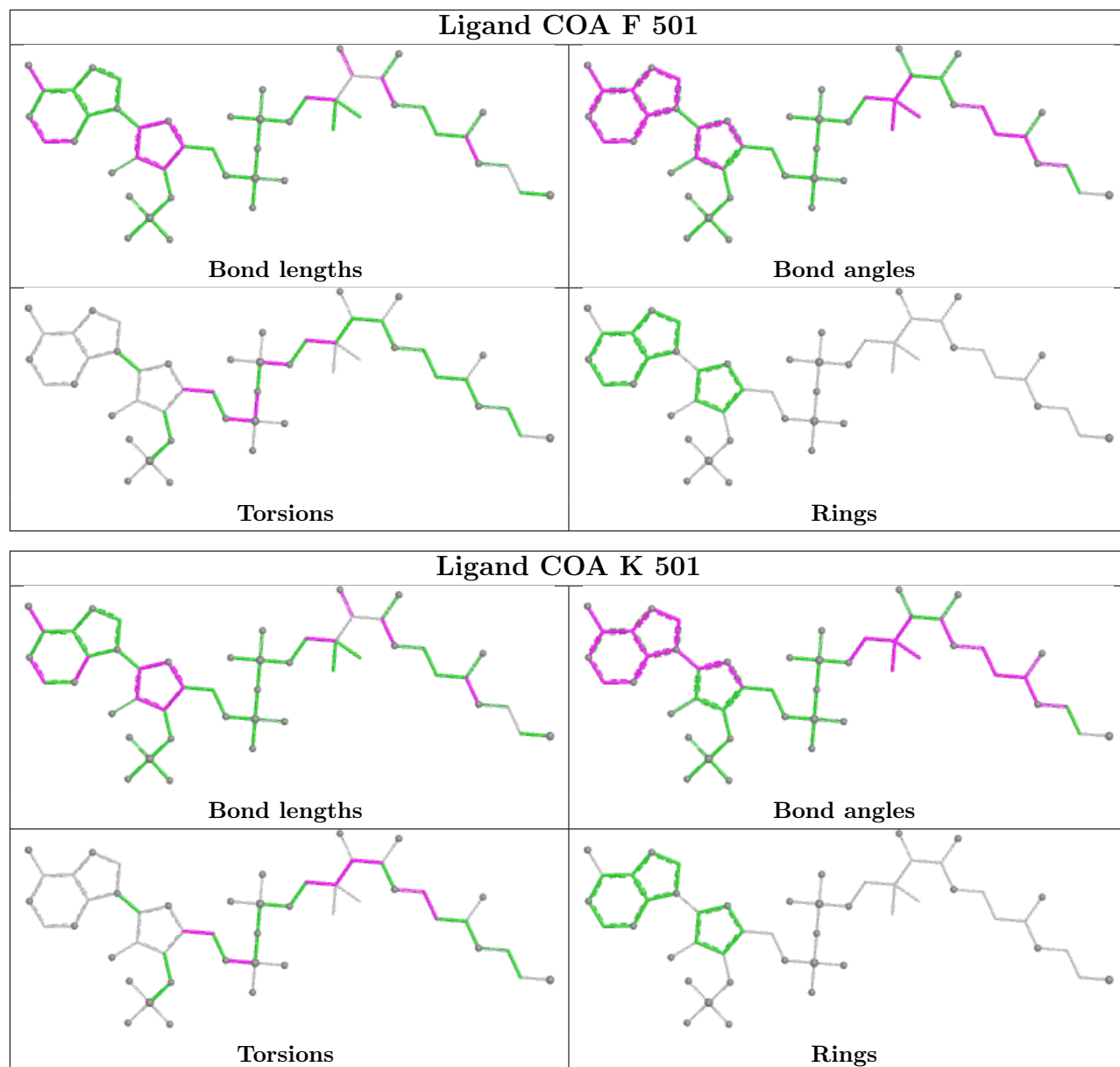
There are no ring outliers.

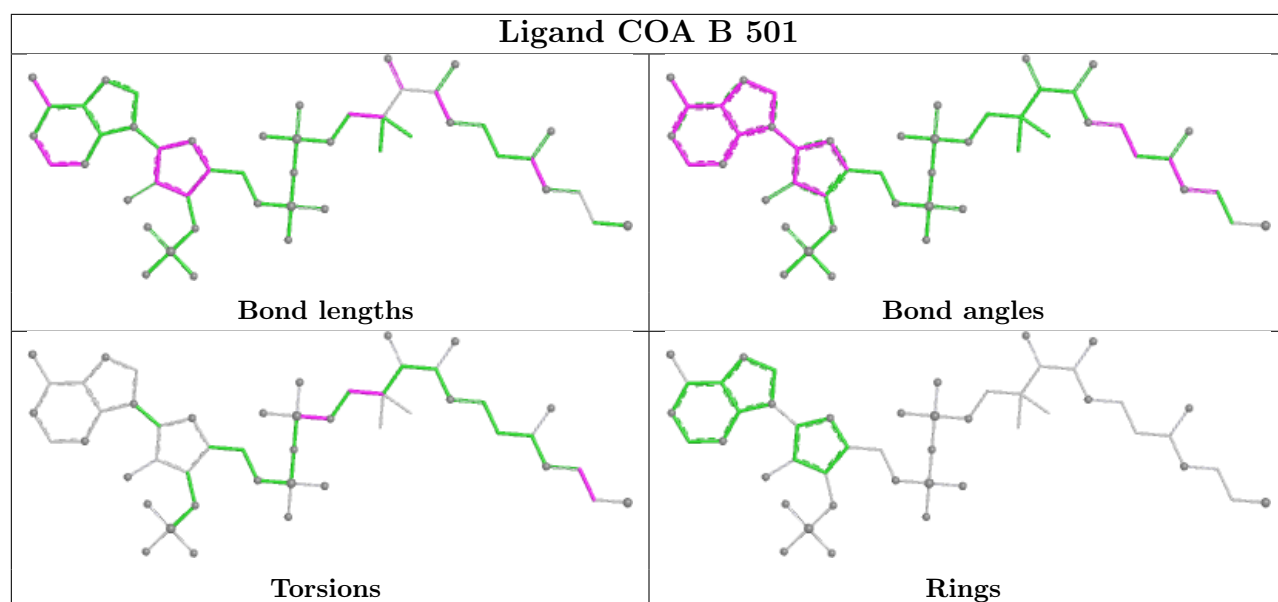
3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	COA	5	0
2	D	501	COA	8	0
2	K	501	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 [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	398/407 (97%)	-1.42	0 100 100	22, 37, 57, 67	1 (0%)
1	B	398/407 (97%)	-1.48	0 100 100	22, 32, 50, 63	0
1	C	398/407 (97%)	-1.39	0 100 100	21, 37, 62, 74	0
1	D	397/407 (97%)	-1.49	0 100 100	21, 32, 54, 73	0
1	E	396/407 (97%)	-1.35	0 100 100	25, 43, 65, 75	0
1	F	399/407 (98%)	-1.45	0 100 100	24, 36, 57, 81	0
1	G	402/407 (98%)	-1.39	0 100 100	24, 37, 62, 86	0
1	H	397/407 (97%)	-1.49	0 100 100	23, 33, 53, 72	0
1	J	396/407 (97%)	-1.42	0 100 100	23, 38, 59, 74	0
1	K	400/407 (98%)	-1.44	0 100 100	21, 33, 58, 73	0
1	L	400/407 (98%)	-1.28	0 100 100	24, 46, 75, 82	0
1	M	397/407 (97%)	-1.39	0 100 100	27, 41, 61, 75	0
All	All	4778/4884 (97%)	-1.42	0 100 100	21, 37, 61, 86	1 (0%)

There are no RSRZ outliers to report.

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](#)

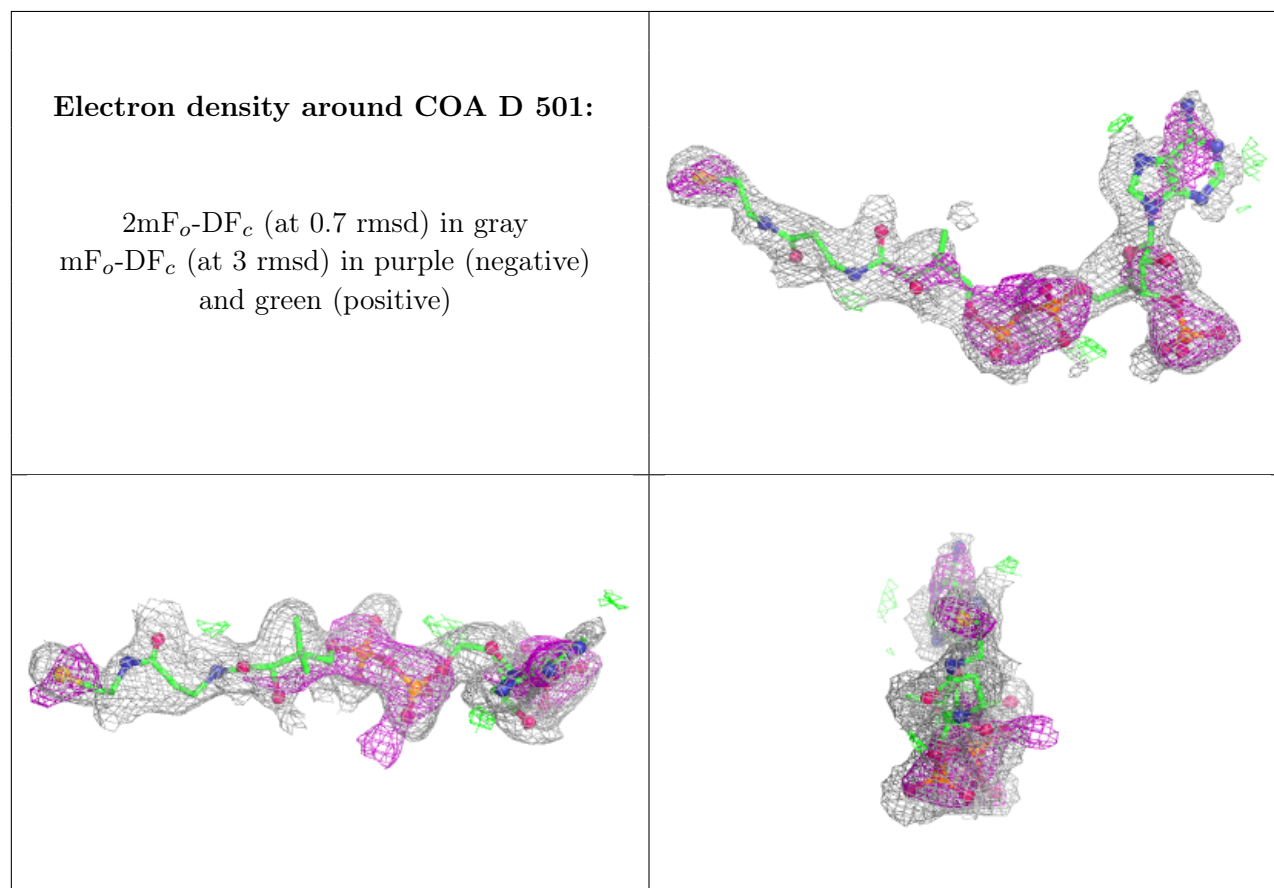
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

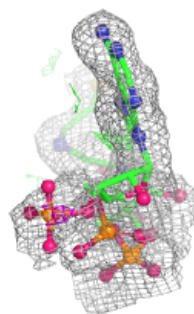
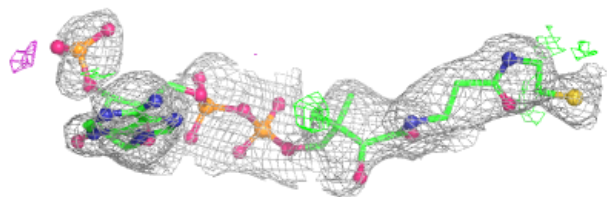
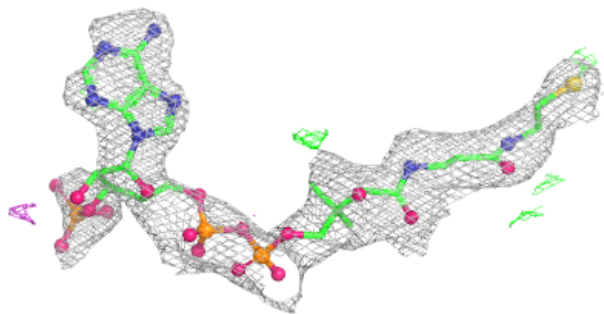
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COA	D	501	48/48	0.98	0.05	20,20,20,20	0
2	COA	H	501	48/48	0.98	0.05	38,57,78,98	0
2	COA	F	501	48/48	0.99	0.04	39,56,72,78	0
2	COA	B	501	48/48	0.99	0.04	29,50,73,91	0
2	COA	K	501	48/48	0.99	0.04	34,58,66,70	0

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.

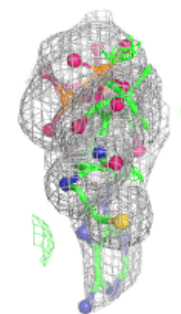
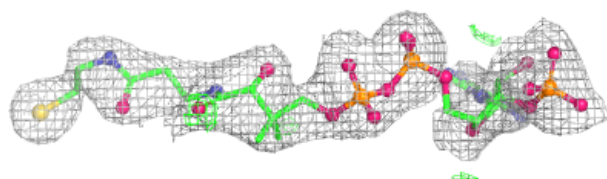
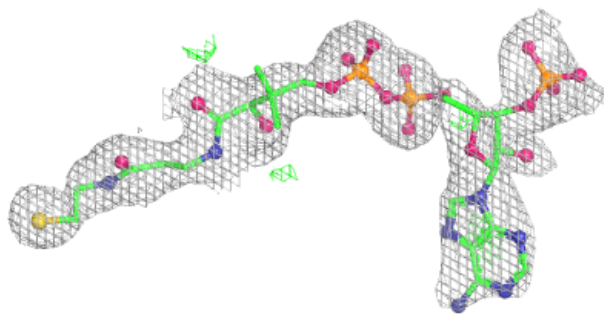


Electron density around COA H 501:

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

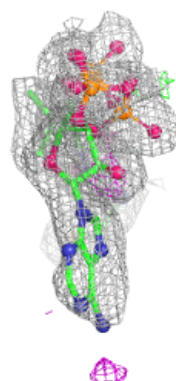
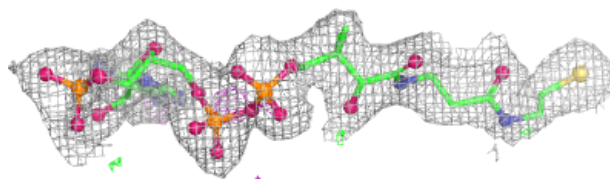
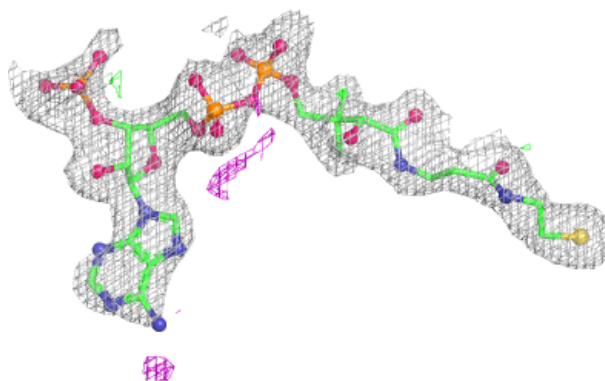
**Electron density around COA F 501:**

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

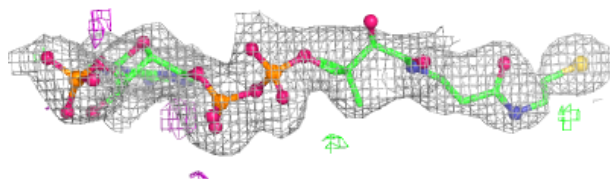
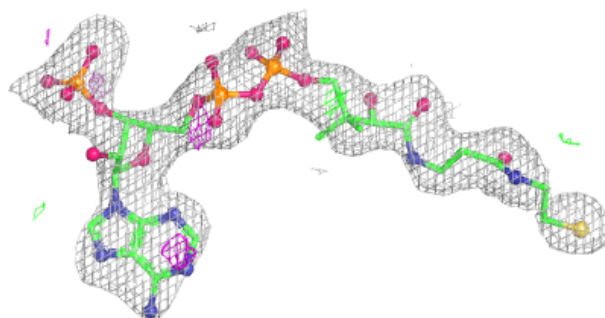


Electron density around COA B 501:

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

**Electron density around COA K 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.