Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:25 am BST

PDB ID	:	4B3J
Title	:	Crystal structure of Mycobacterium tuberculosis fatty acid beta- oxidation complex with CoenzymeA bound at the hydratase and thiolase active sites
Authors	:	Venkatesan, R.; Wierenga, R.K.
Deposited on	:	2012-07-24
Resolution	:	2.50 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:

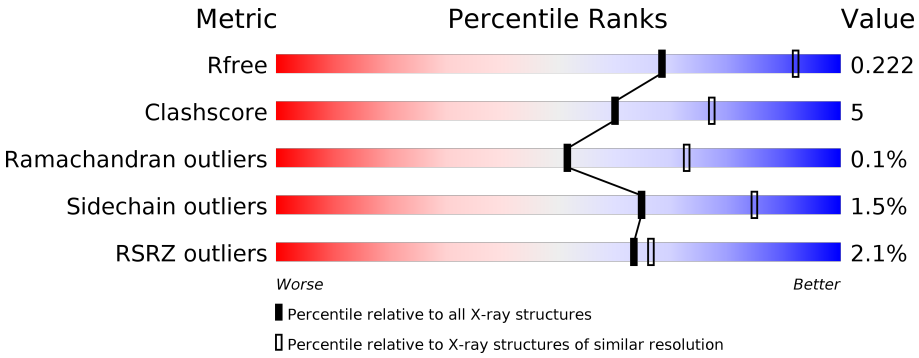
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	736	2% 89% 9%
1	B	736	2% 89% 9%
2	C	403	2% 87% 12%
2	D	403	2% 87% 11%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18116 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 FATTY ACID BETA-OXIDATION COMPLEX ALPHA-CHAIN FADB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	8	0
			5463	3461	936	1043	23			
1	B	726	Total	C	N	O	S	0	12	0
			5440	3447	933	1038	22			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	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	-	expression tag	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

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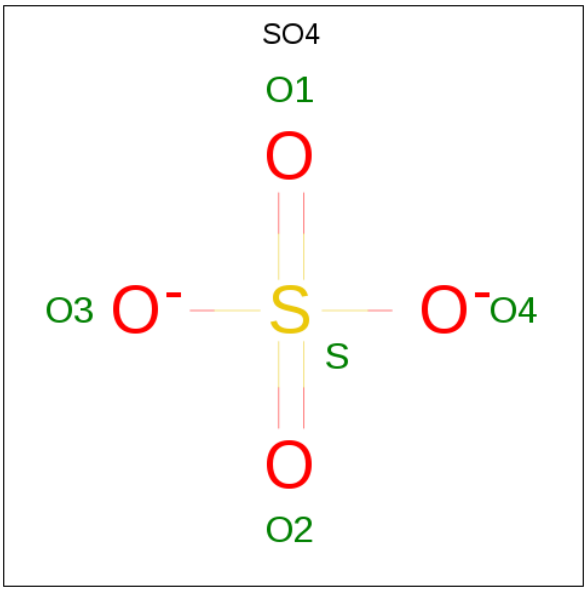
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP O53872
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression tag	UNP O53872
B	0	SER	-	expression tag	UNP O53872

- Molecule 2 is a protein called FATTY ACID BETA-OXIDATION COMPLEX BETA-CHAIN FADA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	402	Total	C	N	O	S	0	6	0
			2997	1876	529	577	15			
2	D	400	Total	C	N	O	S	0	4	0
			2961	1848	524	573	16			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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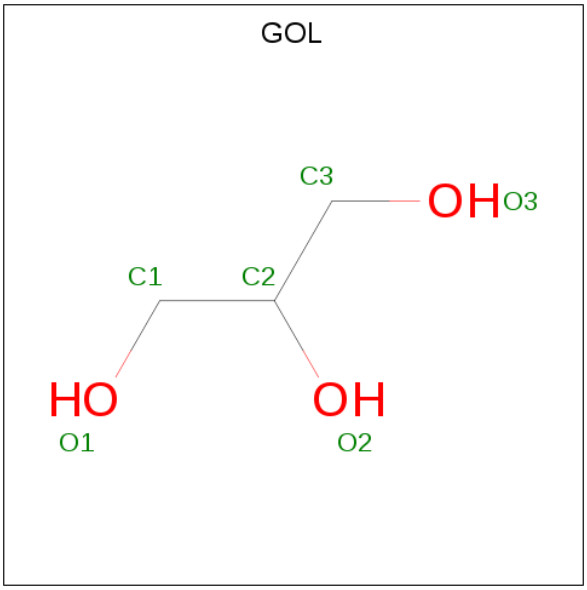
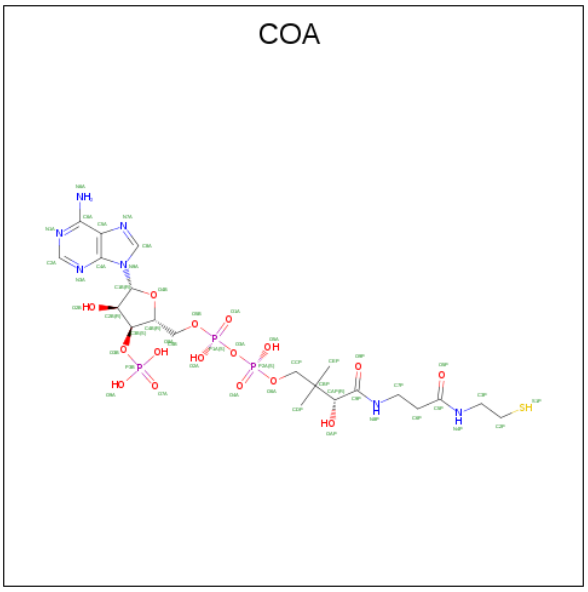
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



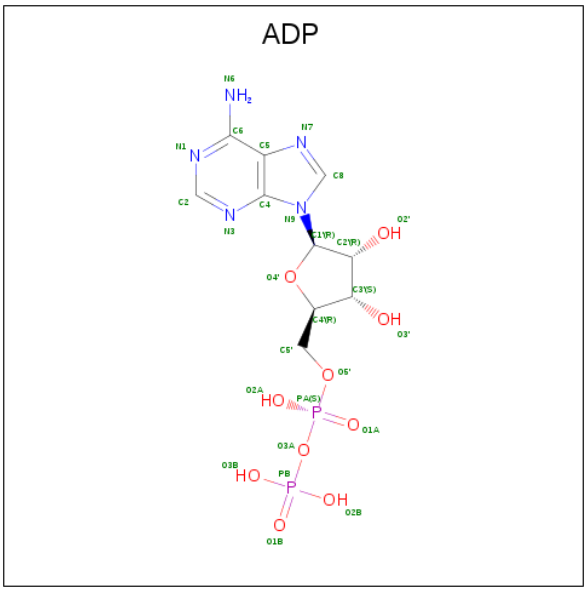
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is water.

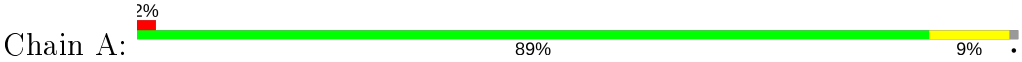
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	251	Total	O	0	0
			251	251		
7	B	284	Total	O	0	0
			284	284		
7	C	177	Total	O	0	0
			177	177		
7	D	125	Total	O	0	0
			125	125		

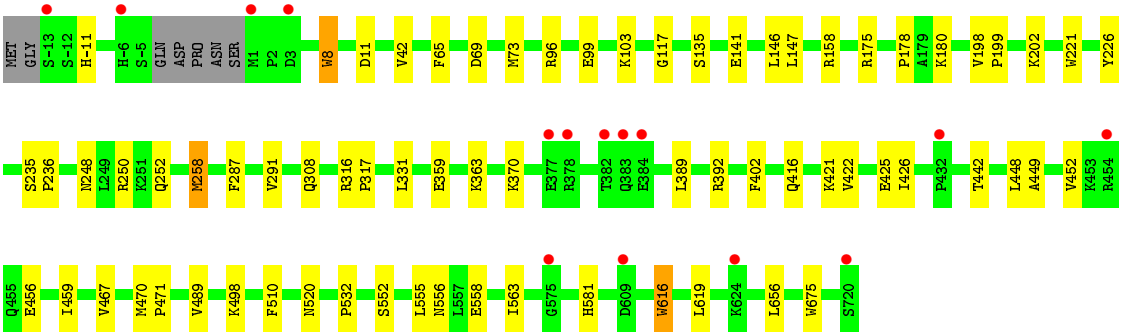
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: FATTY ACID BETA-OXIDATION COMPLEX ALPHA-CHAIN FADB

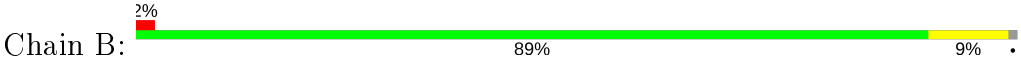
Chain A:

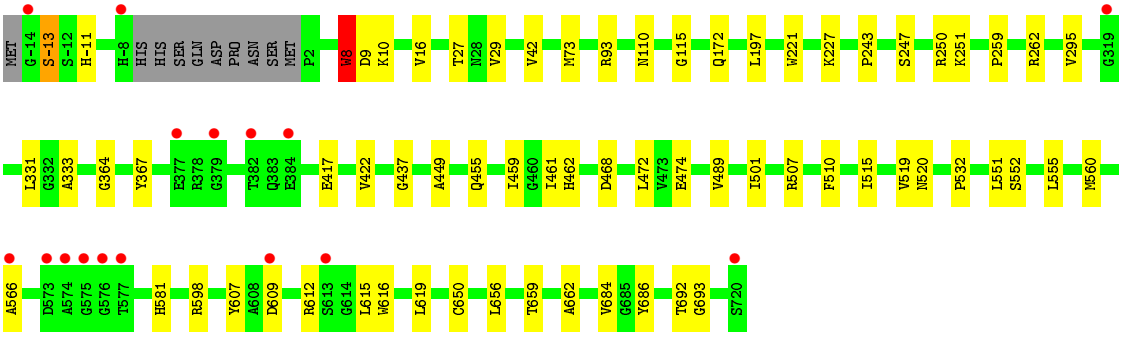




• Molecule 1: FATTY ACID BETA-OXIDATION COMPLEX ALPHA-CHAIN FADB

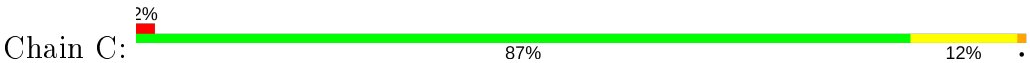
Chain B:

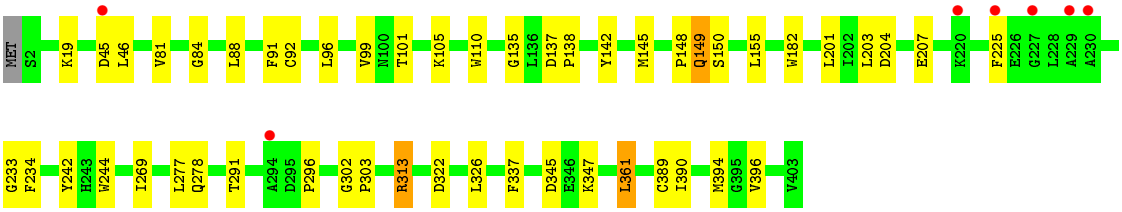




• Molecule 2: FATTY ACID BETA-OXIDATION COMPLEX BETA-CHAIN FADA

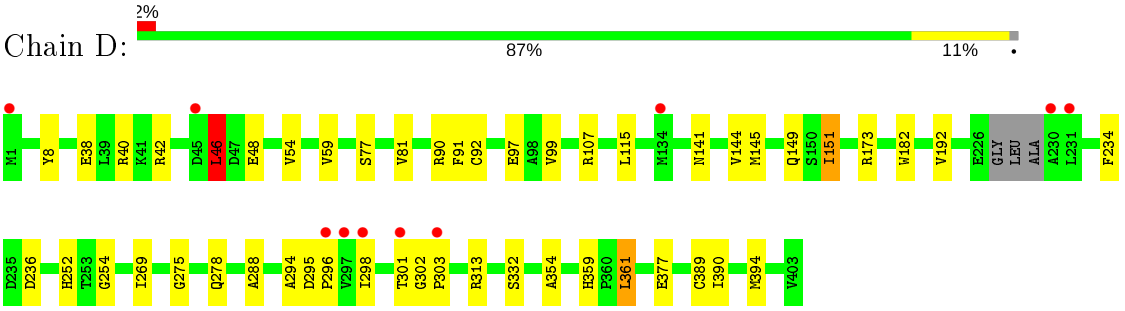
Chain C:





• Molecule 2: FATTY ACID BETA-OXIDATION COMPLEX BETA-CHAIN FADA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	248.30Å 135.25Å 118.58Å 90.00° 110.64° 90.00°	Depositor
Resolution (Å)	48.30 – 2.50 48.30 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.30-2.50) 99.7 (48.30-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.181 , 0.221 0.182 , 0.222	Depositor DCC
R_{free} test set	6303 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18116	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, 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	0.43	3/5592 (0.1%)	0.54	0/7570
1	B	0.44	3/5576 (0.1%)	0.54	0/7550
2	C	0.46	2/3061 (0.1%)	0.60	0/4144
2	D	0.44	1/3016 (0.0%)	0.58	1/4082 (0.0%)
All	All	0.44	9/17245 (0.1%)	0.56	1/23346 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	244	TRP	CD2-CE2	5.38	1.47	1.41
2	C	182	TRP	CD2-CE2	5.31	1.47	1.41
1	A	616	TRP	CD2-CE2	5.16	1.47	1.41
1	B	221	TRP	CD2-CE2	5.16	1.47	1.41
2	D	182	TRP	CD2-CE2	5.12	1.47	1.41
1	A	8[A]	TRP	CD2-CE2	5.07	1.47	1.41
1	A	8[B]	TRP	CD2-CE2	5.07	1.47	1.41
1	B	8[A]	TRP	CD2-CE2	5.01	1.47	1.41
1	B	8[B]	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	46	LEU	CA-CB-CG	5.77	128.57	115.30

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	5463	0	5495	37	0
1	B	5440	0	5475	44	0
2	C	2997	0	3025	40	0
2	D	2961	0	2979	33	0
3	A	30	0	0	0	0
3	B	40	0	0	1	0
3	C	35	0	0	0	0
3	D	25	0	0	0	0
4	A	24	0	28	2	0
4	B	6	0	8	1	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	48	0	29	3	0
5	B	48	0	32	5	0
5	C	48	0	32	11	0
5	D	48	0	32	5	0
6	C	27	0	12	0	0
6	D	27	0	12	0	0
7	A	251	0	0	1	0
7	B	284	0	0	4	0
7	C	177	0	0	2	0
7	D	125	0	0	1	0
All	All	18116	0	17175	158	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 5.

All (158) 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)
4:A:1730:GOL:O2	5:A:1731:COA:C3P	1.91	1.12
5:C:1412:COA:H52A	5:C:1412:COA:H8A	1.33	1.10
5:D:1409:COA:O9P	5:D:1409:COA:H131	1.52	1.08
5:C:1412:COA:H131	5:C:1412:COA:O9P	1.52	1.04
1:A:103:LYS:HE3	7:A:2020:HOH:O	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1730:COA:H4B	5:B:1730:COA:O9A	1.67	0.94
1:B:262[B]:ARG:NH1	7:B:2133:HOH:O	2.01	0.94
5:C:1412:COA:C8A	5:C:1412:COA:H52A	2.00	0.92
5:C:1412:COA:O9P	5:C:1412:COA:CDP	2.22	0.85
2:D:92:CYS:SG	5:D:1409:COA:H21	2.17	0.85
2:C:149:GLN:HE22	5:C:1412:COA:H32	1.45	0.80
5:D:1409:COA:CDP	5:D:1409:COA:O9P	2.27	0.80
2:C:149:GLN:NE2	5:C:1412:COA:H32	1.99	0.78
2:C:84:GLY:HA2	2:D:394:MET:HE3	1.67	0.77
5:B:1730:COA:C4B	5:B:1730:COA:O9A	2.33	0.75
2:D:295:ASP:HB3	2:D:298:ILE:HG22	1.68	0.74
2:D:40:ARG:HD2	2:D:48:GLU:OE2	1.88	0.73
2:C:92:CYS:SG	5:C:1412:COA:H21	2.29	0.72
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.71	0.71
4:A:1730:GOL:O2	5:A:1731:COA:N4P	2.24	0.71
5:B:1730:COA:O9P	5:B:1730:COA:H142	1.92	0.69
2:C:313[A]:ARG:HD2	7:C:2139:HOH:O	1.93	0.68
2:D:91:PHE:HB2	2:D:390:ILE:HG23	1.75	0.67
1:B:510:PHE:HB2	1:B:656[A]:LEU:HD21	1.76	0.66
2:C:91:PHE:HB2	2:C:390:ILE:CG2	2.27	0.65
2:D:298:ILE:O	2:D:298:ILE:HG23	1.97	0.64
1:A:331:LEU:HD13	1:A:422:VAL:HG12	1.78	0.64
2:D:302:GLY:N	2:D:303:PRO:HD2	2.12	0.64
1:B:520:ASN:HB3	1:B:581:HIS:CE1	2.33	0.63
2:C:302:GLY:N	2:C:303:PRO:HD2	2.16	0.61
2:C:96:LEU:HD23	2:C:396[A]:VAL:HG13	1.82	0.60
1:B:616:TRP:O	1:B:619:LEU:HB2	2.02	0.59
2:D:390:ILE:HB	2:D:394:MET:HB2	1.85	0.59
1:B:8[A]:TRP:CZ3	1:B:10:LYS:HB2	2.39	0.58
2:D:90:ARG:HD3	2:D:394:MET:HE2	1.87	0.57
5:B:1730:COA:H22	5:B:1730:COA:O5P	2.05	0.57
1:A:69:ASP:O	1:A:73[A]:MET:HG3	2.06	0.56
2:C:203:LEU:HD11	2:C:207:GLU:HG3	1.89	0.55
2:D:40:ARG:NH2	2:D:77:SER:O	2.32	0.55
2:C:92:CYS:SG	5:C:1412:COA:C2P	2.93	0.55
2:C:390:ILE:HB	2:C:394:MET:HB2	1.89	0.54
1:A:135:SER:O	1:A:178:PRO:HD3	2.07	0.54
1:A:141:GLU:HG3	1:A:147:LEU:C	2.28	0.54
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.42	0.54
1:A:616:TRP:HE3	1:A:619:LEU:HD13	1.73	0.54
1:B:437:GLY:HA3	1:B:461:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-13:SER:HB3	1:B:93:ARG:NE	2.24	0.53
2:C:91:PHE:HB2	2:C:390:ILE:HG22	1.89	0.53
2:C:81:VAL:HG11	2:D:296:PRO:HD3	1.91	0.53
1:A:416:GLN:HG3	1:A:448:LEU:HD23	1.90	0.53
2:C:149:GLN:HE22	5:C:1412:COA:C3P	2.20	0.52
2:C:296:PRO:HD3	2:D:81:VAL:HG21	1.91	0.52
1:B:73[A]:MET:HE2	4:B:1729:GOL:O1	2.10	0.52
1:B:459:ILE:HD13	1:B:489:VAL:HG21	1.91	0.51
1:A:552:SER:O	1:A:555:LEU:O	2.29	0.50
1:A:258:MET:HG2	1:A:675:TRP:HB3	1.94	0.50
1:A:11[A]:ASP:CG	1:A:202:LYS:HZ2	2.15	0.50
1:A:616:TRP:O	1:A:619:LEU:HB2	2.12	0.50
1:B:243:PRO:HA	2:C:135:GLY:O	2.11	0.50
1:B:515:ILE:HD11	1:B:551:LEU:HD21	1.93	0.50
1:A:250:ARG:NH1	2:D:145:MET:HG2	2.27	0.49
2:D:38:GLU:OE2	2:D:42:ARG:HD2	2.12	0.49
2:D:252:HIS:HE1	2:D:332:SER:H	1.58	0.49
1:B:598:ARG:NH1	7:B:2249:HOH:O	2.44	0.49
5:A:1731:COA:O1A	5:A:1731:COA:OAP	2.17	0.48
1:B:-11:HIS:CE1	1:B:42:VAL:HG12	2.49	0.48
1:A:359:GLU:HG2	1:A:363:LYS:HE2	1.95	0.48
1:B:532:PRO:HB2	1:B:615:LEU:HD13	1.95	0.48
2:D:90:ARG:HH21	2:D:97:GLU:CD	2.16	0.48
1:B:110:ASN:HA	1:B:197:LEU:HD11	1.95	0.48
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.96	0.48
1:A:65:PHE:HB3	1:A:117:GLY:HA2	1.97	0.47
2:D:354:ALA:HB1	2:D:359:HIS:HB2	1.97	0.47
1:B:115:GLY:HA3	5:B:1730:COA:H21	1.95	0.47
2:C:303:PRO:HD3	2:C:389:CYS:HA	1.95	0.47
1:A:248:ASN:O	1:A:252:GLN:HG2	2.14	0.47
1:A:556:ASN:OD1	1:A:558:GLU:HB2	2.15	0.47
2:C:291:THR:HG22	2:C:396[A]:VAL:HG23	1.97	0.47
1:B:9:ASP:O	1:B:16:VAL:HA	2.15	0.47
1:B:331:LEU:HD13	1:B:422:VAL:CG1	2.45	0.47
1:A:402:PHE:CD2	1:A:426:ILE:HG12	2.51	0.46
1:A:287:PHE:CE2	1:A:291:VAL:HG21	2.50	0.46
1:A:467:VAL:O	1:A:498:LYS:NZ	2.40	0.46
2:D:389:CYS:C	2:D:390:ILE:HG13	2.35	0.46
1:B:656[B]:LEU:HD13	1:B:662:ALA:HB2	1.97	0.46
2:C:361:LEU:HD22	5:C:1412:COA:H22	1.97	0.46
2:D:141:ASN:O	2:D:144:VAL:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:CYS:HB3	1:B:656[A]:LEU:HD23	1.97	0.46
1:B:686:TYR:O	1:B:692:THR:HA	2.16	0.46
2:C:150:SER:HB2	2:C:225:PHE:CD2	2.51	0.46
5:D:1409:COA:H132	7:D:2092:HOH:O	2.16	0.46
1:A:456[B]:GLU:OE1	1:A:456[B]:GLU:CA	2.64	0.46
1:B:552:SER:O	1:B:555:LEU:O	2.34	0.46
2:C:99:VAL:HG13	2:C:269:ILE:HD11	1.98	0.46
2:C:150:SER:HB2	2:C:225:PHE:CG	2.52	0.45
1:B:507:ARG:HG2	1:B:566:ALA:HB1	1.97	0.45
2:D:46:LEU:HD22	2:D:278:GLN:HB3	1.98	0.45
1:B:472:LEU:HD11	1:B:501:ILE:HG23	1.98	0.45
1:A:389:LEU:HA	1:A:392:ARG:NH1	2.31	0.45
1:B:519:VAL:HG21	1:B:560:MET:SD	2.56	0.45
1:B:333:ALA:HB1	1:B:364:GLY:HA3	1.98	0.45
2:C:101:THR:HG22	2:C:105:LYS:HD2	1.99	0.45
1:A:141:GLU:HB2	1:A:146:LEU:HB2	1.98	0.45
1:B:8[A]:TRP:HZ3	1:B:10:LYS:HB2	1.82	0.44
1:A:258:MET:CG	1:A:675:TRP:HB3	2.48	0.44
2:D:38:GLU:HG2	2:D:192:VAL:HG21	2.00	0.44
2:D:254:GLY:HA2	5:D:1409:COA:H143	2.00	0.44
2:D:294:ALA:HB3	2:D:301:THR:HG23	2.00	0.44
1:B:510:PHE:CG	1:B:656[A]:LEU:HD21	2.52	0.44
1:A:421:LYS:HE3	1:A:425:GLU:OE2	2.18	0.44
1:B:367:TYR:HB2	7:B:2195:HOH:O	2.18	0.44
1:A:459:ILE:HG21	1:A:489:VAL:HG21	1.99	0.44
1:B:449:ALA:O	1:B:455:GLN:HG2	2.17	0.43
1:B:367:TYR:OH	1:B:468:ASP:OD1	2.31	0.43
2:D:59:VAL:HG21	2:D:361:LEU:HB3	2.00	0.43
1:A:520:ASN:HB3	1:A:581:HIS:CE1	2.53	0.43
1:B:259:PRO:HD2	1:B:295:VAL:HG11	1.99	0.43
1:B:437:GLY:HA2	1:B:459:ILE:O	2.18	0.43
1:A:449:ALA:O	1:A:452:VAL:HG22	2.18	0.43
1:A:442:THR:HG21	1:A:563:ILE:HG12	2.01	0.43
2:C:149:GLN:HE22	5:C:1412:COA:C5P	2.30	0.43
2:D:54:VAL:HG22	2:D:115:LEU:HB2	2.01	0.43
2:D:302:GLY:N	2:D:303:PRO:CD	2.79	0.42
1:A:96:ARG:NH1	1:A:99:GLU:OE1	2.48	0.42
2:D:151:ILE:HD13	2:D:234:PHE:HB2	2.01	0.42
2:C:137:ASP:HA	2:C:138:PRO:HD3	1.93	0.42
2:C:91:PHE:HB2	2:C:390:ILE:HG23	2.00	0.42
1:B:684:VAL:O	1:B:693:GLY:HA2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:TYR:CZ	2:D:275:GLY:HA3	2.55	0.42
1:B:437:GLY:HA3	1:B:461:ILE:CD1	2.49	0.42
1:A:-11:HIS:CE1	1:A:42:VAL:HG12	2.55	0.42
1:B:250:ARG:NH1	2:C:145:MET:HG2	2.34	0.42
1:B:607:TYR:CE1	1:B:612[B]:ARG:HG3	2.55	0.42
2:C:92:CYS:HB2	2:C:389:CYS:O	2.20	0.42
1:B:659:THR:HG23	3:B:1728:SO4:O2	2.20	0.41
1:A:510:PHE:CD1	1:A:656:LEU:HD11	2.55	0.41
2:D:90:ARG:HH11	2:D:394:MET:CE	2.34	0.41
2:C:148:PRO:HD3	2:C:234:PHE:CD1	2.56	0.41
2:C:201:LEU:HD11	2:C:204:ASP:HB3	2.03	0.41
1:B:27:THR:HG23	1:B:29:VAL:HG23	2.03	0.41
1:A:198:VAL:HB	1:A:199:PRO:HD3	2.03	0.41
1:B:520:ASN:HB3	1:B:581:HIS:NE2	2.35	0.41
2:C:46:LEU:HD22	2:C:278:GLN:HB3	2.02	0.41
1:A:470:MET:HA	1:A:471:PRO:HD3	1.96	0.41
1:B:247:SER:HB3	7:B:2123:HOH:O	2.20	0.41
2:C:322:ASP:O	2:C:347:LYS:HG2	2.21	0.41
1:B:251:LYS:HD2	2:C:233:GLY:HA2	2.03	0.41
1:A:221:TRP:HA	1:A:226:TYR:CD1	2.56	0.40
1:A:235:SER:HA	1:A:236:PRO:HD3	1.86	0.40
1:A:316:ARG:HA	1:A:317:PRO:HD2	1.92	0.40
1:B:227:LYS:HA	1:B:227:LYS:HD3	1.92	0.40
2:C:155:LEU:HD21	2:C:242:TYR:CD2	2.56	0.40
2:C:326:LEU:HD22	2:C:337:PHE:CG	2.57	0.40
1:A:510:PHE:CE1	1:A:656:LEU:HD11	2.56	0.40
2:C:313[B]:ARG:HG3	7:C:2139:HOH:O	2.21	0.40
2:C:110:TRP:CH2	2:D:107:ARG:HD2	2.55	0.40
2:C:110:TRP:CZ2	2:D:288:ALA:HA	2.56	0.40
2:C:88:LEU:HD12	2:C:88:LEU:C	2.42	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	733/736 (100%)	712 (97%)	21 (3%)	0	100	100
1	B	734/736 (100%)	714 (97%)	19 (3%)	1 (0%)	51	73
2	C	406/403 (101%)	393 (97%)	12 (3%)	1 (0%)	47	68
2	D	400/403 (99%)	385 (96%)	14 (4%)	1 (0%)	41	61
All	All	2273/2278 (100%)	2204 (97%)	66 (3%)	3 (0%)	51	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	361	LEU
2	D	361	LEU
1	B	609	ASP

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	564/566 (100%)	554 (98%)	10 (2%)	59	81
1	B	561/566 (99%)	556 (99%)	5 (1%)	78	92
2	C	314/310 (101%)	305 (97%)	9 (3%)	42	69
2	D	309/310 (100%)	302 (98%)	7 (2%)	50	76
All	All	1748/1752 (100%)	1717 (98%)	31 (2%)	65	81

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8[A]	TRP
1	A	8[B]	TRP
1	A	158	ARG
1	A	175	ARG
1	A	180	LYS

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Mol	Chain	Res	Type
1	A	258	MET
1	A	308[A]	GLN
1	A	308[B]	GLN
1	A	370	LYS
1	A	532	PRO
1	B	-13	SER
1	B	8[A]	TRP
1	B	8[B]	TRP
1	B	172	GLN
1	B	417	GLU
2	C	19	LYS
2	C	45	ASP
2	C	142[A]	TYR
2	C	142[B]	TYR
2	C	149	GLN
2	C	277	LEU
2	C	313[A]	ARG
2	C	313[B]	ARG
2	C	345	ASP
2	D	46	LEU
2	D	149	GLN
2	D	151	ILE
2	D	173	ARG
2	D	236	ASP
2	D	377[A]	GLU
2	D	377[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	149	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

39 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	1726	-	4,4,4	0.34	0	6,6,6	0.17	0
3	SO4	C	1406	-	4,4,4	0.36	0	6,6,6	0.19	0
6	ADP	D	1410	-	24,29,29	1.07	3 (12%)	29,45,45	1.46	4 (13%)
5	COA	C	1412	-	41,50,50	0.84	1 (2%)	52,75,75	1.22	4 (7%)
3	SO4	B	1727	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	C	1409	-	4,4,4	0.39	0	6,6,6	0.22	0
4	GOL	B	1729	-	5,5,5	0.43	0	5,5,5	0.59	0
3	SO4	C	1408	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	B	1721	-	4,4,4	0.30	0	6,6,6	0.24	0
4	GOL	A	1727	-	5,5,5	0.36	0	5,5,5	0.16	0
3	SO4	B	1725	-	4,4,4	0.34	0	6,6,6	0.14	0
3	SO4	B	1722	-	4,4,4	0.39	0	6,6,6	0.14	0
3	SO4	C	1405	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	B	1724	-	4,4,4	0.35	0	6,6,6	0.11	0
3	SO4	B	1723	-	4,4,4	0.40	0	6,6,6	0.16	0
3	SO4	C	1404	-	4,4,4	0.30	0	6,6,6	0.39	0
4	GOL	D	1411	-	5,5,5	0.45	0	5,5,5	0.49	0
4	GOL	C	1411	-	5,5,5	0.41	0	5,5,5	0.43	0
4	GOL	A	1728	-	5,5,5	0.38	0	5,5,5	0.21	0
3	SO4	C	1407	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	B	1728	-	4,4,4	0.36	0	6,6,6	0.13	0
3	SO4	D	1406	-	4,4,4	0.35	0	6,6,6	0.15	0
3	SO4	A	1724	-	4,4,4	0.35	0	6,6,6	0.17	0
3	SO4	A	1721	-	4,4,4	0.41	0	6,6,6	0.16	0
3	SO4	D	1407	-	4,4,4	0.30	0	6,6,6	0.12	0
5	COA	D	1409	-	41,50,50	0.83	1 (2%)	52,75,75	1.16	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	COA	A	1731	-	41,50,50	0.83	2 (4%)	52,75,75	1.11	5 (9%)
3	SO4	D	1404	-	4,4,4	0.32	0	6,6,6	0.30	0
3	SO4	B	1726	-	4,4,4	0.31	0	6,6,6	0.27	0
3	SO4	A	1725	-	4,4,4	0.35	0	6,6,6	0.10	0
4	GOL	A	1730	-	5,5,5	0.23	0	5,5,5	0.36	0
6	ADP	C	1413	-	24,29,29	1.08	2 (8%)	29,45,45	1.34	4 (13%)
3	SO4	A	1722	-	4,4,4	0.34	0	6,6,6	0.14	0
3	SO4	D	1408	-	4,4,4	0.33	0	6,6,6	0.11	0
3	SO4	A	1723	-	4,4,4	0.33	0	6,6,6	0.10	0
3	SO4	D	1405	-	4,4,4	0.34	0	6,6,6	0.16	0
5	COA	B	1730	-	41,50,50	0.83	1 (2%)	52,75,75	1.22	5 (9%)
3	SO4	C	1410	-	4,4,4	0.37	0	6,6,6	0.24	0
4	GOL	A	1729	-	5,5,5	0.34	0	5,5,5	0.15	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
4	GOL	B	1729	-	-	1/4/4/4	-
5	COA	D	1409	-	-	22/44/64/64	0/3/3/3
5	COA	C	1412	-	-	23/44/64/64	0/3/3/3
4	GOL	D	1411	-	-	4/4/4/4	-
4	GOL	C	1411	-	-	2/4/4/4	-
4	GOL	A	1728	-	-	2/4/4/4	-
6	ADP	C	1413	-	-	0/12/32/32	0/3/3/3
5	COA	A	1731	-	-	13/44/64/64	0/3/3/3
5	COA	B	1730	-	-	27/44/64/64	0/3/3/3
6	ADP	D	1410	-	-	8/12/32/32	0/3/3/3
4	GOL	A	1727	-	-	4/4/4/4	-
4	GOL	A	1730	-	-	2/4/4/4	-
4	GOL	A	1729	-	-	0/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1413	ADP	C5-C4	2.77	1.48	1.40
6	D	1410	ADP	C5-C4	2.76	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1413	ADP	O4'-C1'	2.59	1.44	1.41
5	B	1730	COA	C5A-C4A	2.56	1.47	1.40
5	A	1731	COA	C5A-C4A	2.47	1.47	1.40
5	C	1412	COA	C5A-C4A	2.45	1.47	1.40
5	D	1409	COA	C5A-C4A	2.41	1.47	1.40
6	D	1410	ADP	O4'-C1'	2.25	1.44	1.41
5	A	1731	COA	O4B-C1B	2.15	1.44	1.41
6	D	1410	ADP	C2-N3	2.11	1.35	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1410	ADP	C3'-C2'-C1'	4.11	107.17	100.98
5	B	1730	COA	P2A-O3A-P1A	-3.83	119.68	132.83
6	D	1410	ADP	N3-C2-N1	-3.66	122.95	128.68
5	A	1731	COA	N3A-C2A-N1A	-3.63	123.00	128.68
6	C	1413	ADP	N3-C2-N1	-3.50	123.20	128.68
5	D	1409	COA	N3A-C2A-N1A	-3.45	123.29	128.68
5	C	1412	COA	N3A-C2A-N1A	-3.30	123.51	128.68
5	B	1730	COA	N3A-C2A-N1A	-3.26	123.58	128.68
5	A	1731	COA	P2A-O3A-P1A	-3.11	122.15	132.83
6	C	1413	ADP	C3'-C2'-C1'	3.06	105.59	100.98
5	D	1409	COA	P2A-O3A-P1A	-3.02	122.47	132.83
5	B	1730	COA	C4A-C5A-N7A	-2.87	106.41	109.40
5	C	1412	COA	P2A-O3A-P1A	-2.84	123.09	132.83
5	D	1409	COA	C4A-C5A-N7A	-2.70	106.59	109.40
5	A	1731	COA	C4A-C5A-N7A	-2.67	106.62	109.40
5	C	1412	COA	C4A-C5A-N7A	-2.67	106.62	109.40
6	C	1413	ADP	C4-C5-N7	-2.53	106.76	109.40
5	C	1412	COA	O6A-CCP-CBP	-2.42	106.65	110.55
6	C	1413	ADP	PA-O3A-PB	-2.26	125.08	132.83
5	B	1730	COA	C3B-C2B-C1B	2.18	104.73	99.89
6	D	1410	ADP	C4-C5-N7	-2.18	107.13	109.40
5	A	1731	COA	C1B-N9A-C4A	-2.15	122.87	126.64
5	A	1731	COA	C2A-N1A-C6A	2.12	122.38	118.75
5	B	1730	COA	O6A-CCP-CBP	-2.05	107.24	110.55
6	D	1410	ADP	PA-O3A-PB	-2.03	125.87	132.83

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	1410	ADP	PA-O3A-PB-O2B
6	D	1410	ADP	PA-O3A-PB-O3B
6	D	1410	ADP	O4'-C4'-C5'-O5'
6	D	1410	ADP	C3'-C4'-C5'-O5'
5	C	1412	COA	C3B-O3B-P3B-O8A
5	C	1412	COA	C5B-O5B-P1A-O2A
5	C	1412	COA	C5B-O5B-P1A-O3A
5	C	1412	COA	CCP-O6A-P2A-O4A
5	C	1412	COA	CCP-O6A-P2A-O5A
5	C	1412	COA	CAP-CBP-CCP-O6A
5	C	1412	COA	OAP-CAP-CBP-CCP
5	C	1412	COA	C9P-CAP-CBP-CCP
5	C	1412	COA	OAP-CAP-CBP-CDP
5	C	1412	COA	C9P-CAP-CBP-CDP
5	C	1412	COA	OAP-CAP-CBP-CEP
5	C	1412	COA	C9P-CAP-CBP-CEP
5	C	1412	COA	C5P-C6P-C7P-N8P
5	C	1412	COA	C6P-C5P-N4P-C3P
5	C	1412	COA	O5P-C5P-N4P-C3P
4	A	1727	GOL	O1-C1-C2-C3
4	A	1727	GOL	C1-C2-C3-O3
4	A	1727	GOL	O2-C2-C3-O3
4	D	1411	GOL	C1-C2-C3-O3
4	C	1411	GOL	O1-C1-C2-C3
5	D	1409	COA	C5B-O5B-P1A-O2A
5	D	1409	COA	CCP-O6A-P2A-O4A
5	D	1409	COA	CCP-O6A-P2A-O5A
5	D	1409	COA	OAP-CAP-CBP-CCP
5	D	1409	COA	C9P-CAP-CBP-CCP
5	D	1409	COA	OAP-CAP-CBP-CDP
5	D	1409	COA	C9P-CAP-CBP-CDP
5	D	1409	COA	C9P-CAP-CBP-CEP
5	D	1409	COA	O9P-C9P-CAP-CBP
5	D	1409	COA	N8P-C9P-CAP-CBP
5	D	1409	COA	N8P-C9P-CAP-OAP
5	D	1409	COA	C5P-C6P-C7P-N8P
5	D	1409	COA	S1P-C2P-C3P-N4P
5	A	1731	COA	C5B-O5B-P1A-O2A
5	A	1731	COA	CDP-CBP-CCP-O6A
5	A	1731	COA	CEP-CBP-CCP-O6A
5	A	1731	COA	CAP-CBP-CCP-O6A
5	A	1731	COA	S1P-C2P-C3P-N4P
5	B	1730	COA	C4B-C3B-O3B-P3B

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Mol	Chain	Res	Type	Atoms
5	B	1730	COA	C3B-O3B-P3B-O7A
5	B	1730	COA	C5B-O5B-P1A-O1A
5	B	1730	COA	C5B-O5B-P1A-O2A
5	B	1730	COA	CCP-O6A-P2A-O4A
5	B	1730	COA	CCP-O6A-P2A-O5A
5	B	1730	COA	CDP-CBP-CCP-O6A
5	B	1730	COA	CEP-CBP-CCP-O6A
5	B	1730	COA	CAP-CBP-CCP-O6A
5	B	1730	COA	OAP-CAP-CBP-CCP
5	B	1730	COA	C9P-CAP-CBP-CCP
5	B	1730	COA	OAP-CAP-CBP-CDP
5	B	1730	COA	C9P-CAP-CBP-CDP
5	B	1730	COA	OAP-CAP-CBP-CEP
5	B	1730	COA	C9P-CAP-CBP-CEP
5	B	1730	COA	CAP-C9P-N8P-C7P
5	B	1730	COA	C6P-C5P-N4P-C3P
5	B	1730	COA	C2P-C3P-N4P-C5P
5	A	1731	COA	O5P-C5P-N4P-C3P
5	B	1730	COA	O5P-C5P-N4P-C3P
5	A	1731	COA	C6P-C5P-N4P-C3P
5	B	1730	COA	O9P-C9P-N8P-C7P
5	A	1731	COA	O4B-C4B-C5B-O5B
5	B	1730	COA	O4B-C4B-C5B-O5B
5	A	1731	COA	C3B-C4B-C5B-O5B
5	B	1730	COA	C3B-C4B-C5B-O5B
4	D	1411	GOL	O2-C2-C3-O3
4	C	1411	GOL	O1-C1-C2-O2
6	D	1410	ADP	C4'-C5'-O5'-PA
5	D	1409	COA	O5P-C5P-N4P-C3P
5	D	1409	COA	O9P-C9P-CAP-OAP
4	A	1727	GOL	O1-C1-C2-O2
5	D	1409	COA	OAP-CAP-CBP-CEP
4	B	1729	GOL	O2-C2-C3-O3
4	A	1730	GOL	O1-C1-C2-O2
5	C	1412	COA	P2A-O3A-P1A-O5B
5	A	1731	COA	P1A-O3A-P2A-O6A
5	D	1409	COA	C6P-C5P-N4P-C3P
5	C	1412	COA	C4B-C5B-O5B-P1A
5	C	1412	COA	CCP-O6A-P2A-O3A
4	A	1728	GOL	O2-C2-C3-O3
4	D	1411	GOL	O1-C1-C2-O2
5	D	1409	COA	C5B-O5B-P1A-O3A

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Mol	Chain	Res	Type	Atoms
5	A	1731	COA	C5B-O5B-P1A-O3A
4	D	1411	GOL	O1-C1-C2-C3
6	D	1410	ADP	C5'-O5'-PA-O2A
5	D	1409	COA	C5B-O5B-P1A-O1A
5	C	1412	COA	CDP-CBP-CCP-O6A
5	C	1412	COA	CEP-CBP-CCP-O6A
5	D	1409	COA	CEP-CBP-CCP-O6A
5	C	1412	COA	O9P-C9P-CAP-CBP
5	B	1730	COA	O9P-C9P-CAP-CBP
5	D	1409	COA	CDP-CBP-CCP-O6A
5	C	1412	COA	N8P-C9P-CAP-CBP
5	B	1730	COA	N8P-C9P-CAP-CBP
5	A	1731	COA	C4B-C5B-O5B-P1A
4	A	1728	GOL	C1-C2-C3-O3
6	D	1410	ADP	PA-O3A-PB-O1B
6	D	1410	ADP	C5'-O5'-PA-O3A
5	D	1409	COA	CCP-O6A-P2A-O3A
5	B	1730	COA	C3B-O3B-P3B-O9A
5	B	1730	COA	C5B-O5B-P1A-O3A
5	B	1730	COA	CCP-O6A-P2A-O3A
4	A	1730	GOL	O1-C1-C2-C3
5	A	1731	COA	C5B-O5B-P1A-O1A
5	C	1412	COA	O4B-C4B-C5B-O5B

There are no ring outliers.

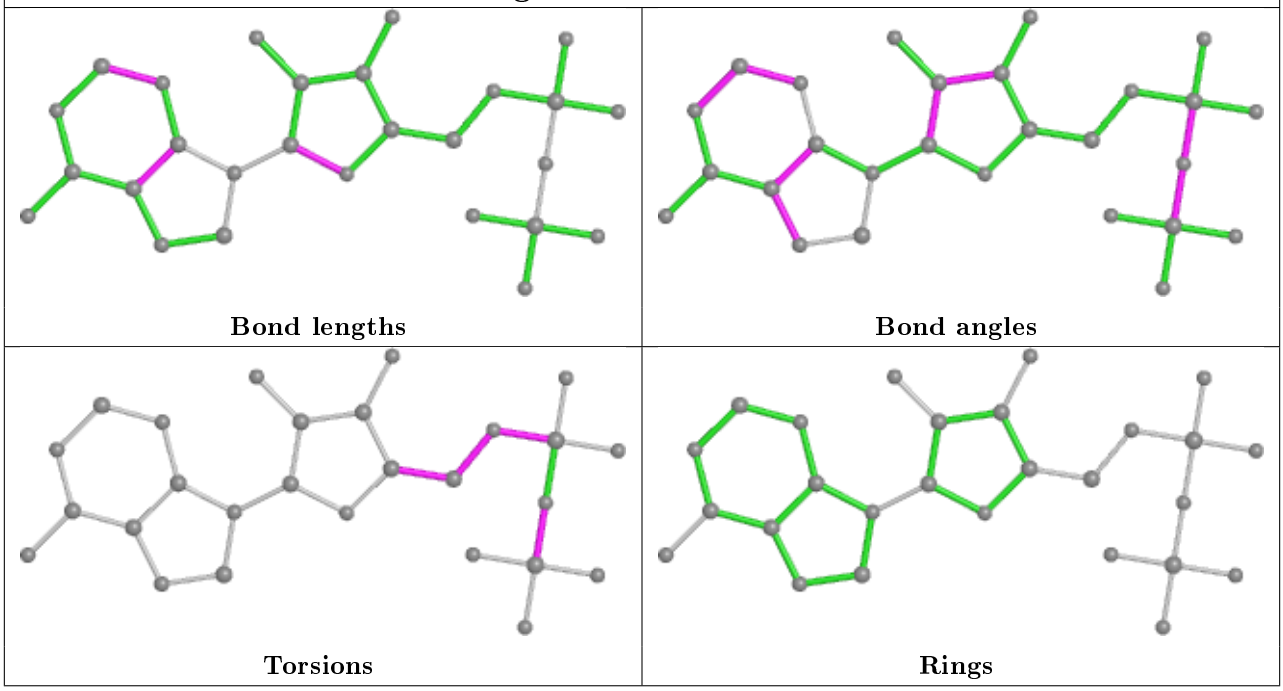
7 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1412	COA	11	0
4	B	1729	GOL	1	0
3	B	1728	SO4	1	0
5	D	1409	COA	5	0
5	A	1731	COA	3	0
4	A	1730	GOL	2	0
5	B	1730	COA	5	0

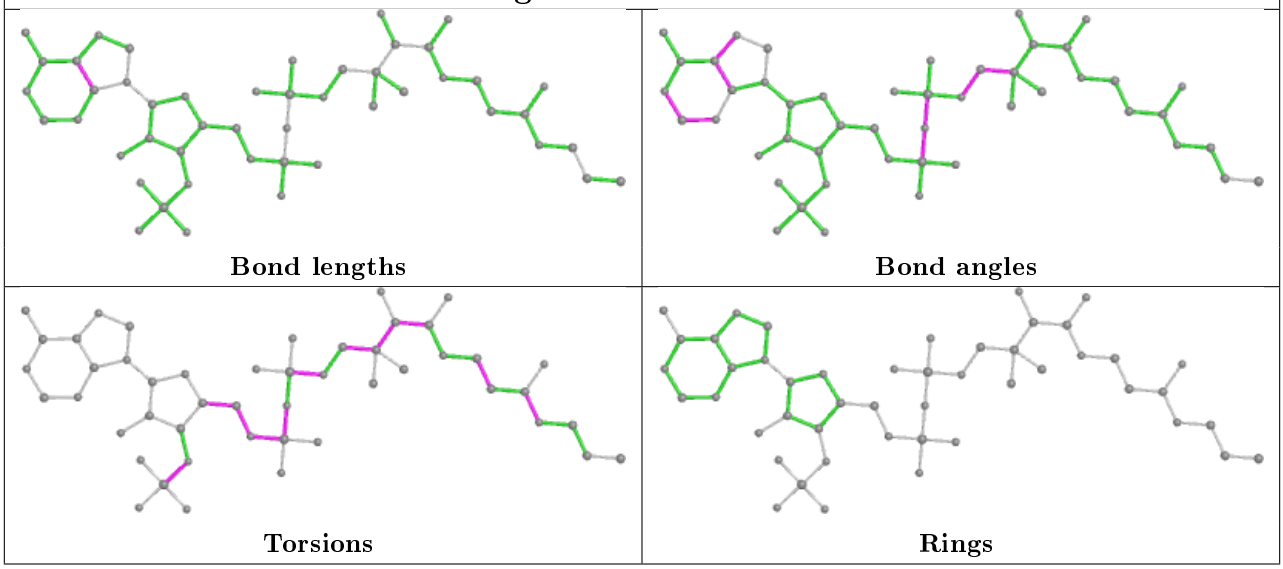
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

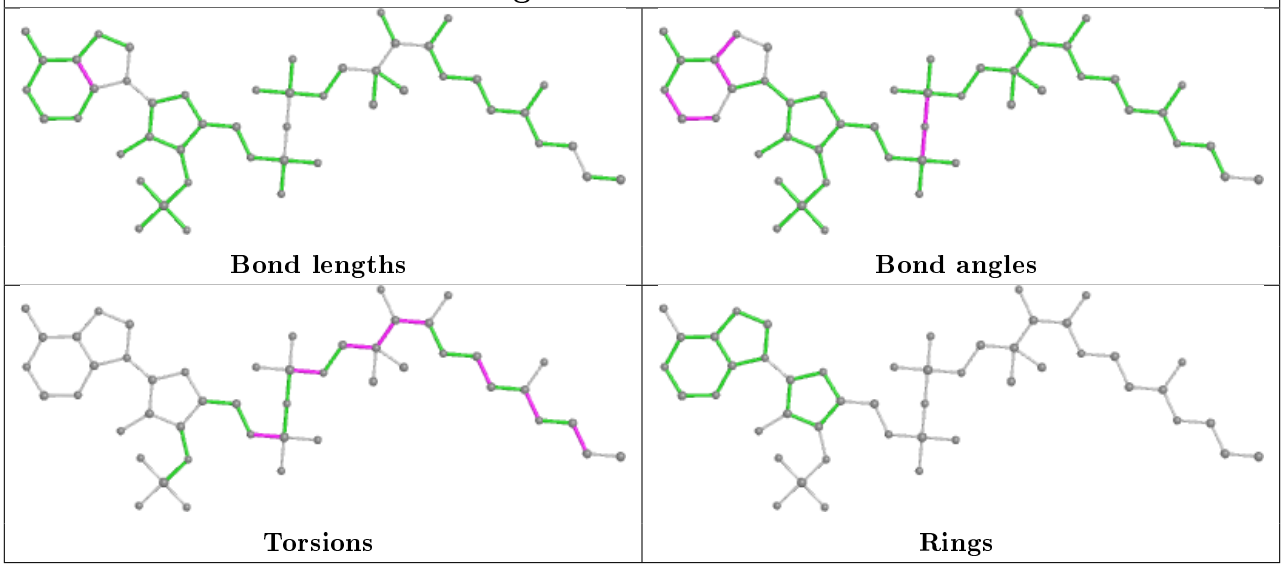
Ligand ADP D 1410



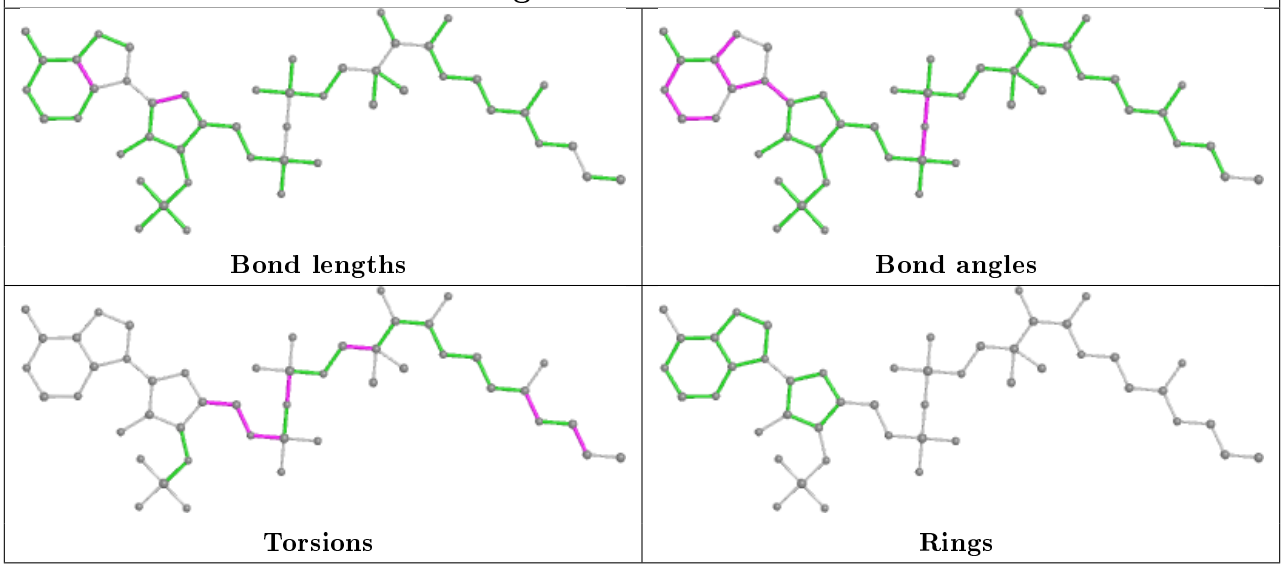
Ligand COA C 1412



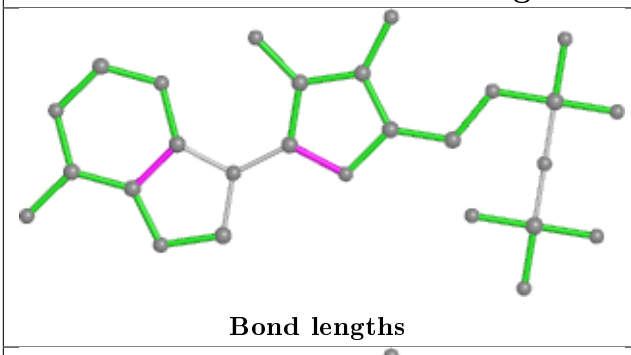
Ligand COA D 1409



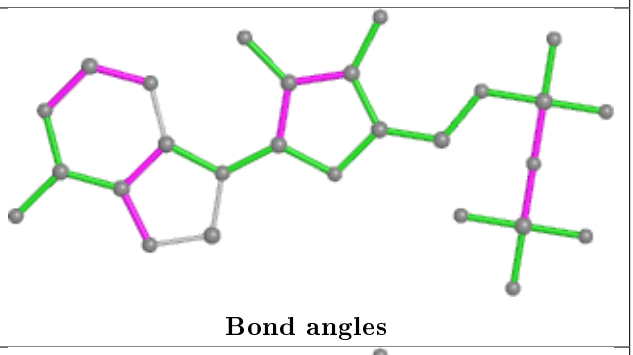
Ligand COA A 1731



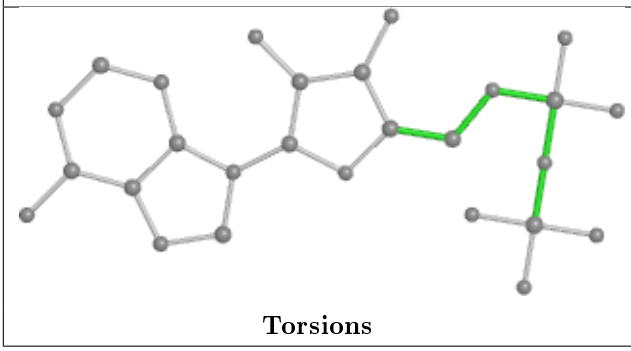
Ligand ADP C 1413



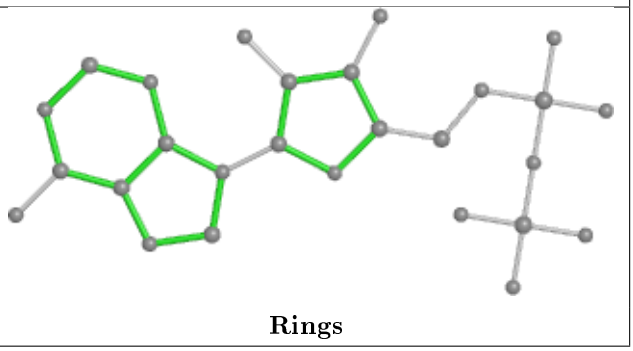
Bond lengths



Bond angles

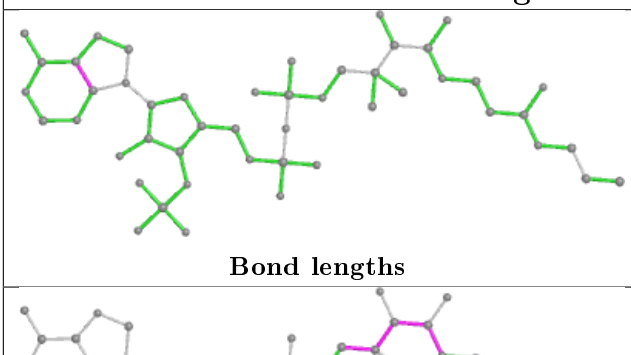


Torsions

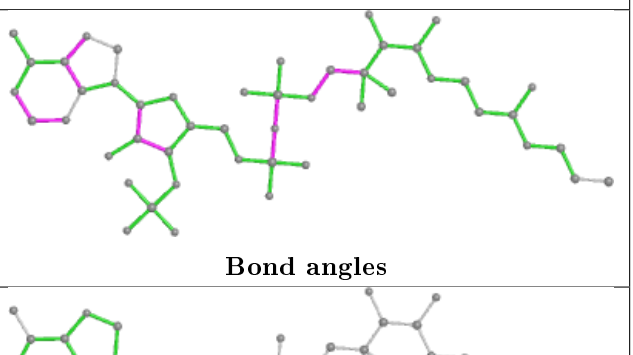


Rings

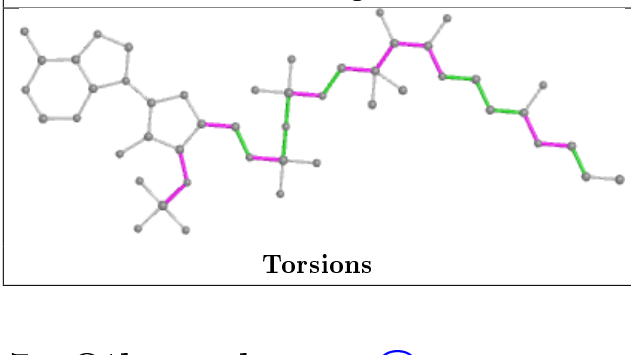
Ligand COA B 1730



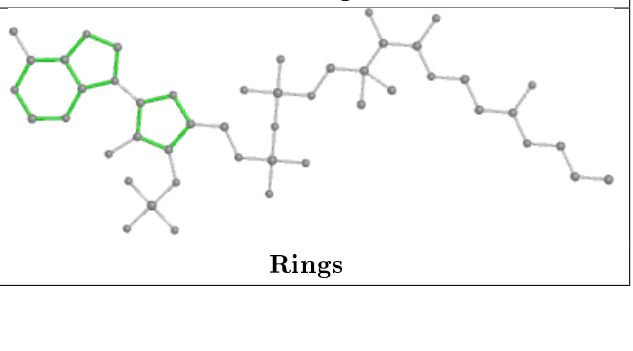
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.18	15 (2%)	63	66	19, 39, 62, 99	0
1	B	726/736 (98%)	-0.22	16 (2%)	62	65	19, 34, 64, 99	0
2	C	402/403 (99%)	-0.14	7 (1%)	70	72	19, 29, 57, 96	0
2	D	400/403 (99%)	-0.09	10 (2%)	57	61	20, 31, 65, 98	0
All	All	2257/2278 (99%)	-0.17	48 (2%)	63	66	19, 35, 63, 99	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	230	ALA	5.5
2	D	231	LEU	4.8
1	A	-6	HIS	4.0
2	C	229	ALA	4.0
2	D	1	MET	3.7
1	B	-8	HIS	3.6
2	D	296	PRO	3.6
1	A	378	ARG	3.5
2	D	298	ILE	3.4
1	B	377	GLU	3.3
2	C	227	GLY	3.2
1	B	720	SER	3.1
2	C	45	ASP	3.1
1	A	377	GLU	3.1
1	A	384	GLU	3.0
1	A	454	ARG	3.0
1	B	575	GLY	2.9
2	D	303	PRO	2.8
1	A	382	THR	2.8
1	A	720	SER	2.8
1	B	573	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	576	GLY	2.7
2	C	225	PHE	2.7
1	A	3	ASP	2.7
1	A	575	GLY	2.7
1	A	609	ASP	2.6
1	A	624	LYS	2.6
1	B	384	GLU	2.4
1	B	566	ALA	2.4
1	B	-14	GLY	2.4
2	D	45	ASP	2.4
1	A	1	MET	2.4
1	A	383	GLN	2.4
2	D	301	THR	2.3
1	B	574	ALA	2.3
2	C	294	ALA	2.3
2	C	220	LYS	2.2
1	A	-13	SER	2.2
1	B	319	GLY	2.2
2	D	230	ALA	2.2
1	A	432	PRO	2.2
1	B	577	THR	2.1
1	B	379	GLY	2.1
2	D	297	VAL	2.1
1	B	382	THR	2.1
1	B	609	ASP	2.0
1	B	613	SER	2.0
2	D	134[A]	MET	2.0

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

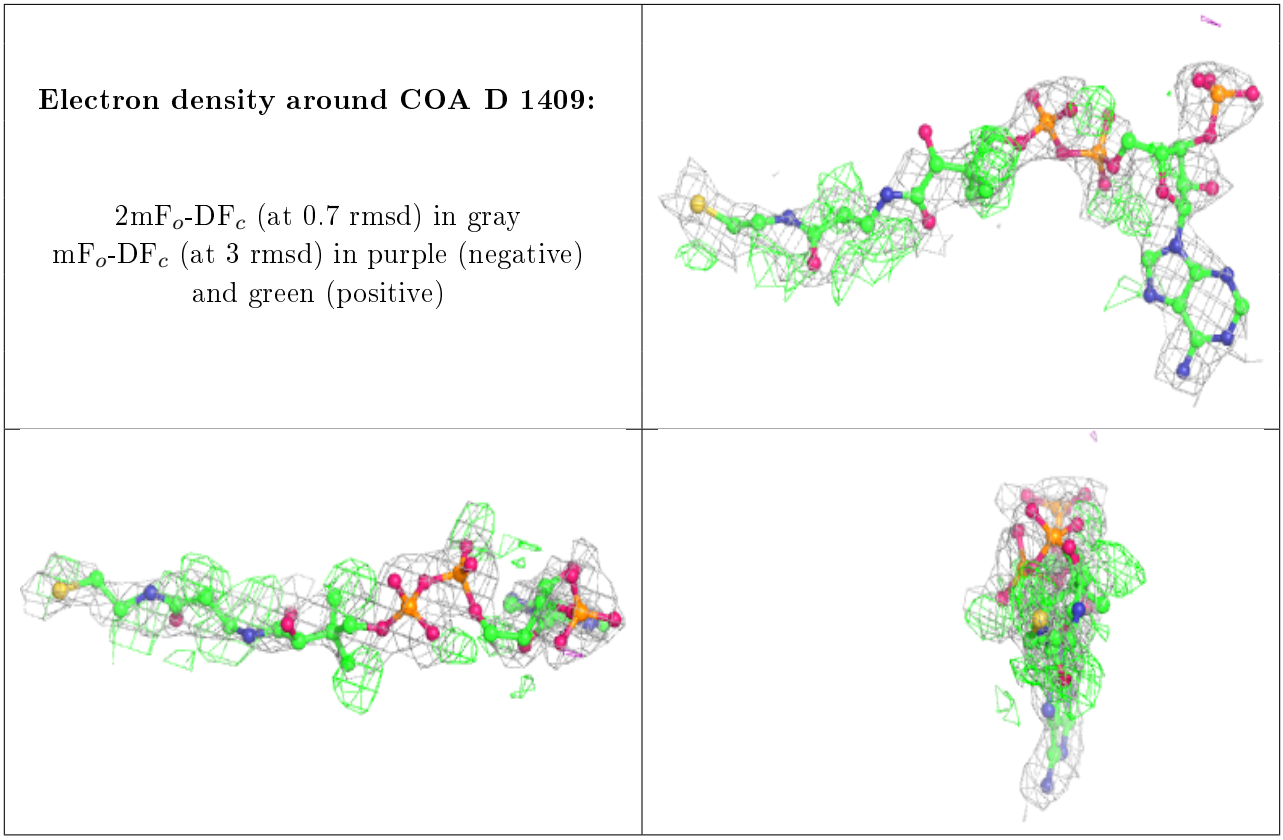
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	COA	D	1409	48/48	0.69	0.36	40,44,46,49	48
6	ADP	D	1410	27/27	0.73	0.30	60,92,132,135	0
3	SO4	B	1726	5/5	0.77	0.32	65,65,66,67	5
6	ADP	C	1413	27/27	0.81	0.24	48,80,133,138	0
5	COA	B	1730	48/48	0.83	0.30	41,50,57,57	48
4	GOL	D	1411	6/6	0.84	0.33	37,37,39,40	0
3	SO4	A	1724	5/5	0.84	0.23	65,65,68,68	5
5	COA	C	1412	48/48	0.84	0.25	32,38,46,51	48
3	SO4	B	1727	5/5	0.86	0.30	63,64,66,67	5
4	GOL	A	1728	6/6	0.87	0.22	50,55,55,56	0
3	SO4	B	1725	5/5	0.87	0.20	51,51,52,53	5
5	COA	A	1731	48/48	0.87	0.24	37,45,53,62	48
4	GOL	C	1411	6/6	0.90	0.28	50,53,54,55	0
3	SO4	D	1408	5/5	0.90	0.12	80,81,84,84	5
4	GOL	A	1727	6/6	0.90	0.24	48,52,53,55	0
3	SO4	C	1410	5/5	0.90	0.18	65,67,70,73	0
3	SO4	B	1728	5/5	0.91	0.18	40,40,42,42	5
4	GOL	B	1729	6/6	0.91	0.20	41,46,47,48	0
3	SO4	B	1724	5/5	0.91	0.27	65,66,67,68	5
3	SO4	A	1726	5/5	0.91	0.36	62,62,64,64	5
3	SO4	C	1408	5/5	0.92	0.34	51,54,55,55	5
3	SO4	C	1406	5/5	0.92	0.20	73,73,75,77	0
3	SO4	C	1409	5/5	0.93	0.32	39,40,41,41	5
4	GOL	A	1730	6/6	0.94	0.17	23,23,24,24	6
3	SO4	A	1723	5/5	0.95	0.20	76,76,78,78	0
3	SO4	A	1725	5/5	0.95	0.12	73,74,78,79	0
3	SO4	D	1404	5/5	0.95	0.10	59,61,65,65	0
3	SO4	B	1722	5/5	0.96	0.12	54,57,59,59	0
4	GOL	A	1729	6/6	0.96	0.21	49,51,54,56	0
3	SO4	C	1407	5/5	0.97	0.25	72,72,74,74	0
3	SO4	D	1405	5/5	0.97	0.27	63,66,67,69	0
3	SO4	B	1723	5/5	0.97	0.10	62,63,66,66	0
3	SO4	A	1722	5/5	0.97	0.12	48,49,50,51	0
3	SO4	D	1406	5/5	0.97	0.27	63,65,66,66	0
3	SO4	B	1721	5/5	0.98	0.10	39,40,40,41	0
3	SO4	A	1721	5/5	0.98	0.13	44,46,47,47	0
3	SO4	C	1405	5/5	0.98	0.25	57,58,59,60	0
3	SO4	C	1404	5/5	0.98	0.11	46,47,50,50	0
3	SO4	D	1407	5/5	0.99	0.24	62,63,64,64	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

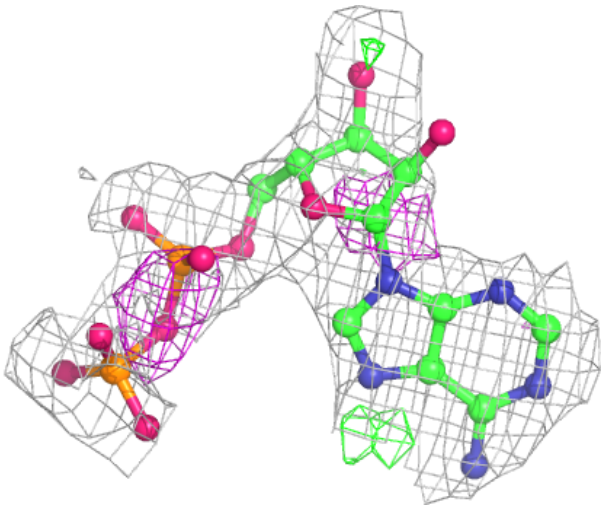
Electron density around COA D 1409:

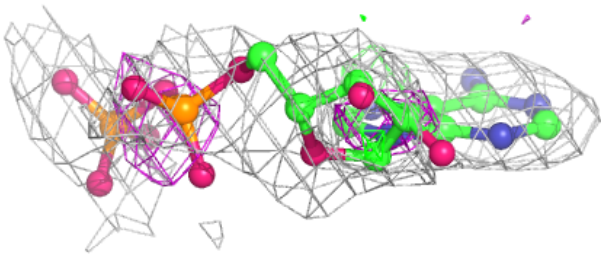
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

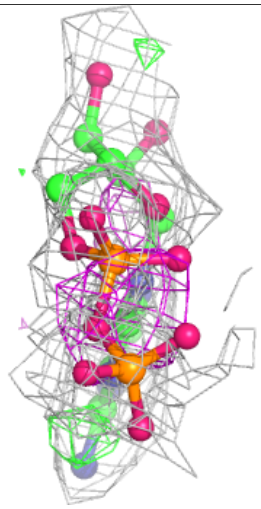


Electron density around ADP D 1410:

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

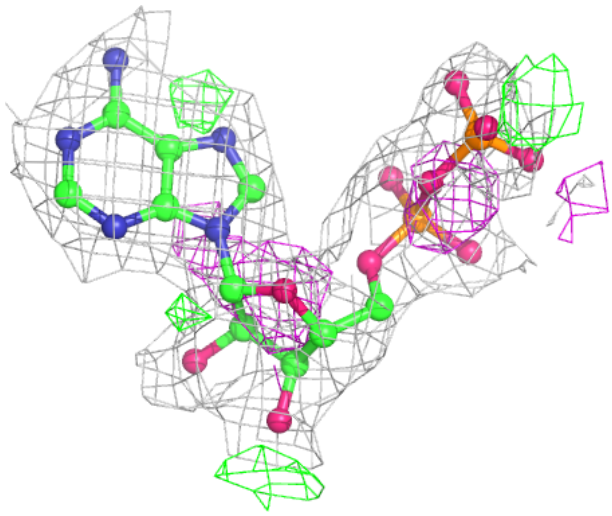


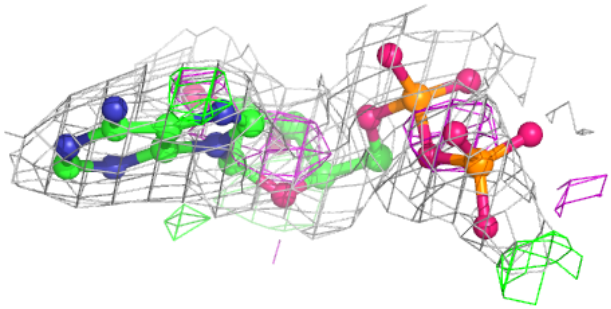


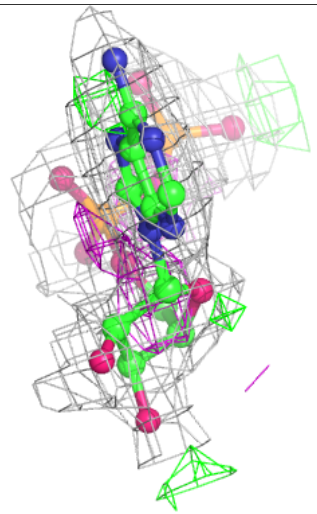


Electron density around ADP C 1413:

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

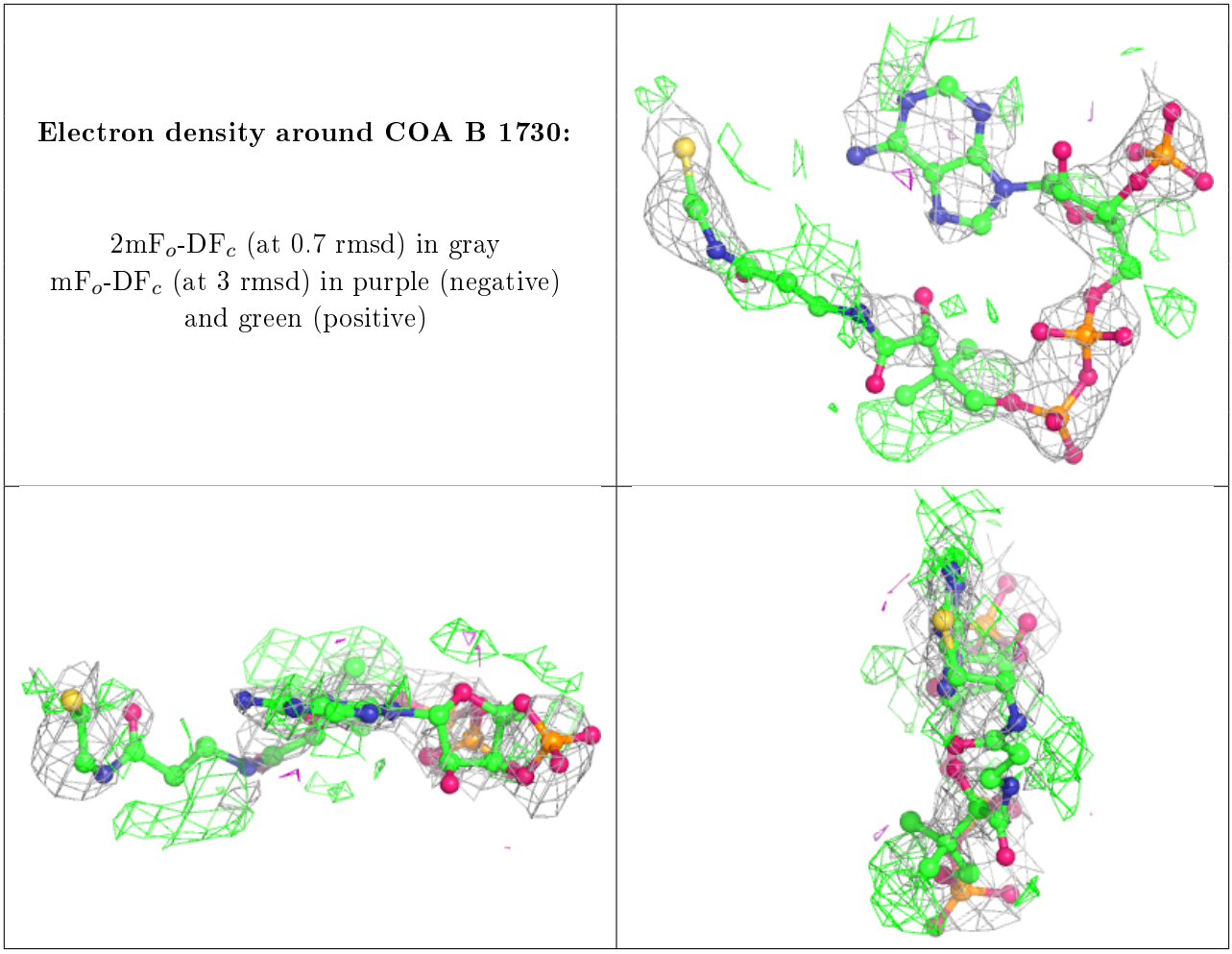






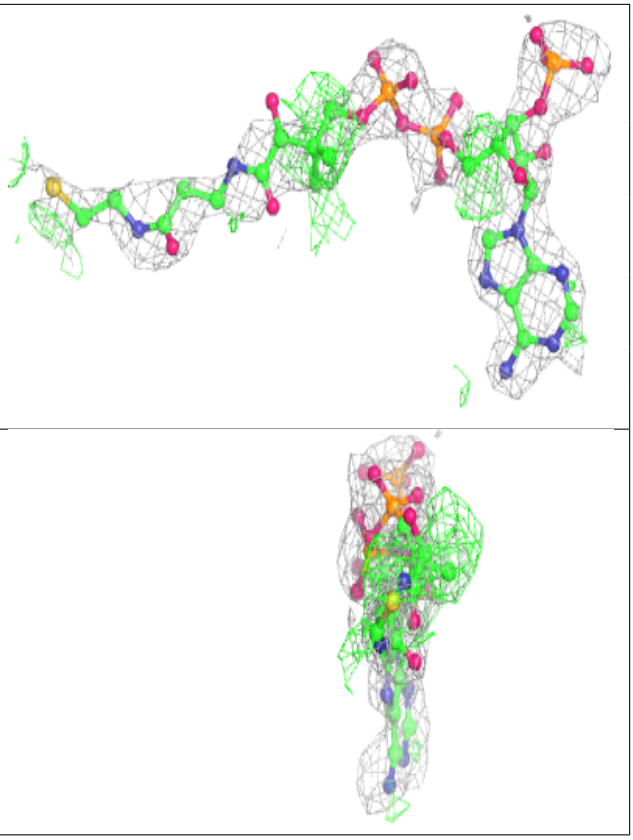
Electron density around COA B 1730:

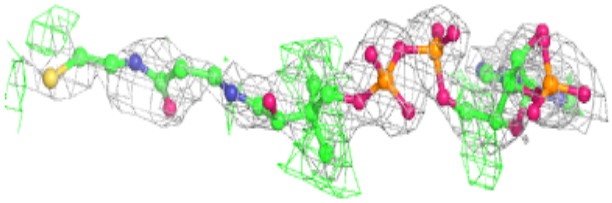
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around COA C 1412:

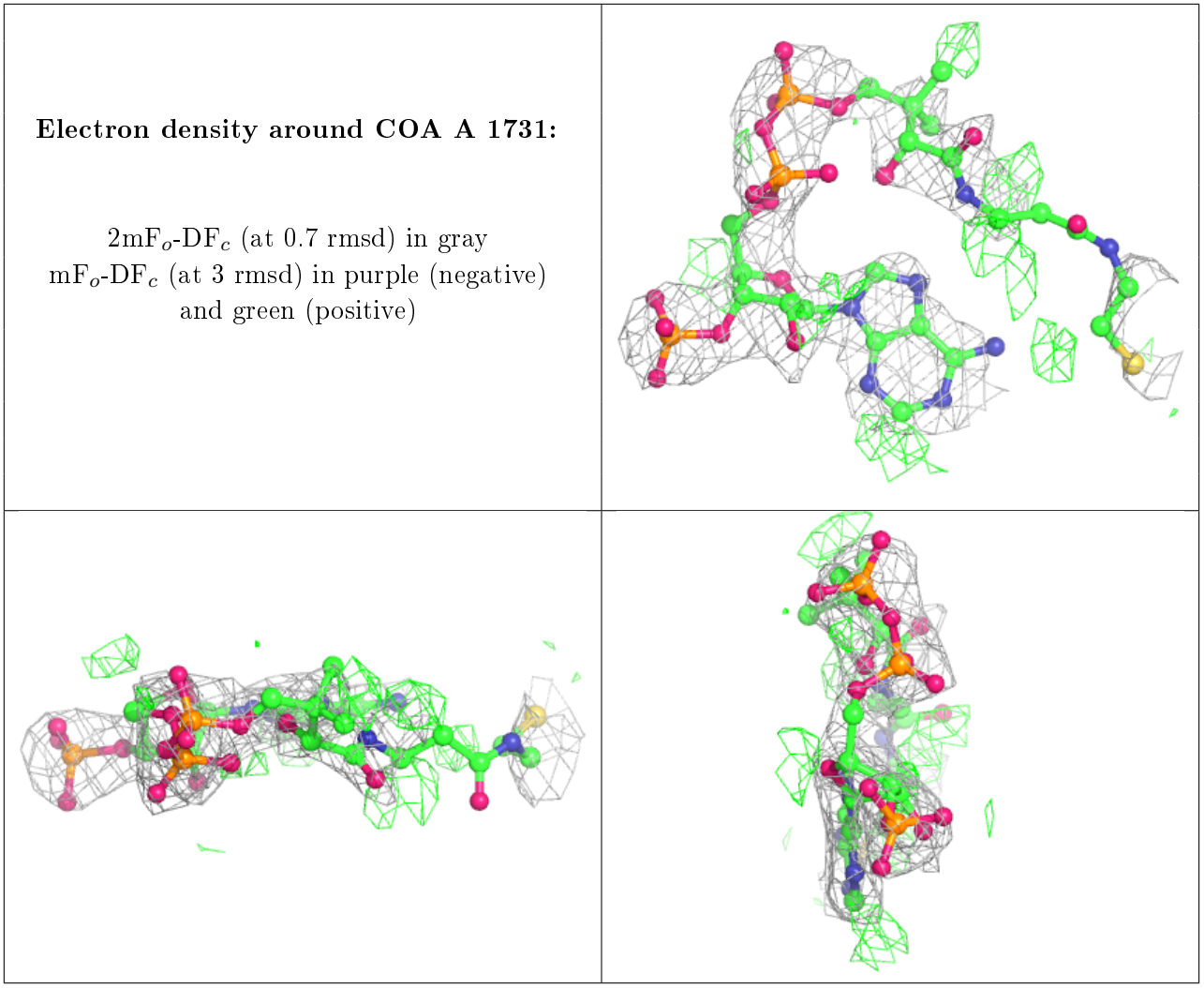
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around COA A 1731:

$2mF_o$-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.