Full wwPDB X-ray Structure Validation Report ⓘ

May 1, 2024 – 12:27 am BST

PDB ID	:	4B3I
Title	:	Crystal structure of Mycobacterium tuberculosis fatty acid beta- oxidation complex with CoenzymeA bound at the hydratase active sites
Authors	:	Venkatesan, R.; Wierenga, R.K.
Deposited on	:	2012-07-24
Resolution	:	2.63 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:

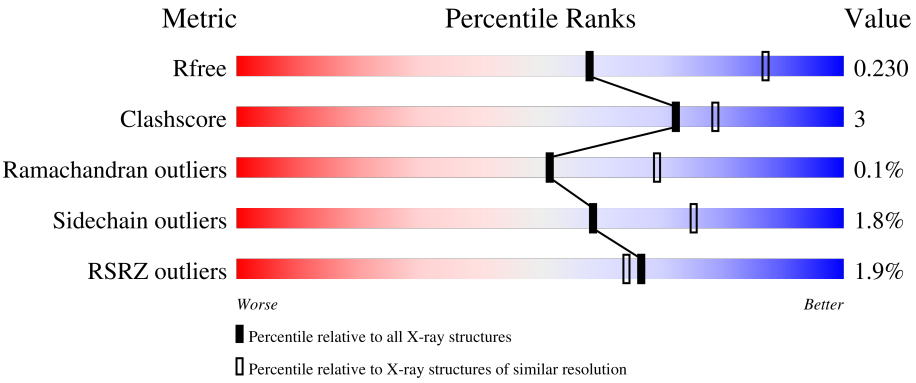
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 <=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	90% 9%
1	B	736	3% 91% 7%
2	C	403	2% 92% 7%
2	D	403	2% 92% 8%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17910 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	731	Total	C	N	O	S	0	5	0
			5454	3453	940	1040	21			
1	B	728	Total	C	N	O	S	0	6	0
			5405	3423	925	1037	20			

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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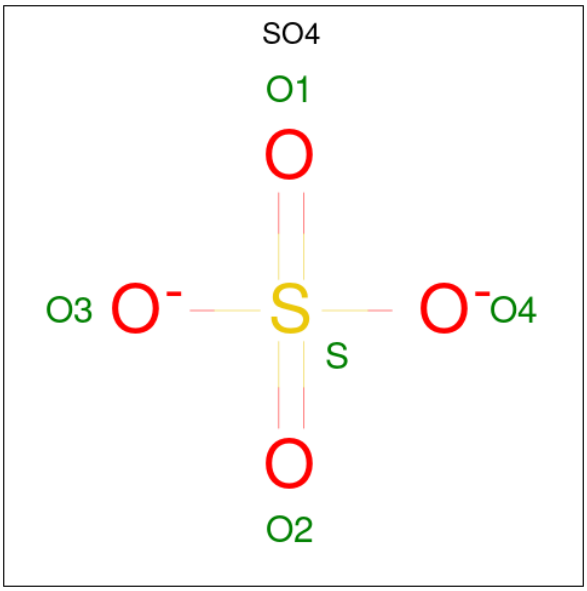
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP O53872
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression tag	UNP O53872
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	3	0
			2976	1859	529	573	15			
2	D	403	Total	C	N	O	S	0	2	0
			2968	1854	525	574	15			

- 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	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	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	C	1	Total O S 5 4 1	0	0

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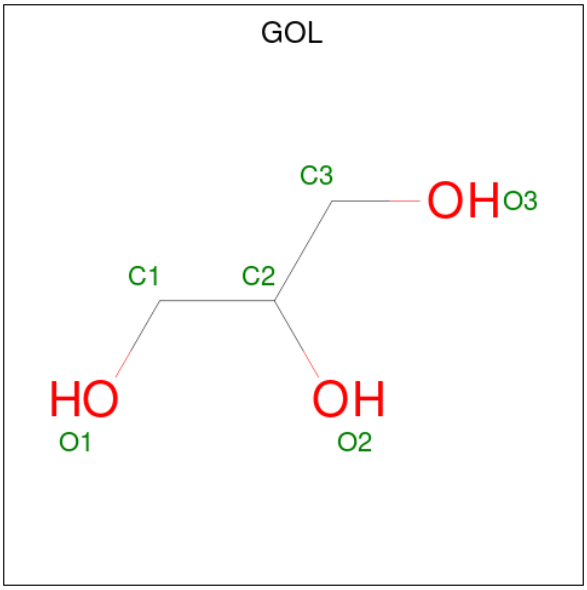
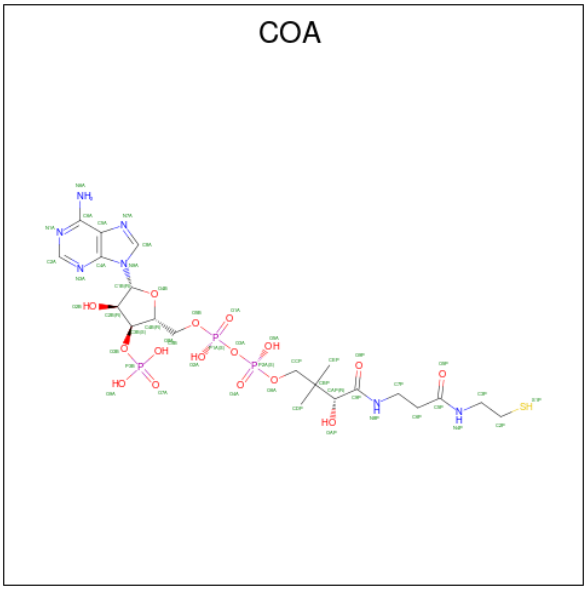
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

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



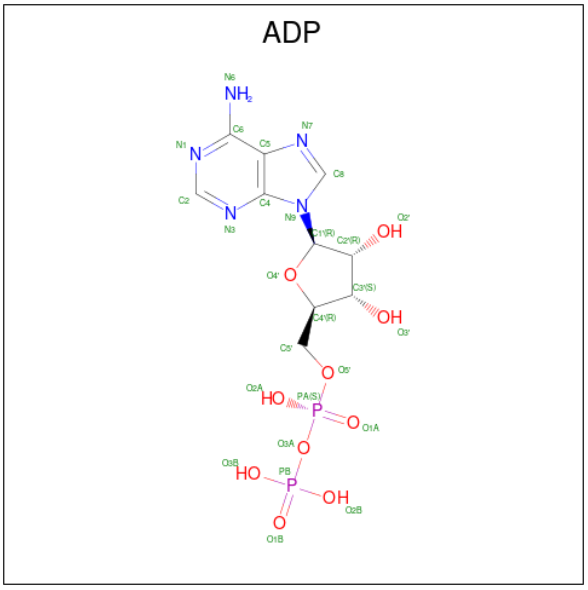
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- 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		

- 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	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is water.

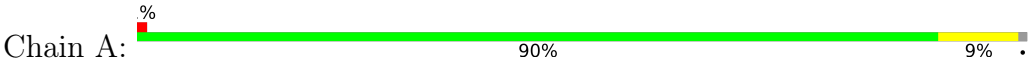
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	235	Total	O	0	0
			235	235		
7	B	254	Total	O	0	0
			254	254		
7	C	168	Total	O	0	0
			168	168		
7	D	122	Total	O	0	0
			122	122		

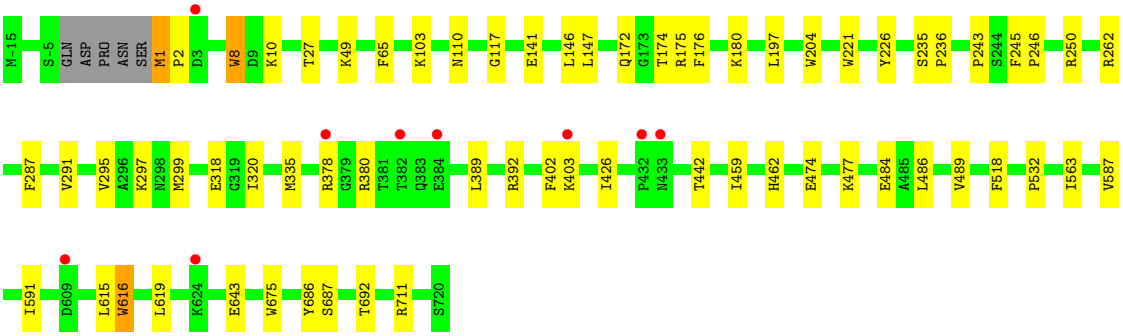
3 Residue-property plots (i)

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: FATTY ACID BETA-OXIDATION COMPLEX ALPHA-CHAIN FADB

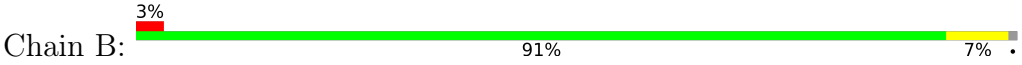
Chain A:





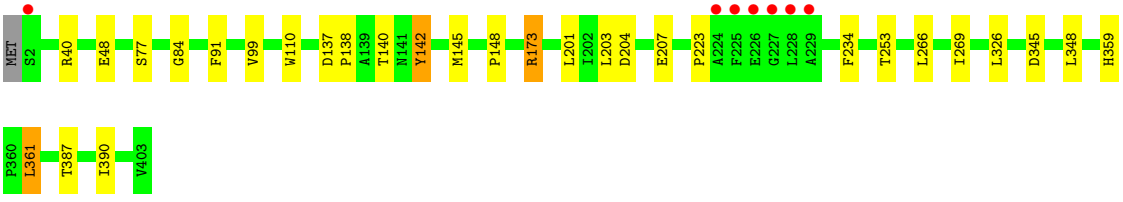
• Molecule 1: FATTY ACID BETA-OXIDATION COMPLEX ALPHA-CHAIN FADB

Chain B:



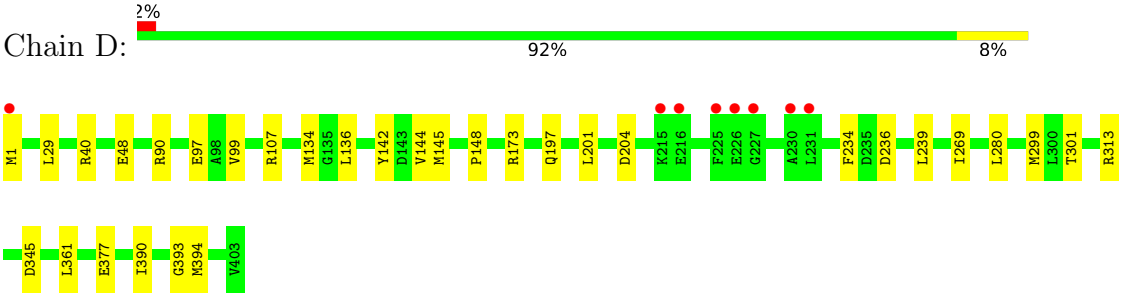
• Molecule 2: FATTY ACID BETA-OXIDATION COMPLEX BETA-CHAIN FADA

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	248.16Å 135.97Å 118.16Å 90.00° 110.43° 90.00°	Depositor
Resolution (Å)	50.00 – 2.63 49.68 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.63) 100.0 (49.68-2.63)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.229 0.187 , 0.230	Depositor DCC
R_{free} test set	5447 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17910	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, ADP, SO4, GOL

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	0.40	3/5574 (0.1%)	0.51	0/7547
1	B	0.41	2/5527 (0.0%)	0.51	0/7490
2	C	0.40	0/3030	0.55	0/4103
2	D	0.40	0/3019	0.54	0/4092
All	All	0.40	5/17150 (0.0%)	0.52	0/23232

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	221	TRP	CD2-CE2	5.23	1.47	1.41
1	A	675	TRP	CD2-CE2	5.16	1.47	1.41
1	A	616	TRP	CD2-CE2	5.05	1.47	1.41
1	B	204	TRP	CD2-CE2	5.03	1.47	1.41
1	A	204	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5454	0	5477	40	0
1	B	5405	0	5399	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2976	0	2996	25	0
2	D	2968	0	2975	25	0
3	A	35	0	0	0	0
3	B	45	0	0	0	0
3	C	50	0	0	0	0
3	D	30	0	0	0	0
4	A	12	0	16	2	0
4	B	6	0	8	0	0
5	A	48	0	32	0	0
5	B	48	0	32	0	0
6	A	27	0	12	0	0
6	C	27	0	12	0	0
7	A	235	0	0	3	0
7	B	254	0	0	3	0
7	C	168	0	0	0	0
7	D	122	0	0	1	0
All	All	17910	0	16959	116	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 (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262[A]:ARG:NE	2:C:142[A]:TYR:CE2	1.98	1.29
1:A:262[B]:ARG:HG3	1:A:262[B]:ARG:HH11	1.06	1.12
1:B:262[A]:ARG:HD3	2:C:142[A]:TYR:CD2	1.86	1.10
7:B:2147:HOH:O	2:D:197[A]:GLN:NE2	1.89	1.01
1:A:262[B]:ARG:HH11	1:A:262[B]:ARG:CG	1.73	0.99
1:B:262[A]:ARG:CD	2:C:142[A]:TYR:CD2	2.47	0.97
1:A:103:LYS:HE3	7:A:2018:HOH:O	1.66	0.93
1:A:262[B]:ARG:HG3	1:A:262[B]:ARG:NH1	1.80	0.90
1:B:262[A]:ARG:NE	2:C:142[A]:TYR:CD2	2.42	0.87
7:B:2147:HOH:O	2:D:197[A]:GLN:CD	2.15	0.80
2:D:90:ARG:HD3	2:D:394:MET:HE2	1.65	0.76
1:B:27:THR:HG21	1:B:66:ALA:HB3	1.67	0.75
1:B:84:VAL:HG11	1:B:291:VAL:HG11	1.68	0.74
7:B:2147:HOH:O	2:D:197[A]:GLN:OE1	2.05	0.72
2:C:84:GLY:HA2	2:D:394:MET:HE3	1.73	0.70
2:D:90:ARG:HH11	2:D:394:MET:HE1	1.57	0.70
2:D:40:ARG:HD2	2:D:48:GLU:OE2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLN:HG3	1:B:448:LEU:HD23	1.77	0.67
1:B:563:ILE:HA	1:B:566:ALA:HB3	1.77	0.66
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.77	0.65
2:C:110:TRP:HD1	2:D:313:ARG:HD3	1.62	0.64
2:C:173:ARG:NH2	2:C:348:LEU:O	2.30	0.64
1:A:287:PHE:CE2	1:A:291:VAL:HG21	2.33	0.64
1:B:262[A]:ARG:HD3	2:C:142[A]:TYR:CG	2.33	0.63
1:B:559:LEU:O	1:B:563:ILE:HG23	1.99	0.63
1:A:711:ARG:HB3	4:A:1728:GOL:H2	1.80	0.63
1:A:262[B]:ARG:CG	1:A:262[B]:ARG:NH1	2.45	0.62
2:D:197[B]:GLN:OE1	7:D:2074:HOH:O	0.62	0.62
1:A:389:LEU:HA	1:A:392:ARG:NH1	2.15	0.61
1:A:297:LYS:HE3	7:A:2132:HOH:O	2.02	0.59
1:B:27:THR:CG2	1:B:66:ALA:HB3	2.32	0.58
2:C:40:ARG:NH2	2:C:77:SER:O	2.32	0.58
1:B:262[A]:ARG:CD	2:C:142[A]:TYR:CE2	2.80	0.58
1:B:8[A]:TRP:CZ3	1:B:10:LYS:HB2	2.40	0.57
1:A:65:PHE:HB3	1:A:117:GLY:HA2	1.87	0.56
1:B:262[A]:ARG:CZ	2:C:142[A]:TYR:CE2	2.86	0.54
1:A:711:ARG:HH11	4:A:1728:GOL:H12	1.73	0.54
1:B:162:ILE:HD12	1:B:238:LEU:HD21	1.89	0.54
2:C:110:TRP:CH2	2:D:107:ARG:HD2	2.43	0.53
2:D:90:ARG:HH11	2:D:394:MET:CE	2.20	0.53
1:A:146:LEU:HD22	1:A:291:VAL:HG22	1.91	0.53
1:A:402:PHE:CD2	1:A:426:ILE:HG12	2.44	0.53
1:B:616:TRP:O	1:B:619:LEU:HB2	2.09	0.53
1:B:65:PHE:HB3	1:B:117:GLY:HA2	1.90	0.53
2:C:203:LEU:HD11	2:C:207:GLU:HG3	1.91	0.52
2:D:201:LEU:HD11	2:D:204:ASP:HB3	1.92	0.52
1:B:552:SER:O	1:B:555:LEU:O	2.28	0.51
1:A:141:GLU:HG3	1:A:147:LEU:C	2.31	0.51
2:C:201:LEU:HD11	2:C:204:ASP:HB3	1.93	0.51
1:B:515:ILE:HD11	1:B:551:LEU:HD21	1.94	0.50
1:B:336:MET:SD	1:B:465:SER:HB3	2.52	0.50
2:D:134:MET:HB2	2:D:144:VAL:HG21	1.94	0.50
1:A:243:PRO:HG3	2:D:136:LEU:HD23	1.94	0.49
1:A:686:TYR:O	1:A:692:THR:HA	2.12	0.49
1:A:8[A]:TRP:CZ3	1:A:10:LYS:HB2	2.47	0.49
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.94	0.49
1:B:84:VAL:HG11	1:B:291:VAL:CG1	2.39	0.49
1:B:262[A]:ARG:NE	2:C:142[A]:TYR:HE2	1.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8[A]:TRP:HZ3	1:A:10:LYS:HB2	1.78	0.48
1:A:65:PHE:HB3	1:A:117:GLY:CA	2.43	0.48
1:B:325:ILE:HB	1:B:349:TYR:CE1	2.49	0.47
1:B:327:ARG:HB3	1:B:404:GLY:O	2.15	0.47
2:D:148:PRO:HD3	2:D:234:PHE:CD1	2.50	0.47
2:C:140:THR:HG21	2:D:29:LEU:HD23	1.96	0.46
1:A:442:THR:HG21	1:A:563:ILE:HG12	1.98	0.46
1:A:245:PHE:HB2	1:A:246:PRO:HD3	1.98	0.46
1:B:8[A]:TRP:HZ3	1:B:10:LYS:HB2	1.79	0.46
1:B:250:ARG:NH1	2:C:145:MET:HG2	2.31	0.46
1:A:221:TRP:HA	1:A:226:TYR:CD1	2.50	0.46
1:B:27:THR:HG21	1:B:66:ALA:CB	2.42	0.45
2:C:223:PRO:HA	2:C:253:THR:HG22	1.98	0.45
1:A:295:VAL:HG12	1:A:299:MET:HE3	1.98	0.45
1:A:518:PHE:HB2	1:A:643:GLU:CD	2.37	0.45
1:B:442:THR:HG21	1:B:563:ILE:CG2	2.46	0.45
1:B:656:LEU:HD13	1:B:662:ALA:HB2	1.98	0.45
2:D:390:ILE:HB	2:D:394:MET:HB2	1.97	0.45
1:A:459:ILE:HG21	1:A:489:VAL:HG21	1.99	0.44
1:A:587:VAL:O	1:A:591:ILE:HG12	2.17	0.44
1:A:378:ARG:HH21	1:A:380:ARG:NH2	2.15	0.44
7:A:2110:HOH:O	2:D:142[B]:TYR:CZ	2.68	0.44
2:C:40:ARG:HD3	2:C:48:GLU:OE2	2.18	0.44
2:D:299:MET:O	2:D:393:GLY:HA2	2.17	0.44
2:D:301:THR:HG22	2:D:301:THR:O	2.18	0.44
1:A:616:TRP:O	1:A:619:LEU:HB2	2.17	0.44
1:A:250:ARG:HD2	2:D:142[B]:TYR:CE2	2.53	0.44
1:B:510:PHE:CD1	1:B:656:LEU:HD11	2.53	0.44
2:C:91:PHE:HB2	2:C:390:ILE:HG23	2.00	0.44
1:A:378:ARG:HH21	1:A:380:ARG:HH22	1.65	0.43
2:D:1:MET:HA	2:D:107:ARG:HH21	1.82	0.43
1:A:235:SER:HA	1:A:236:PRO:HD3	1.90	0.43
1:B:65:PHE:HB3	1:B:117:GLY:CA	2.49	0.43
1:B:518:PHE:HB2	1:B:643:GLU:CD	2.39	0.43
1:B:560:MET:HA	1:B:563:ILE:HG12	1.99	0.43
2:D:90:ARG:HH21	2:D:97:GLU:CD	2.21	0.43
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.99	0.43
1:A:287:PHE:O	1:A:291:VAL:HG23	2.19	0.43
1:A:616:TRP:HE3	1:A:619:LEU:HD13	1.83	0.43
1:B:470:MET:HA	1:B:471:PRO:HD3	1.79	0.43
2:C:326:LEU:HD13	2:C:387:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:99:VAL:HG13	2:C:269:ILE:HD11	2.01	0.42
2:C:359:HIS:CE1	2:C:361:LEU:HA	2.54	0.42
1:B:325:ILE:HB	1:B:349:TYR:HE1	1.83	0.42
1:A:532:PRO:HB2	1:A:615:LEU:HD13	2.02	0.42
1:A:1:MET:HA	1:A:2:PRO:HD3	1.94	0.42
2:D:1:MET:HA	2:D:107:ARG:NH2	2.34	0.42
2:C:148:PRO:HD3	2:C:234:PHE:CD1	2.55	0.41
1:A:320:ILE:HG21	1:A:484:GLU:HA	2.01	0.41
1:A:176:PHE:CD1	1:A:180:LYS:HD2	2.56	0.41
1:A:477:LYS:HB2	1:A:486:LEU:HD21	2.02	0.41
1:B:104:PRO:HG2	1:B:205:ILE:HG23	2.02	0.41
1:B:563:ILE:HA	1:B:566:ALA:CB	2.49	0.41
1:A:110:ASN:HA	1:A:197:LEU:HD11	2.03	0.41
1:B:153:VAL:O	1:B:157:VAL:HG23	2.21	0.40
2:C:137:ASP:HA	2:C:138:PRO:HD3	1.95	0.40
1:B:288:ALA:HA	1:B:291:VAL:HG12	2.04	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	732/736 (100%)	708 (97%)	23 (3%)	1 (0%)	51	69
1	B	730/736 (99%)	710 (97%)	20 (3%)	0	100	100
2	C	403/403 (100%)	390 (97%)	12 (3%)	1 (0%)	47	64
2	D	403/403 (100%)	391 (97%)	11 (3%)	1 (0%)	47	64
All	All	2268/2278 (100%)	2199 (97%)	66 (3%)	3 (0%)	51	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	361	LEU
2	D	361	LEU
1	A	318	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	560/566 (99%)	549 (98%)	11 (2%)	55 72
1	B	553/566 (98%)	543 (98%)	10 (2%)	59 75
2	C	309/310 (100%)	304 (98%)	5 (2%)	62 78
2	D	307/310 (99%)	300 (98%)	7 (2%)	50 68
All	All	1729/1752 (99%)	1696 (98%)	33 (2%)	59 74

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8[A]	TRP
1	A	8[B]	TRP
1	A	27	THR
1	A	49	LYS
1	A	172	GLN
1	A	174	THR
1	A	175	ARG
1	A	335	MET
1	A	403	LYS
1	A	687	SER
1	B	-13	SER
1	B	8[A]	TRP
1	B	8[B]	TRP
1	B	172	GLN
1	B	174	THR
1	B	402	PHE
1	B	441	SER
1	B	443	LEU

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Mol	Chain	Res	Type
1	B	494	LEU
1	B	567	THR
2	C	142[A]	TYR
2	C	142[B]	TYR
2	C	173	ARG
2	C	266	LEU
2	C	345	ASP
2	D	145	MET
2	D	173	ARG
2	D	236	ASP
2	D	239	LEU
2	D	280	LEU
2	D	345	ASP
2	D	377	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	1725	-	4,4,4	0.30	0	6,6,6	0.25	0
3	SO4	C	1409	-	4,4,4	0.34	0	6,6,6	0.13	0
3	SO4	A	1721	-	4,4,4	0.34	0	6,6,6	0.17	0
3	SO4	C	1405	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	D	1408	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	D	1405	-	4,4,4	0.34	0	6,6,6	0.12	0
5	COA	A	1730	-	41,50,50	0.86	2 (4%)	52,75,75	1.08	4 (7%)
3	SO4	B	1722	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	B	1726	-	4,4,4	0.34	0	6,6,6	0.12	0
3	SO4	A	1724	-	4,4,4	0.35	0	6,6,6	0.16	0
3	SO4	C	1410	-	4,4,4	0.31	0	6,6,6	0.18	0
3	SO4	A	1727	-	4,4,4	0.31	0	6,6,6	0.12	0
3	SO4	C	1404	-	4,4,4	0.29	0	6,6,6	0.29	0
3	SO4	B	1724	-	4,4,4	0.32	0	6,6,6	0.12	0
3	SO4	C	1407	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	D	1404	-	4,4,4	0.34	0	6,6,6	0.10	0
3	SO4	D	1409	-	4,4,4	0.34	0	6,6,6	0.09	0
4	GOL	A	1728	-	5,5,5	0.34	0	5,5,5	0.22	0
3	SO4	D	1406	-	4,4,4	0.34	0	6,6,6	0.14	0
6	ADP	C	1414	-	24,29,29	1.09	3 (12%)	29,45,45	1.35	3 (10%)
3	SO4	A	1722	-	4,4,4	0.37	0	6,6,6	0.13	0
3	SO4	C	1406	-	4,4,4	0.32	0	6,6,6	0.11	0
3	SO4	B	1723	-	4,4,4	0.34	0	6,6,6	0.09	0
3	SO4	A	1726	-	4,4,4	0.34	0	6,6,6	0.13	0
3	SO4	C	1413	-	4,4,4	0.36	0	6,6,6	0.10	0
3	SO4	C	1408	-	4,4,4	0.33	0	6,6,6	0.12	0
3	SO4	C	1412	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	D	1407	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	C	1411	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	B	1727	-	4,4,4	0.35	0	6,6,6	0.09	0
5	COA	B	1731	-	41,50,50	0.87	3 (7%)	52,75,75	1.13	5 (9%)
6	ADP	A	1731	-	24,29,29	1.01	2 (8%)	29,45,45	1.38	4 (13%)
3	SO4	B	1729	-	4,4,4	0.34	0	6,6,6	0.14	0
3	SO4	B	1721	-	4,4,4	0.33	0	6,6,6	0.18	0
3	SO4	A	1725	-	4,4,4	0.34	0	6,6,6	0.18	0
3	SO4	A	1723	-	4,4,4	0.33	0	6,6,6	0.14	0
4	GOL	B	1730	-	5,5,5	0.35	0	5,5,5	0.36	0
3	SO4	B	1728	-	4,4,4	0.35	0	6,6,6	0.15	0
4	GOL	A	1729	-	5,5,5	0.35	0	5,5,5	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	A	1731	-	-	5/12/32/32	0/3/3/3
4	GOL	A	1728	-	-	2/4/4/4	-
6	ADP	C	1414	-	-	2/12/32/32	0/3/3/3
4	GOL	B	1730	-	-	2/4/4/4	-
5	COA	A	1730	-	-	5/44/64/64	0/3/3/3
5	COA	B	1731	-	-	12/44/64/64	0/3/3/3
4	GOL	A	1729	-	-	4/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1414	ADP	C5-C4	2.84	1.48	1.40
5	B	1731	COA	C5A-C4A	2.66	1.48	1.40
5	A	1730	COA	C5A-C4A	2.63	1.47	1.40
6	A	1731	ADP	C5-C4	2.61	1.47	1.40
6	C	1414	ADP	C2-N3	2.24	1.35	1.32
5	A	1730	COA	O4B-C1B	2.22	1.44	1.41
6	C	1414	ADP	O4'-C1'	2.18	1.44	1.41
5	B	1731	COA	O4B-C1B	2.08	1.44	1.41
6	A	1731	ADP	C2-N3	2.04	1.35	1.32
5	B	1731	COA	C2A-N3A	2.01	1.35	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1731	COA	N3A-C2A-N1A	-3.75	122.82	128.68
6	A	1731	ADP	N3-C2-N1	-3.72	122.87	128.68
5	A	1730	COA	N3A-C2A-N1A	-3.57	123.10	128.68
6	C	1414	ADP	C3'-C2'-C1'	3.51	106.27	100.98
6	C	1414	ADP	N3-C2-N1	-3.34	123.45	128.68
5	A	1730	COA	P2A-O3A-P1A	-2.99	122.56	132.83
6	A	1731	ADP	C4-C5-N7	-2.77	106.51	109.40
6	A	1731	ADP	PA-O3A-PB	-2.76	123.34	132.83
5	B	1731	COA	C4A-C5A-N7A	-2.61	106.68	109.40
6	C	1414	ADP	C4-C5-N7	-2.59	106.70	109.40
5	B	1731	COA	CEP-CBP-CAP	2.58	113.30	108.82
5	B	1731	COA	P2A-O3A-P1A	-2.56	124.04	132.83
6	A	1731	ADP	C3'-C2'-C1'	2.50	104.74	100.98
5	A	1730	COA	C4A-C5A-N7A	-2.39	106.91	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1730	COA	C2A-N1A-C6A	2.08	122.31	118.75
5	B	1731	COA	C2A-N1A-C6A	2.04	122.25	118.75

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1729	GOL	O1-C1-C2-C3
4	A	1729	GOL	C1-C2-C3-O3
5	A	1730	COA	C6P-C5P-N4P-C3P
5	B	1731	COA	CCP-O6A-P2A-O4A
5	B	1731	COA	CCP-O6A-P2A-O5A
5	B	1731	COA	C9P-CAP-CBP-CCP
5	B	1731	COA	OAP-CAP-CBP-CDP
5	B	1731	COA	C9P-CAP-CBP-CDP
5	B	1731	COA	C9P-CAP-CBP-CEP
5	B	1731	COA	CAP-C9P-N8P-C7P
6	A	1731	ADP	C5'-O5'-PA-O3A
6	A	1731	ADP	C4'-C5'-O5'-PA
6	A	1731	ADP	C3'-C4'-C5'-O5'
5	A	1730	COA	O5P-C5P-N4P-C3P
5	B	1731	COA	O9P-C9P-N8P-C7P
4	B	1730	GOL	C1-C2-C3-O3
4	A	1729	GOL	O1-C1-C2-O2
4	A	1729	GOL	O2-C2-C3-O3
6	A	1731	ADP	O4'-C4'-C5'-O5'
6	C	1414	ADP	C3'-C4'-C5'-O5'
5	B	1731	COA	OAP-CAP-CBP-CEP
6	C	1414	ADP	O4'-C4'-C5'-O5'
4	B	1730	GOL	O2-C2-C3-O3
5	B	1731	COA	P1A-O3A-P2A-O6A
4	A	1728	GOL	C1-C2-C3-O3
6	A	1731	ADP	C5'-O5'-PA-O1A
5	B	1731	COA	OAP-CAP-CBP-CCP
5	A	1730	COA	C3B-O3B-P3B-O7A
5	A	1730	COA	C3B-O3B-P3B-O8A
5	A	1730	COA	C3B-O3B-P3B-O9A
5	B	1731	COA	CCP-O6A-P2A-O3A
4	A	1728	GOL	O2-C2-C3-O3

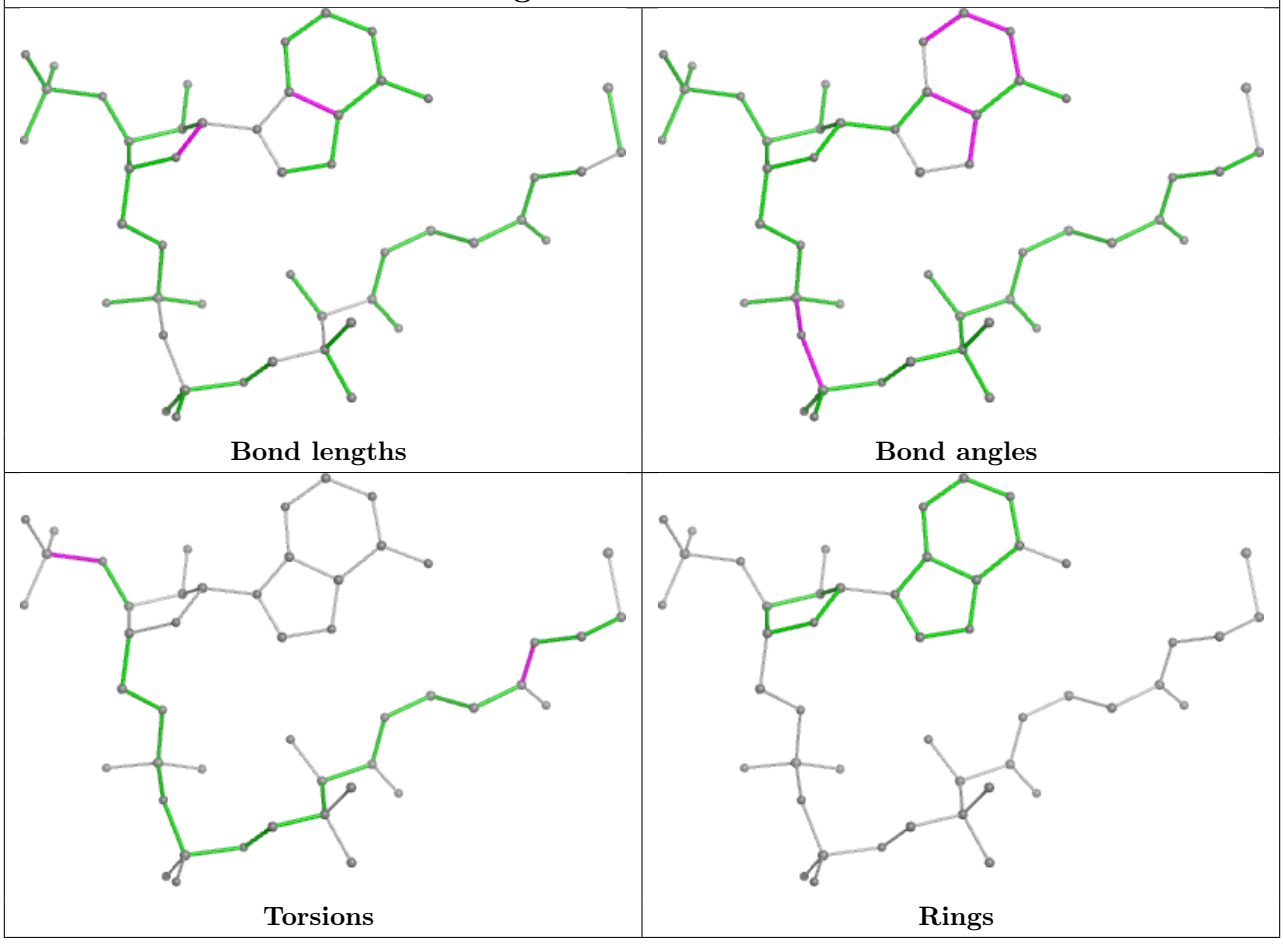
There are no ring outliers.

1 monomer is involved in 2 short contacts:

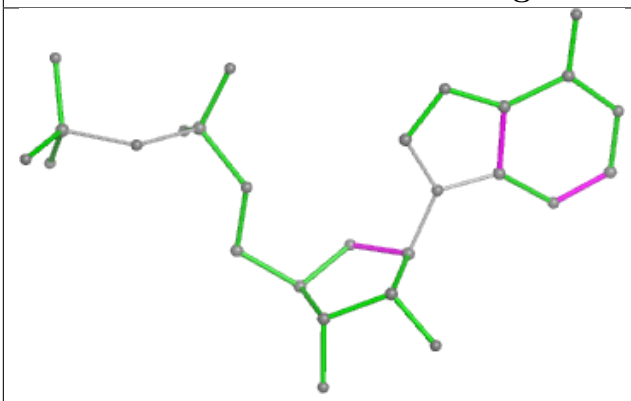
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1728	GOL	2	0

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.

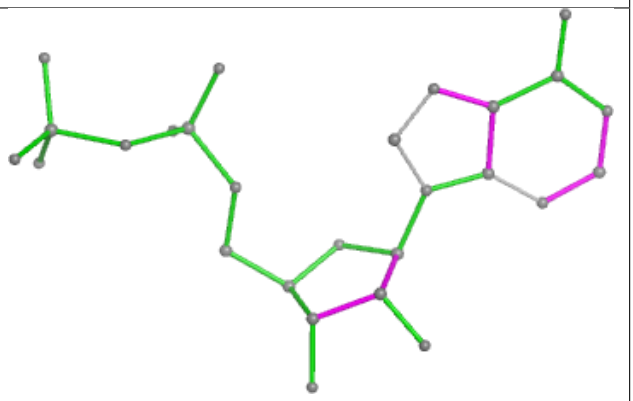
Ligand COA A 1730



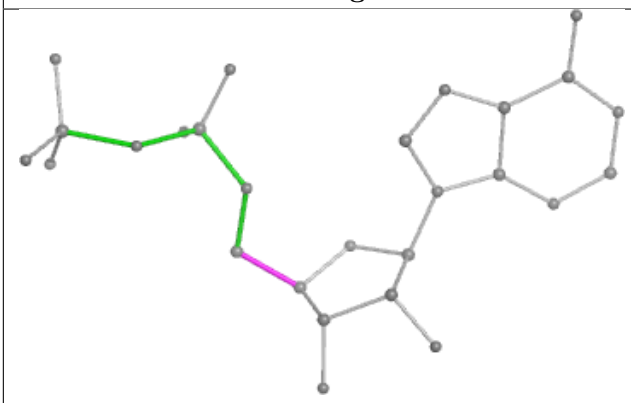
Ligand ADP C 1414



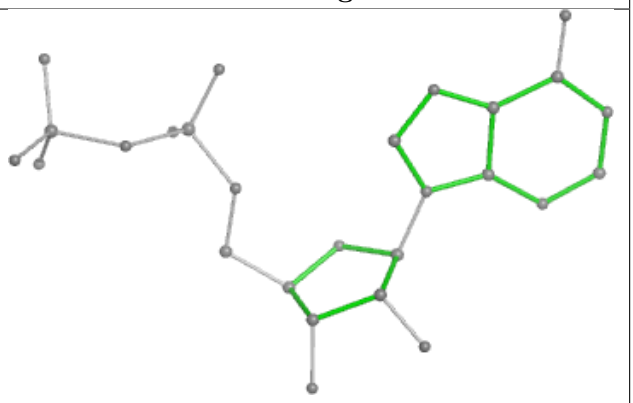
Bond lengths



Bond angles

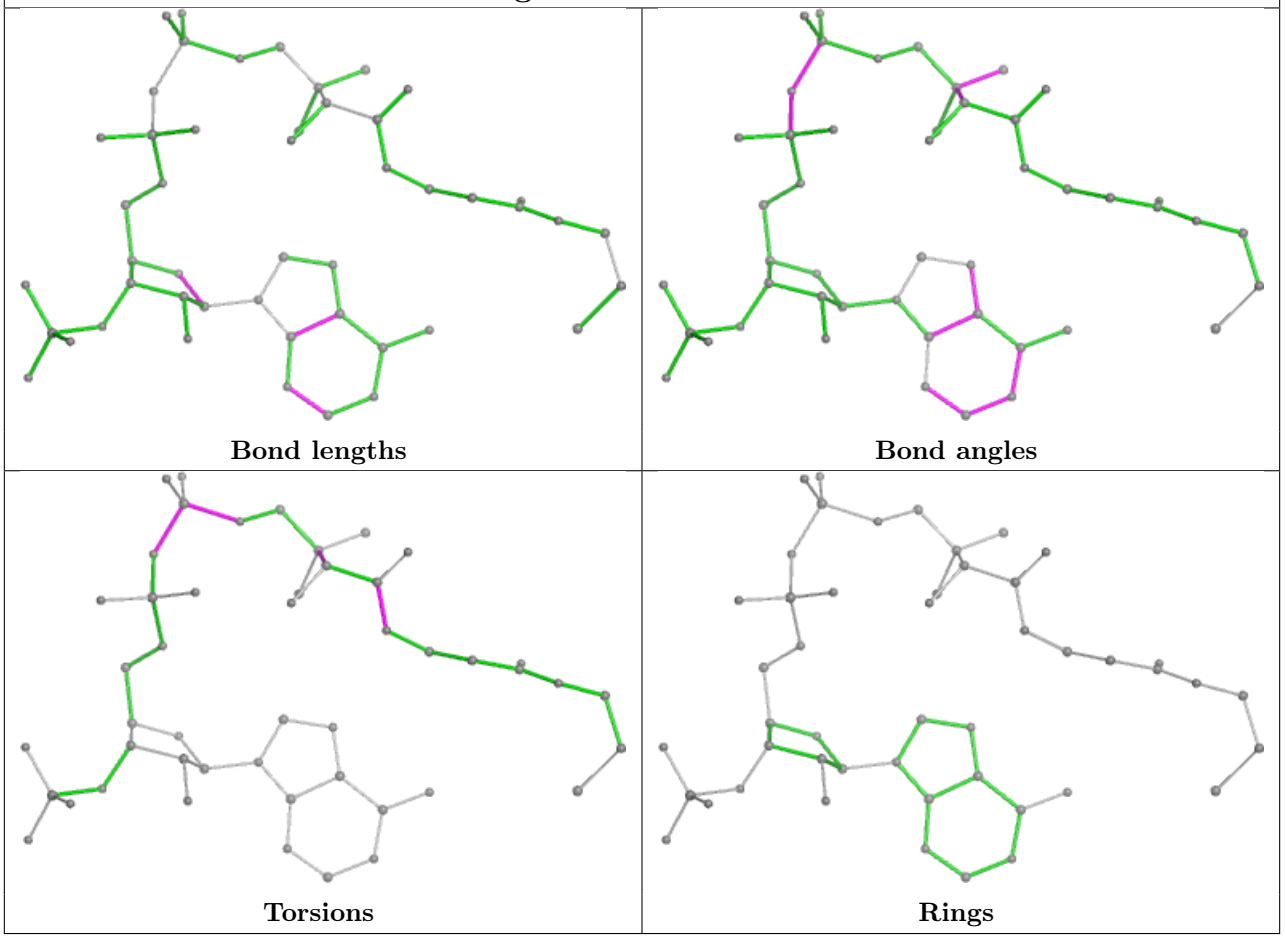


Torsions

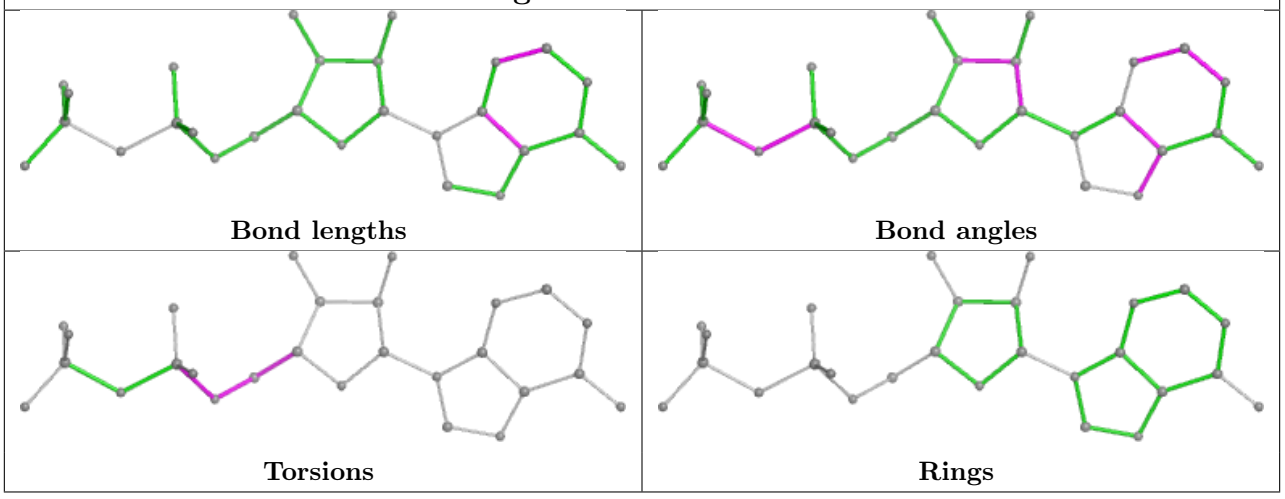


Rings

Ligand COA B 1731



Ligand ADP A 1731



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	731/736 (99%)	-0.30	9 (1%)	79	77	22, 40, 63, 90	0
1	B	728/736 (98%)	-0.22	20 (2%)	54	50	23, 38, 70, 115	0
2	C	402/403 (99%)	-0.29	7 (1%)	70	67	21, 29, 47, 102	0
2	D	403/403 (100%)	-0.28	8 (1%)	65	61	21, 34, 51, 84	0
All	All	2264/2278 (99%)	-0.27	44 (1%)	66	64	21, 36, 64, 115	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	226	GLU	5.3
1	B	573	ASP	5.3
2	D	225	PHE	4.5
2	C	229	ALA	4.4
1	B	566	ALA	4.4
1	B	381	THR	4.0
1	B	576	GLY	4.0
2	C	227	GLY	3.7
1	B	575	GLY	3.7
1	B	-14	GLY	3.6
1	B	574	ALA	3.5
1	B	377	GLU	3.4
1	B	382	THR	3.1
1	B	570	GLY	3.1
1	A	433	ASN	3.1
1	B	572	GLU	3.1
2	C	225	PHE	3.1
1	B	3	ASP	3.0
2	D	227	GLY	3.0
1	A	382	THR	3.0
1	B	571	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	379	GLY	2.9
1	A	3	ASP	2.9
2	C	228	LEU	2.9
2	D	1	MET	2.6
1	A	378	ARG	2.5
1	A	432	PRO	2.4
2	C	2	SER	2.4
1	B	609	ASP	2.4
2	C	224	ALA	2.4
1	B	569	LYS	2.4
1	B	383	GLN	2.3
1	B	380	ARG	2.2
1	A	609	ASP	2.2
2	D	230	ALA	2.2
1	A	403	LYS	2.2
1	B	384	GLU	2.2
1	B	373	ALA	2.2
1	A	624	LYS	2.1
1	A	384	GLU	2.1
2	D	216	GLU	2.1
2	D	226	GLU	2.1
2	D	215	LYS	2.0
2	D	231	LEU	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 monosaccharides 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.

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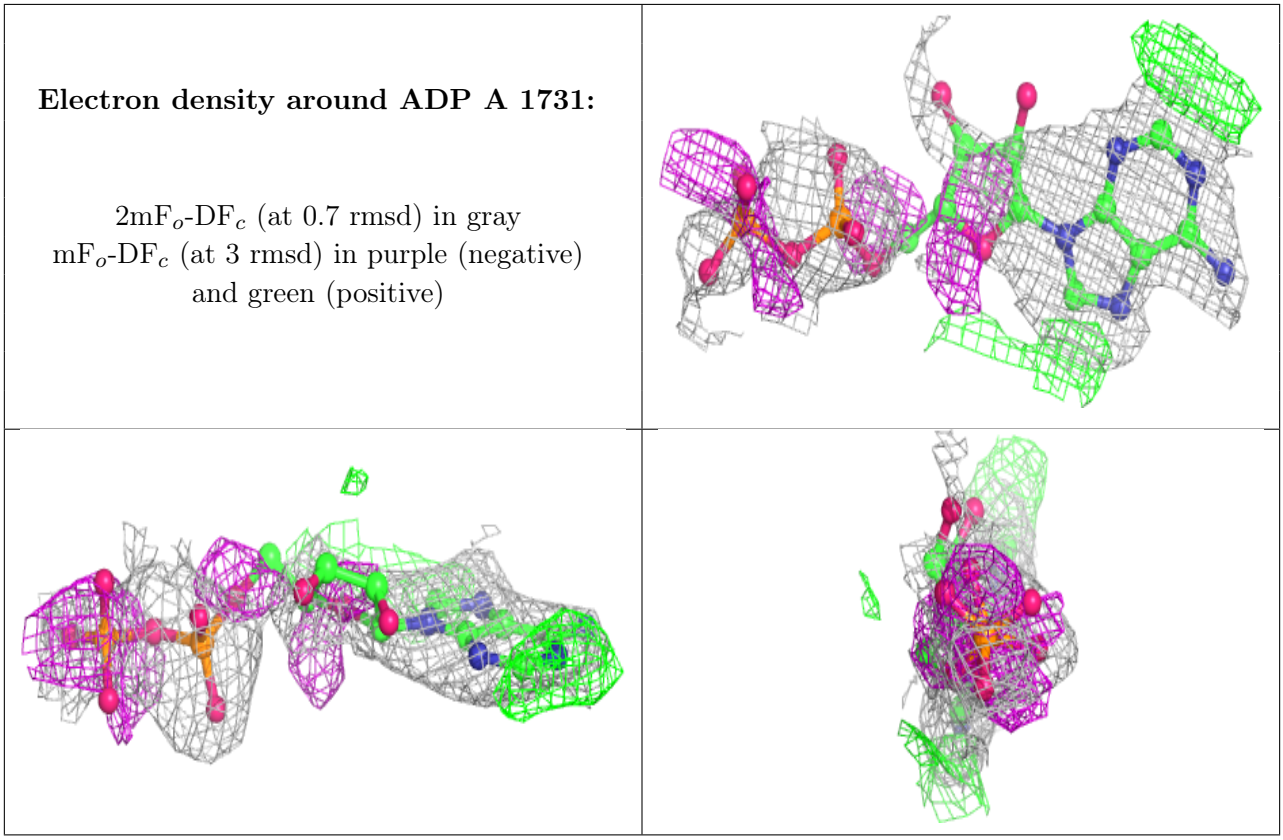
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	1725	5/5	0.73	0.38	57,57,58,58	5
6	ADP	A	1731	27/27	0.73	0.36	92,105,119,121	0
6	ADP	C	1414	27/27	0.76	0.36	67,87,109,110	0
3	SO4	D	1409	5/5	0.78	0.26	93,94,96,97	5
3	SO4	A	1725	5/5	0.83	0.23	39,40,40,41	5
3	SO4	A	1726	5/5	0.83	0.31	48,48,49,50	5
3	SO4	A	1724	5/5	0.85	0.20	66,67,69,69	5
3	SO4	A	1727	5/5	0.86	0.34	23,23,23,23	5
4	GOL	B	1730	6/6	0.87	0.22	53,54,54,54	0
3	SO4	B	1724	5/5	0.89	0.21	43,44,44,44	5
3	SO4	C	1412	5/5	0.89	0.20	47,48,49,49	5
3	SO4	C	1411	5/5	0.90	0.21	47,48,48,49	5
5	COA	B	1731	48/48	0.90	0.21	66,76,82,83	0
3	SO4	B	1727	5/5	0.90	0.16	30,30,31,31	5
3	SO4	B	1729	5/5	0.90	0.19	85,86,87,88	0
3	SO4	B	1723	5/5	0.91	0.32	62,63,64,64	5
4	GOL	A	1729	6/6	0.91	0.23	48,50,50,51	0
3	SO4	B	1726	5/5	0.93	0.20	46,46,48,48	5
3	SO4	C	1410	5/5	0.93	0.16	44,46,46,47	5
3	SO4	C	1409	5/5	0.94	0.27	49,49,51,53	5
4	GOL	A	1728	6/6	0.94	0.14	54,55,56,57	0
5	COA	A	1730	48/48	0.94	0.22	49,59,65,67	0
3	SO4	B	1728	5/5	0.95	0.28	62,63,63,64	0
3	SO4	C	1406	5/5	0.95	0.23	65,67,68,69	0
3	SO4	C	1407	5/5	0.95	0.33	72,74,76,77	0
3	SO4	D	1404	5/5	0.96	0.10	70,72,73,73	0
3	SO4	D	1406	5/5	0.96	0.31	61,62,64,65	0
3	SO4	A	1723	5/5	0.96	0.20	67,68,69,69	0
3	SO4	C	1408	5/5	0.96	0.25	51,52,53,53	5
3	SO4	C	1413	5/5	0.96	0.21	58,61,64,64	0
3	SO4	D	1408	5/5	0.97	0.18	64,64,66,66	0
3	SO4	D	1405	5/5	0.97	0.25	59,60,61,61	0
3	SO4	B	1721	5/5	0.97	0.12	50,51,51,52	0
3	SO4	A	1721	5/5	0.98	0.11	46,47,47,48	0
3	SO4	A	1722	5/5	0.98	0.11	47,49,51,51	0
3	SO4	B	1722	5/5	0.98	0.12	55,55,56,56	0
3	SO4	C	1405	5/5	0.99	0.23	48,49,50,51	0
3	SO4	C	1404	5/5	0.99	0.12	37,40,41,41	0
3	SO4	D	1407	5/5	0.99	0.22	59,60,60,60	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.

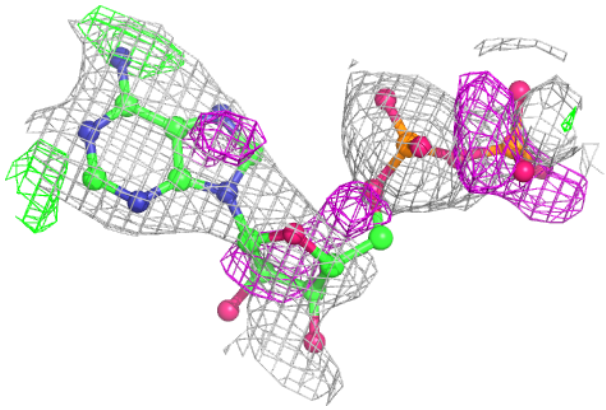
Electron density around ADP A 1731:

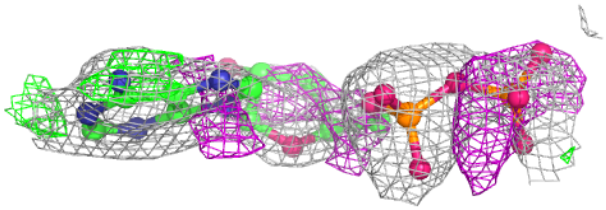
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

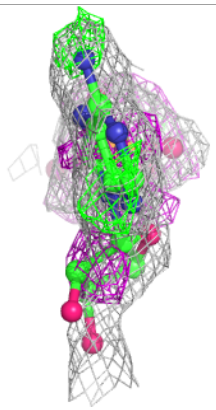


Electron density around ADP C 1414:

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

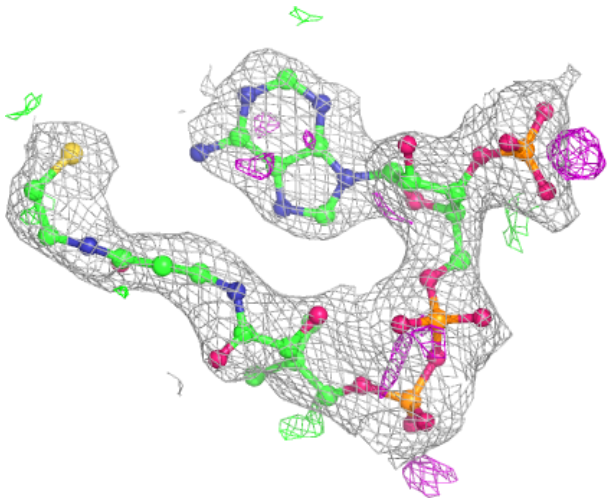


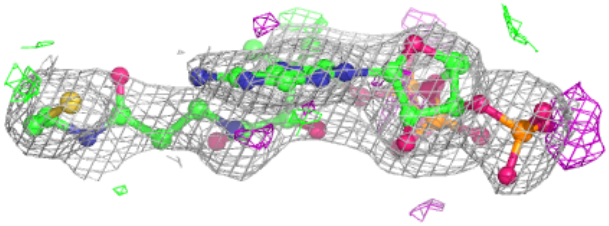


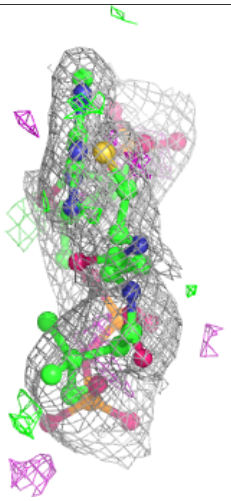


Electron density around COA B 1731:

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

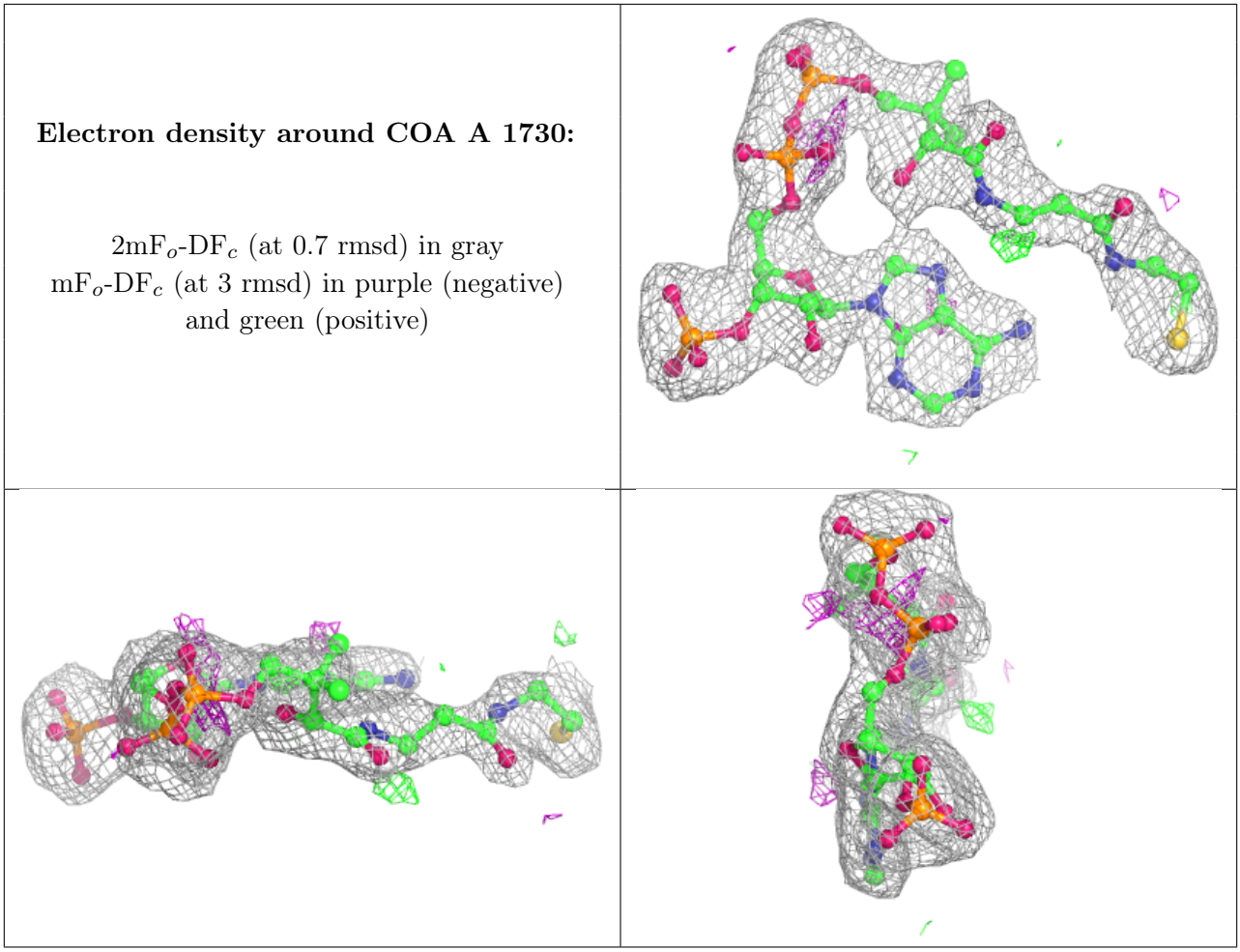






Electron density around COA A 1730:

$2mF_o$-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.