



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:04 AM UTC

PDB ID : 4R1L / pdb_00004r1l
Title : Crystal structure of a Putative Acyl-CoA ligase (BT_0428) from Bacteroides
thetaiotaomicron VPI-5482 at 2.42 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2014-08-06
Resolution : 2.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

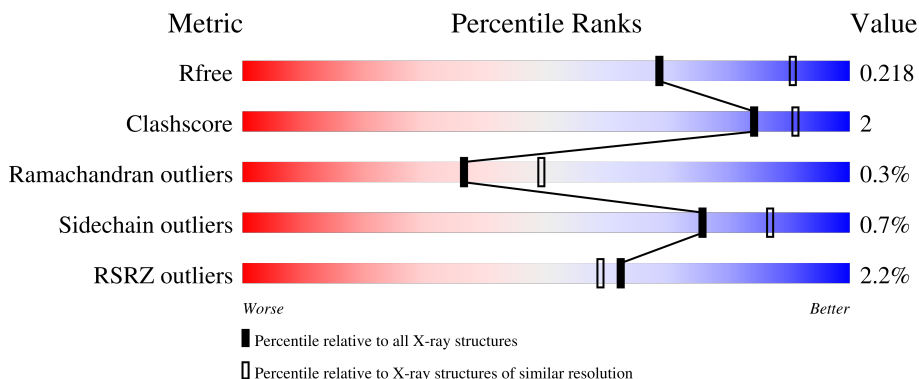
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	436	2% 94% 6%
1	B	436	2% 88% 9%
1	C	436	2% 92% 8%
1	D	436	3% 90% 7%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14432 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 Phenylacetate-coenzyme A ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	Se	0	10	0
			3469	2187	602	659	6	15			
1	B	422	Total	C	N	O	S	Se	0	8	0
			3336	2102	578	635	6	15			
1	C	434	Total	C	N	O	S	Se	0	4	0
			3430	2165	597	647	6	15			
1	D	425	Total	C	N	O	S	Se	0	3	0
			3340	2108	578	633	6	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q8AAN6
B	0	GLY	-	expression tag	UNP Q8AAN6
C	0	GLY	-	expression tag	UNP Q8AAN6
D	0	GLY	-	expression tag	UNP Q8AAN6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

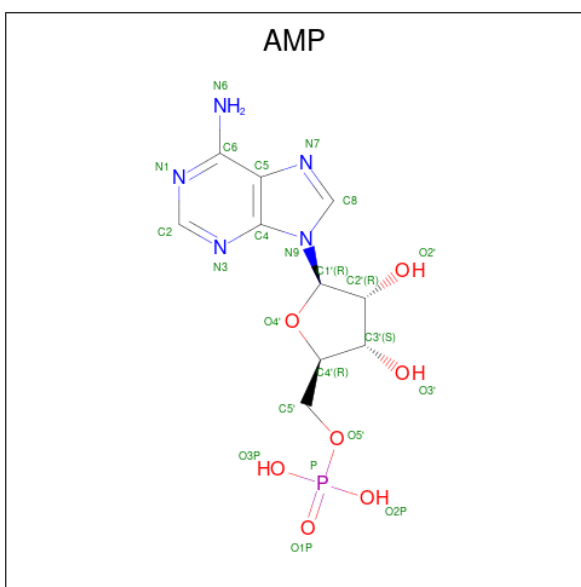
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



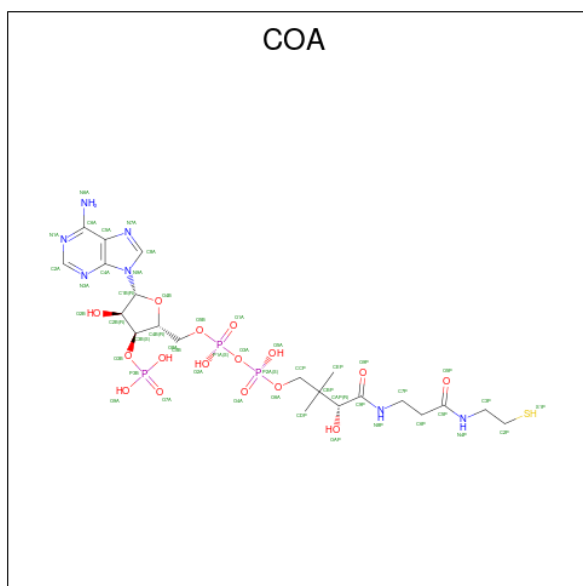
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			23	10	5	7	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is COENZYME A (CCD ID: 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	0	1
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	1
			31	10	5	13	3		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total K 3 3	0	0
6	C	2	Total K 2 2	0	0
6	D	1	Total K 1 1	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



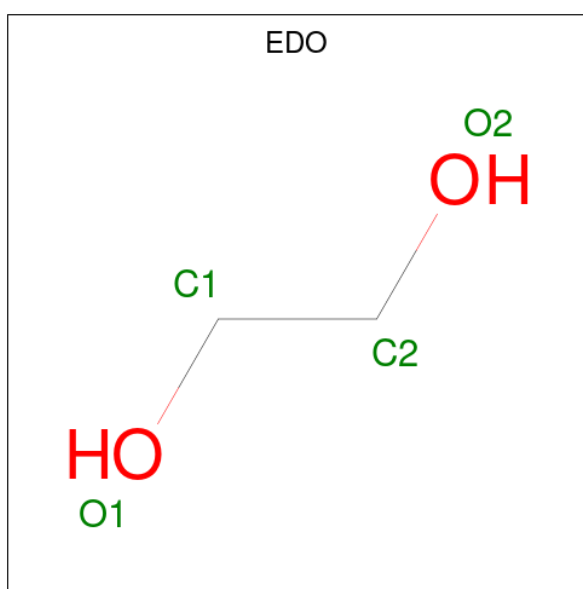
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	1
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



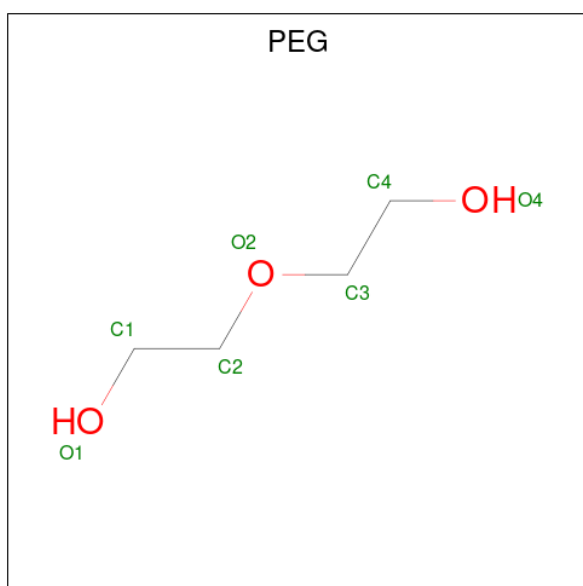
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	173	Total	O	0	1
			174	174		
11	B	124	Total	O	0	0
			124	124		
11	C	114	Total	O	0	1
			115	115		

Continued on next page...

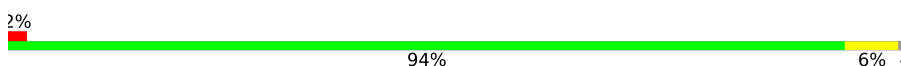
Continued from previous page...

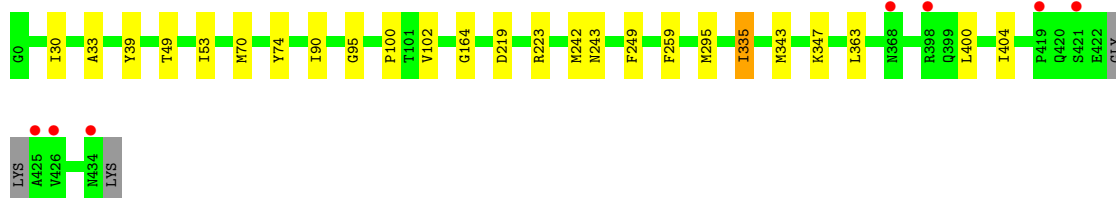
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	145	Total 145	O 145	0	0

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.

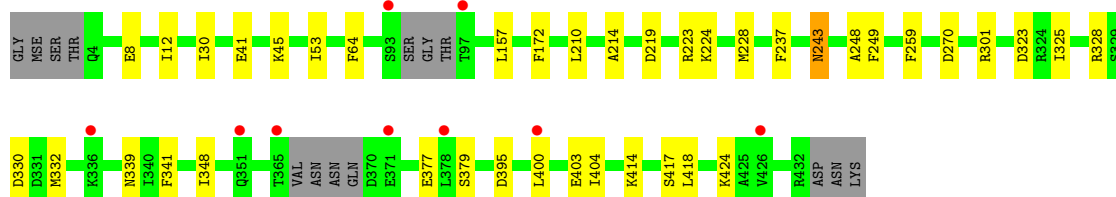
• Molecule 1: Phenylacetate-coenzyme A ligase

Chain A: 



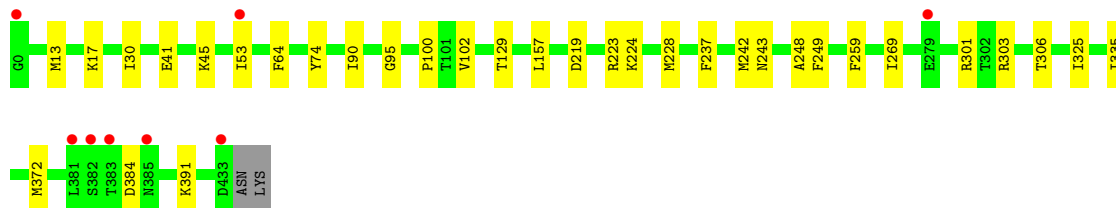
• Molecule 1: Phenylacetate-coenzyme A ligase

Chain B: 



• Molecule 1: Phenylacetate-coenzyme A ligase

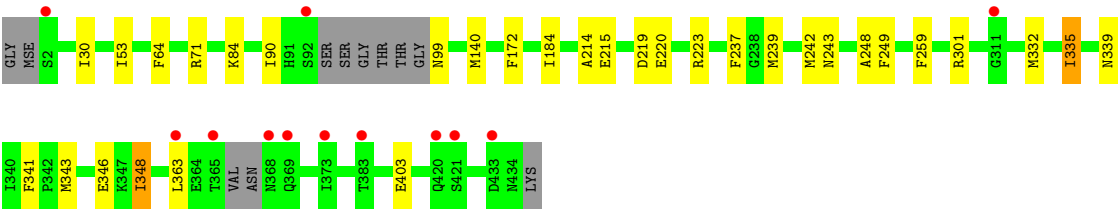
Chain C: 



• Molecule 1: Phenylacetate-coenzyme A ligase

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.70Å 211.14Å 71.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.78 – 2.42 48.78 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.78-2.42) 99.0 (48.78-2.42)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.42Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.172 , 0.213 0.180 , 0.218	Depositor DCC
R_{free} test set	3742 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14432	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, AMP, EDO, PGE, PEG, ADP, COA, SO4, K

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	0.88	1/3542 (0.0%)	1.23	4/4756 (0.1%)
1	B	0.84	0/3402	1.23	11/4573 (0.2%)
1	C	0.84	0/3486	1.22	4/4682 (0.1%)
1	D	0.87	3/3392 (0.1%)	1.22	4/4562 (0.1%)
All	All	0.86	4/13822 (0.0%)	1.22	23/18573 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	140	MSE	SE-CE	-5.83	1.77	1.95
1	A	295	MSE	SE-CE	-5.67	1.78	1.95
1	D	239	MSE	SE-CE	-5.16	1.79	1.95
1	D	348	ILE	CG1-CD1	-5.14	1.31	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	GLY	N-CA-C	8.44	121.74	112.29
1	A	95	GLY	N-CA-C	7.94	121.18	112.29
1	D	249	PHE	CA-CB-CG	7.02	120.82	113.80
1	A	249	PHE	CA-CB-CG	6.91	120.71	113.80
1	C	249	PHE	CA-CB-CG	6.87	120.67	113.80
1	B	249	PHE	CA-CB-CG	6.85	120.65	113.80
1	B	270	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	323	ASP	CA-C-N	5.69	130.43	121.56
1	B	323	ASP	C-N-CA	5.69	130.43	121.56
1	B	325	ILE	CA-C-N	5.56	127.99	120.38
1	B	325	ILE	C-N-CA	5.56	127.99	120.38
1	A	242	MSE	CA-C-N	5.47	132.00	121.54
1	A	242	MSE	C-N-CA	5.47	132.00	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	242	MSE	CA-C-N	5.47	131.99	121.54
1	C	242	MSE	C-N-CA	5.47	131.99	121.54
1	B	172	PHE	CA-CB-CG	5.34	119.14	113.80
1	B	395	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	243	ASN	CA-CB-CG	5.31	117.91	112.60
1	B	379	SER	CA-C-N	5.29	127.79	120.29
1	B	379	SER	C-N-CA	5.29	127.79	120.29
1	D	242	MSE	CA-C-N	5.19	131.46	121.54
1	D	242	MSE	C-N-CA	5.19	131.46	121.54
1	D	172	PHE	CA-CB-CG	5.00	118.81	113.80

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	3469	0	3476	13	0
1	B	3336	0	3279	17	0
1	C	3430	0	3431	16	0
1	D	3340	0	3283	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	D	27	0	12	0	0
4	A	23	0	12	0	0
4	C	23	0	12	0	0
5	A	31	0	11	1	0
5	C	31	0	11	0	0
6	A	3	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
7	A	10	0	14	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	15	0	0	0	0
8	B	5	0	0	0	0
8	C	10	0	0	0	0
8	D	5	0	0	0	0
9	A	16	0	24	2	0
9	B	12	0	18	1	0
9	C	12	0	18	3	0
9	D	8	0	12	0	0
10	D	7	0	10	2	0
11	A	174	0	0	1	0
11	B	124	0	0	1	0
11	C	115	0	0	1	0
11	D	145	0	0	1	0
All	All	14432	0	13647	63	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 2.

All (63) 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:D:332[A]:MSE:HE2	1:D:339:ASN:HB3	1.69	0.74
1:B:332[A]:MSE:HE2	1:B:339:ASN:HB3	1.72	0.71
1:A:219:ASP:O	1:A:223:ARG:HG2	1.93	0.67
1:A:90:ILE:HG23	1:A:102:VAL:HG13	1.76	0.67
9:C:510:EDO:H11	11:C:647:HOH:O	1.95	0.66
1:A:30:ILE:HD13	1:A:53:ILE:HG13	1.77	0.66
1:D:30:ILE:HD13	1:D:53:ILE:HG13	1.77	0.65
1:C:303:ARG:HH11	9:C:510:EDO:H12	1.62	0.64
1:B:30:ILE:HD13	1:B:53:ILE:HG13	1.81	0.62
1:C:30:ILE:HD13	1:C:53:ILE:HG13	1.80	0.61
1:B:224:LYS:O	1:B:228:MSE:HG3	2.03	0.59
1:B:214:ALA:HB1	1:B:424:LYS:HE2	1.85	0.58
1:D:348:ILE:HD11	1:D:403:GLU:CB	2.32	0.58
10:D:504:PEG:H11	11:D:737:HOH:O	2.05	0.56
1:B:400:LEU:O	1:B:404:ILE:HG12	2.08	0.54
1:B:414:LYS:HB3	1:B:417:SER:OG	2.08	0.53
1:D:343:MSE:HE1	1:D:346:GLU:OE1	2.09	0.52
1:C:237:PHE:HB3	1:C:248:ALA:HB3	1.92	0.52
1:A:49:THR:HA	9:A:512:EDO:H21	1.90	0.52
1:C:90:ILE:HG23	1:C:102:VAL:HG13	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ARG:HD3	1:D:99:ASN:HB2	1.91	0.51
1:A:70:MSE:O	9:A:514:EDO:H11	2.12	0.50
1:B:237:PHE:HB3	1:B:248:ALA:HB3	1.93	0.50
1:C:219:ASP:O	1:C:223:ARG:HG2	2.12	0.49
9:B:505:EDO:H11	11:B:653:HOH:O	2.12	0.49
1:D:30:ILE:CD1	1:D:53:ILE:HG13	2.41	0.49
1:D:335:ILE:HD13	1:D:363:LEU:HD22	1.94	0.49
1:A:30:ILE:CD1	1:A:53:ILE:HG13	2.42	0.49
1:A:74:TYR:CE1	1:A:100:PRO:HD2	2.49	0.48
1:D:332[A]:MSE:HE3	1:D:341:PHE:CE2	2.49	0.48
1:C:74:TYR:CE1	1:C:100:PRO:HD2	2.48	0.48
1:B:377:GLU:HG3	1:B:418:LEU:HD12	1.94	0.48
1:D:237:PHE:HB3	1:D:248:ALA:HB3	1.95	0.47
1:C:41:GLU:HG3	1:C:45:LYS:HE2	1.97	0.47
1:C:13:MSE:HG3	1:C:17:LYS:HE3	1.97	0.47
1:A:164:GLY:HA2	5:A:504[A]:COA:H1B	1.96	0.46
1:B:219:ASP:O	1:B:223:ARG:HG2	2.15	0.46
1:B:30:ILE:CD1	1:B:53:ILE:HG13	2.44	0.46
1:B:332[A]:MSE:HE3	1:B:341:PHE:CE2	2.50	0.46
1:D:64:PHE:HB3	1:D:301:ARG:HG3	1.98	0.45
1:C:335:ILE:HD13	1:C:372:MSE:HB2	1.98	0.45
1:C:30:ILE:CD1	1:C:53:ILE:HG13	2.43	0.45
1:B:8:GLU:O	1:B:12:ILE:HG12	2.16	0.45
1:D:219:ASP:O	1:D:223:ARG:HG2	2.16	0.45
1:A:90:ILE:HD11	1:B:157:LEU:HD21	1.98	0.45
1:B:41:GLU:OE2	1:B:45:LYS:HE2	2.16	0.45
1:C:64:PHE:HB3	1:C:301:ARG:HG3	1.98	0.44
1:A:400:LEU:O	1:A:404:ILE:HG12	2.17	0.44
1:A:33:ALA:O	1:A:39:TYR:HB2	2.17	0.43
1:B:64:PHE:HB3	1:B:301:ARG:HG3	2.01	0.43
1:B:348:ILE:HD11	1:B:403:GLU:HB3	2.00	0.43
1:D:214:ALA:HB2	10:D:504:PEG:H12	2.00	0.43
7:A:508:PGE:H6	11:A:772:HOH:O	2.19	0.42
1:C:224:LYS:O	1:C:228:MSE:HG3	2.19	0.42
1:D:184:ILE:HD12	1:D:215:GLU:OE2	2.20	0.41
1:C:129:THR:HB	1:D:84:LYS:HE2	2.02	0.41
1:C:306:THR:HB	1:C:325:ILE:HD13	2.03	0.41
1:D:348:ILE:HD11	1:D:403:GLU:HB3	2.01	0.41
1:C:303:ARG:NH1	9:C:510:EDO:H12	2.34	0.41
1:A:343[B]:MSE:HG3	1:A:347:LYS:HE3	2.03	0.41
1:A:335:ILE:HD13	1:A:363:LEU:HD22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:LEU:HD21	1:D:90:ILE:HD11	2.02	0.41
1:B:328:ARG:HD3	1:B:330:ASP:OD2	2.21	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	439/436 (101%)	420 (96%)	18 (4%)	1 (0%)	43	57
1	B	423/436 (97%)	408 (96%)	14 (3%)	1 (0%)	43	57
1	C	436/436 (100%)	419 (96%)	15 (3%)	2 (0%)	24	35
1	D	422/436 (97%)	406 (96%)	15 (4%)	1 (0%)	43	57
All	All	1720/1744 (99%)	1653 (96%)	62 (4%)	5 (0%)	36	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
1	B	243	ASN
1	C	243	ASN
1	D	243	ASN
1	C	384	ASP

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	382/370 (103%)	380 (100%)	2 (0%)	81	90
1	B	360/370 (97%)	358 (99%)	2 (1%)	78	88
1	C	373/370 (101%)	370 (99%)	3 (1%)	73	85
1	D	358/370 (97%)	355 (99%)	3 (1%)	73	85
All	All	1473/1480 (100%)	1463 (99%)	10 (1%)	76	87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	PHE
1	A	335	ILE
1	B	210	LEU
1	B	259	PHE
1	C	259	PHE
1	C	269	ILE
1	C	391	LYS
1	D	220	GLU
1	D	259	PHE
1	D	335	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	24	GLN
1	A	35	ASN
1	A	252	GLN
1	A	351	GLN
1	A	369	GLN
1	A	385	ASN
1	B	24	GLN
1	B	35	ASN
1	B	99	ASN
1	B	252	GLN
1	B	385	ASN
1	C	22	GLN
1	C	24	GLN
1	C	35	ASN
1	C	252	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	351	GLN
1	D	24	GLN
1	D	252	GLN
1	D	351	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 38 ligands modelled in this entry, 10 are monoatomic - leaving 28 for Mogul analysis.

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	ADP	D	502	-	28,29,29	0.27	0	43,45,45	0.61	1 (2%)
3	ADP	B	502	-	28,29,29	0.34	0	43,45,45	0.51	1 (2%)
7	PGE	A	508	-	9,9,9	0.20	0	8,8,8	0.22	0
8	SO4	C	507	-	4,4,4	0.24	0	6,6,6	0.14	0
5	COA	A	504[A]	-	32,33,50	0.76	2 (6%)	50,52,75	1.24	7 (14%)
9	EDO	A	512	-	3,3,3	0.53	0	2,2,2	0.13	0
9	EDO	D	506	-	3,3,3	0.61	0	2,2,2	0.18	0
9	EDO	C	510	-	3,3,3	0.58	0	2,2,2	0.31	0
8	SO4	A	509[B]	-	4,4,4	0.20	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AMP	C	502	6	25,25,25	0.25	0	37,38,38	0.52	0
4	AMP	A	503[B]	6	25,25,25	0.35	0	37,38,38	0.47	0
9	EDO	C	508	-	3,3,3	0.49	0	2,2,2	0.49	0
8	SO4	B	503	-	4,4,4	0.32	0	6,6,6	0.18	0
10	PEG	D	504	-	6,6,6	0.27	0	5,5,5	0.33	0
3	ADP	A	502[A]	6	28,29,29	0.34	0	43,45,45	0.59	1 (2%)
9	EDO	A	513	-	3,3,3	0.51	0	2,2,2	0.35	0
9	EDO	C	509	-	3,3,3	0.58	0	2,2,2	0.35	0
9	EDO	A	515	-	3,3,3	0.73	0	2,2,2	0.22	0
9	EDO	A	514	-	3,3,3	0.36	0	2,2,2	0.32	0
8	SO4	A	511	-	4,4,4	0.27	0	6,6,6	0.14	0
9	EDO	B	506	-	3,3,3	0.67	0	2,2,2	0.03	0
8	SO4	A	510	-	4,4,4	0.33	0	6,6,6	0.36	0
8	SO4	C	506[B]	-	4,4,4	0.25	0	6,6,6	0.08	0
8	SO4	D	505	-	4,4,4	0.23	0	6,6,6	0.30	0
9	EDO	D	507	-	3,3,3	0.60	0	2,2,2	0.34	0
5	COA	C	503[A]	-	32,33,50	0.78	2 (6%)	50,52,75	1.14	7 (14%)
9	EDO	B	504	-	3,3,3	0.47	0	2,2,2	0.38	0
9	EDO	B	505	-	3,3,3	0.58	0	2,2,2	0.24	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
3	ADP	D	502	-	-	6/16/32/32	0/3/3/3
3	ADP	B	502	-	-	4/16/32/32	0/3/3/3
7	PGE	A	508	-	-	3/7/7/7	-
5	COA	A	504[A]	-	-	0/21/37/64	0/3/3/3
9	EDO	A	512	-	-	0/1/1/1	-
9	EDO	D	506	-	-	0/1/1/1	-
9	EDO	C	510	-	-	1/1/1/1	-
9	EDO	C	508	-	-	0/1/1/1	-
4	AMP	C	502	6	-	0/10/26/26	0/3/3/3
4	AMP	A	503[B]	6	-	0/10/26/26	0/3/3/3
10	PEG	D	504	-	-	1/4/4/4	-
3	ADP	A	502[A]	6	-	6/16/32/32	0/3/3/3
9	EDO	A	513	-	-	0/1/1/1	-
9	EDO	C	509	-	-	0/1/1/1	-
9	EDO	A	515	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	514	-	-	0/1/1/1	-
9	EDO	B	506	-	-	0/1/1/1	-
9	EDO	D	507	-	-	0/1/1/1	-
5	COA	C	503[A]	-	-	0/21/37/64	0/3/3/3
9	EDO	B	504	-	-	0/1/1/1	-
9	EDO	B	505	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503[A]	COA	P1A-O3A	2.80	1.62	1.59
5	A	504[A]	COA	P3B-O3B	2.77	1.64	1.59
5	C	503[A]	COA	P2A-O6A	2.15	1.62	1.54
5	A	504[A]	COA	P1A-O3A	2.06	1.61	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504[A]	COA	O6A-P2A-O3A	4.83	120.83	104.64
5	C	503[A]	COA	O6A-P2A-O3A	4.26	118.91	104.64
5	A	504[A]	COA	O3A-P1A-O1A	-3.11	101.33	110.70
5	A	504[A]	COA	O5A-P2A-O4A	3.06	122.75	110.83
5	A	504[A]	COA	O6A-P2A-O5A	-2.83	97.21	107.80
5	C	503[A]	COA	O3A-P1A-O1A	-2.76	102.42	110.70
5	C	503[A]	COA	O6A-P2A-O5A	-2.51	98.38	107.80
3	D	502	ADP	O5'-PA-O1A	2.48	118.76	108.94
3	B	502	ADP	O5'-PA-O1A	2.31	118.11	108.94
5	A	504[A]	COA	O3B-P3B-O7A	2.28	117.47	109.33
3	A	502[A]	ADP	O5'-PA-O1A	2.28	117.98	108.94
5	C	503[A]	COA	O5A-P2A-O4A	2.23	119.54	110.83
5	A	504[A]	COA	O3A-P2A-O4A	-2.20	99.45	111.04
5	C	503[A]	COA	O2A-P1A-O1A	2.19	122.62	112.44
5	C	503[A]	COA	O3A-P2A-O4A	-2.11	99.95	111.04
5	C	503[A]	COA	O3B-P3B-O7A	2.03	116.56	109.33
5	A	504[A]	COA	O2A-P1A-O1A	2.00	121.75	112.44

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502[A]	ADP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	502[A]	ADP	C5'-O5'-PA-O1A
3	A	502[A]	ADP	C5'-O5'-PA-O2A
3	A	502[A]	ADP	C5'-O5'-PA-O3A
3	B	502	ADP	C5'-O5'-PA-O1A
3	B	502	ADP	C5'-O5'-PA-O2A
3	B	502	ADP	C5'-O5'-PA-O3A
3	D	502	ADP	PA-O3A-PB-O3B
3	D	502	ADP	C5'-O5'-PA-O1A
3	D	502	ADP	C5'-O5'-PA-O2A
3	D	502	ADP	C5'-O5'-PA-O3A
10	D	504	PEG	C1-C2-O2-C3
7	A	508	PGE	C4-C3-O2-C2
7	A	508	PGE	C6-C5-O3-C4
7	A	508	PGE	C3-C4-O3-C5
9	C	510	EDO	O1-C1-C2-O2
3	A	502[A]	ADP	PA-O3A-PB-O1B
3	D	502	ADP	PA-O3A-PB-O1B
3	A	502[A]	ADP	PA-O3A-PB-O3B
3	B	502	ADP	PA-O3A-PB-O3B
3	D	502	ADP	PA-O3A-PB-O2B

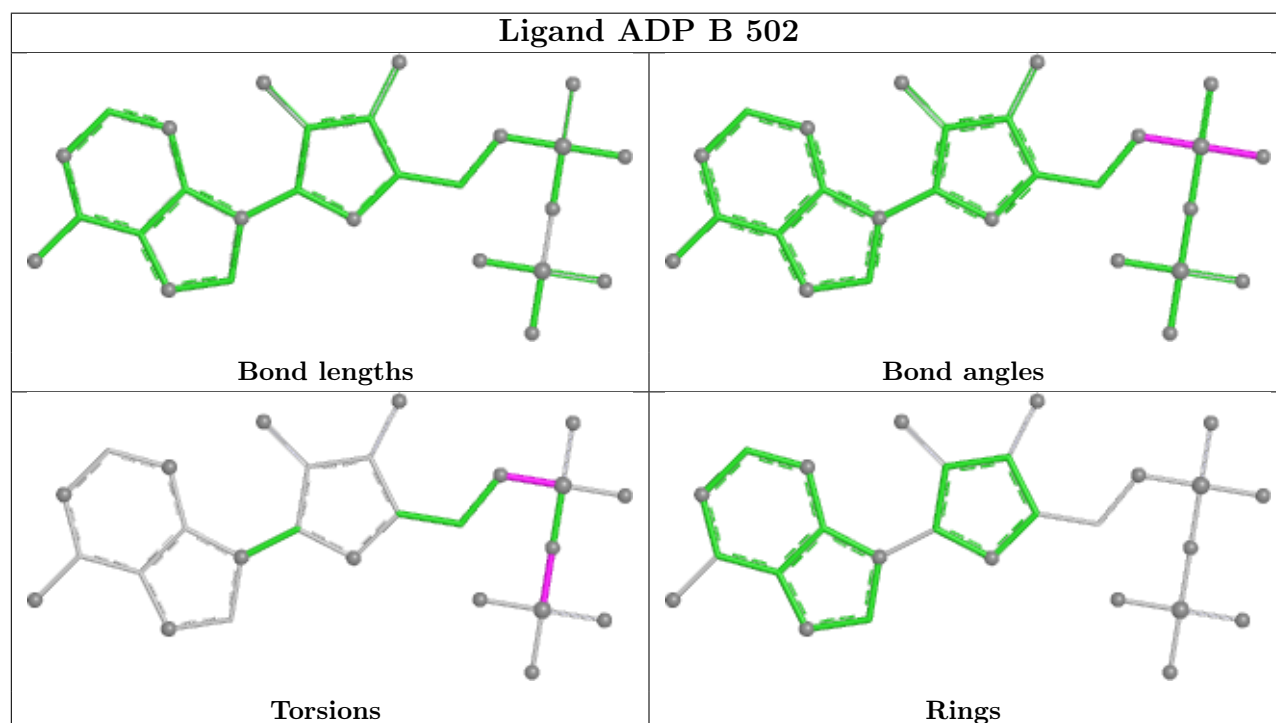
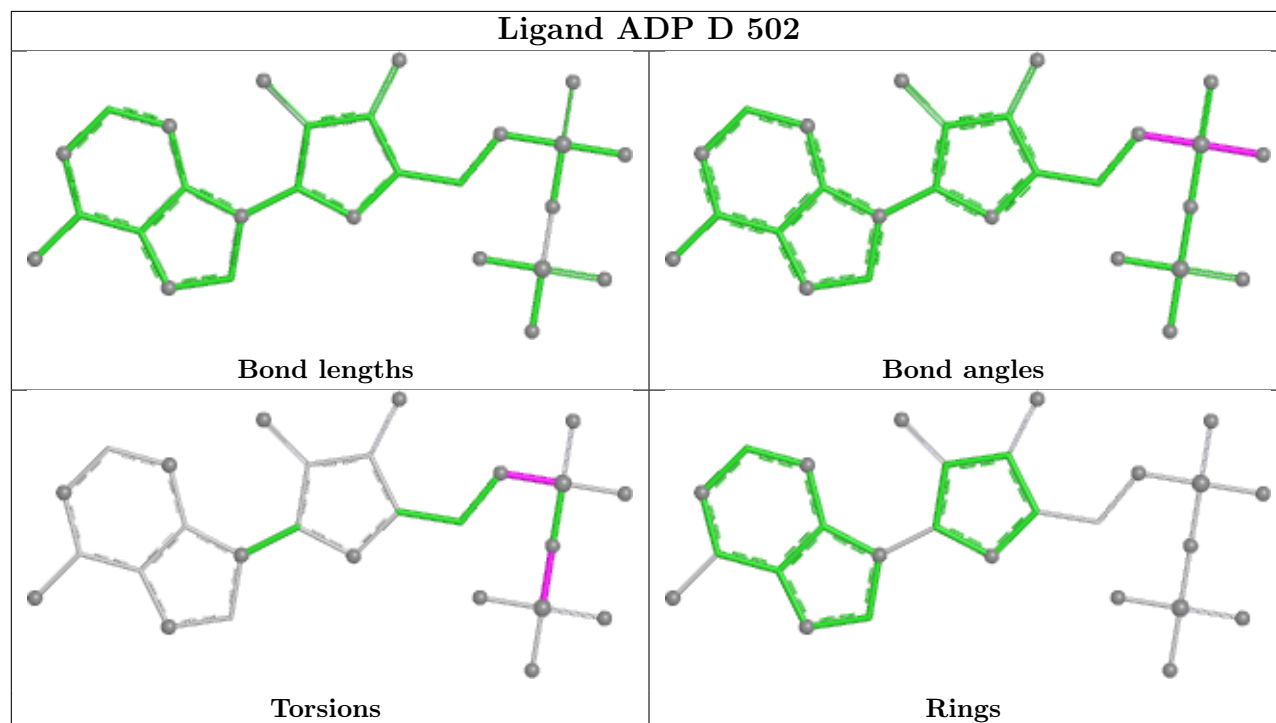
There are no ring outliers.

7 monomers are involved in 10 short contacts:

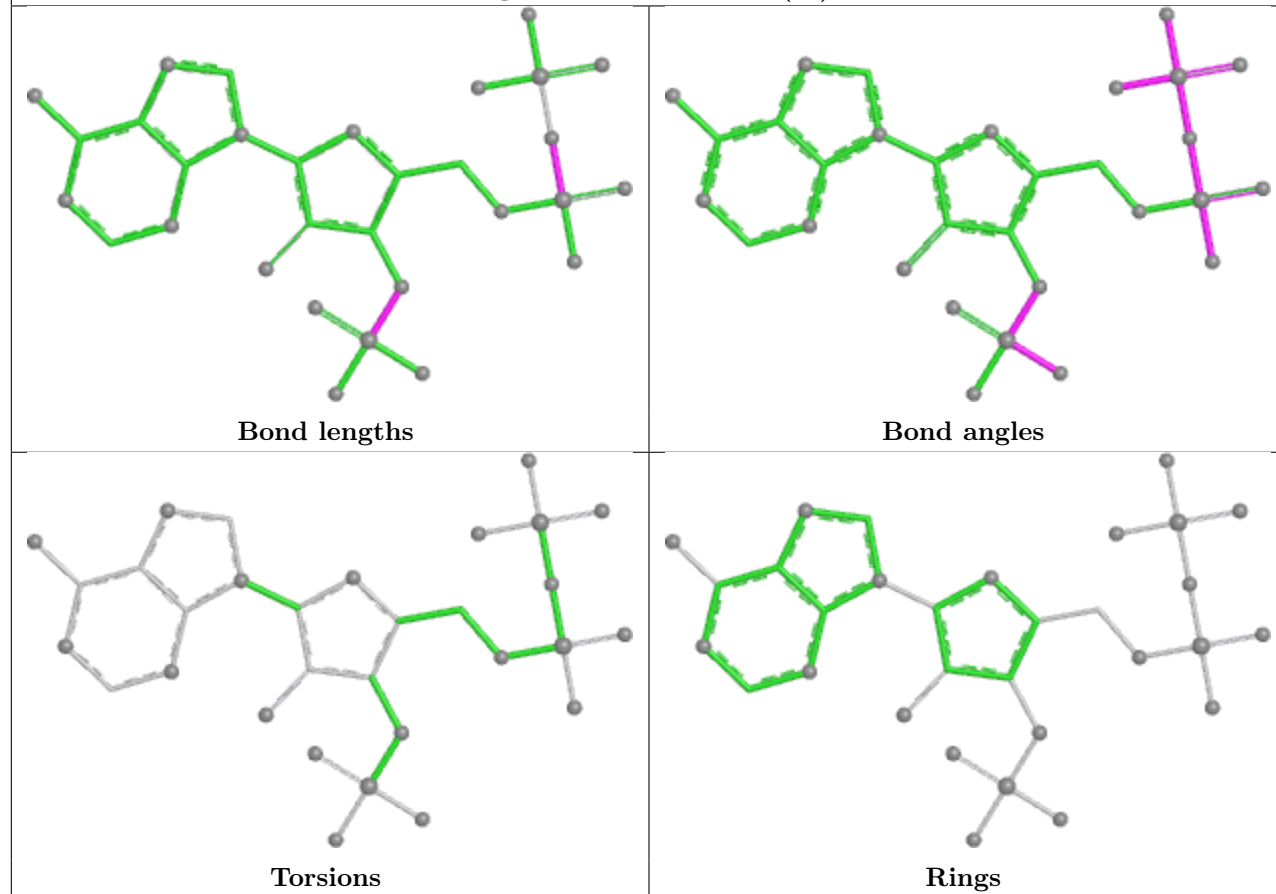
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	508	PGE	1	0
5	A	504[A]	COA	1	0
9	A	512	EDO	1	0
9	C	510	EDO	3	0
10	D	504	PEG	2	0
9	A	514	EDO	1	0
9	B	505	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

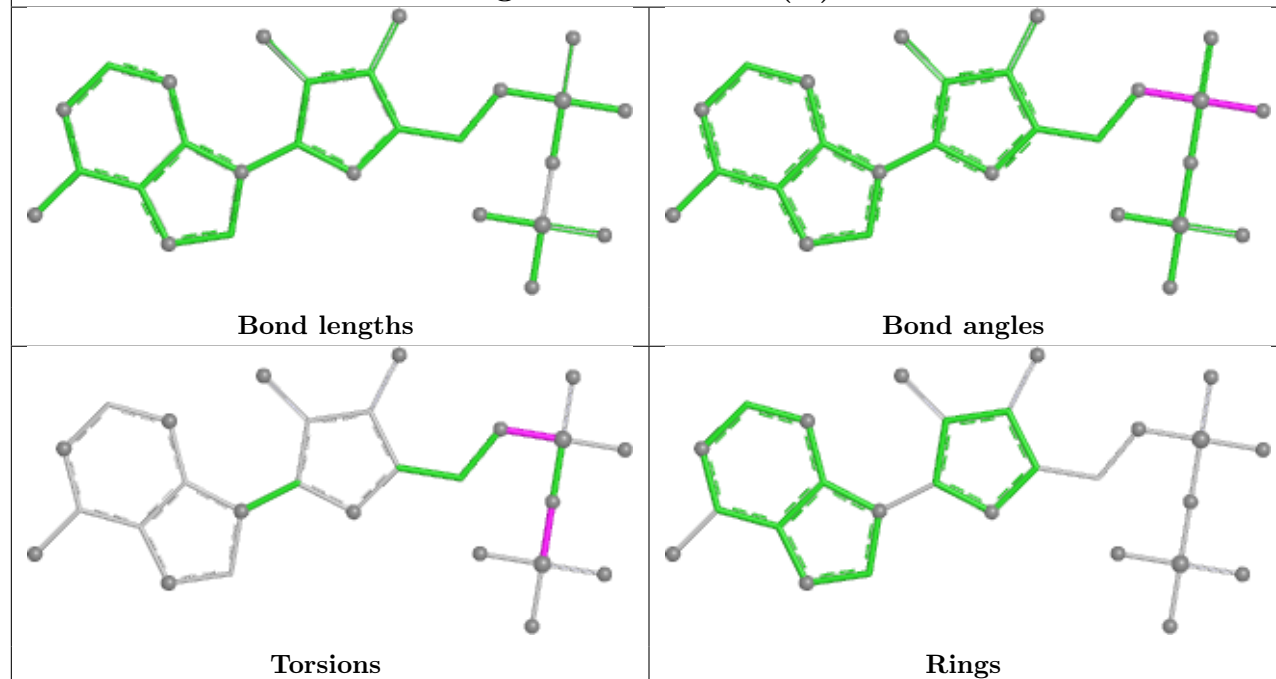
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

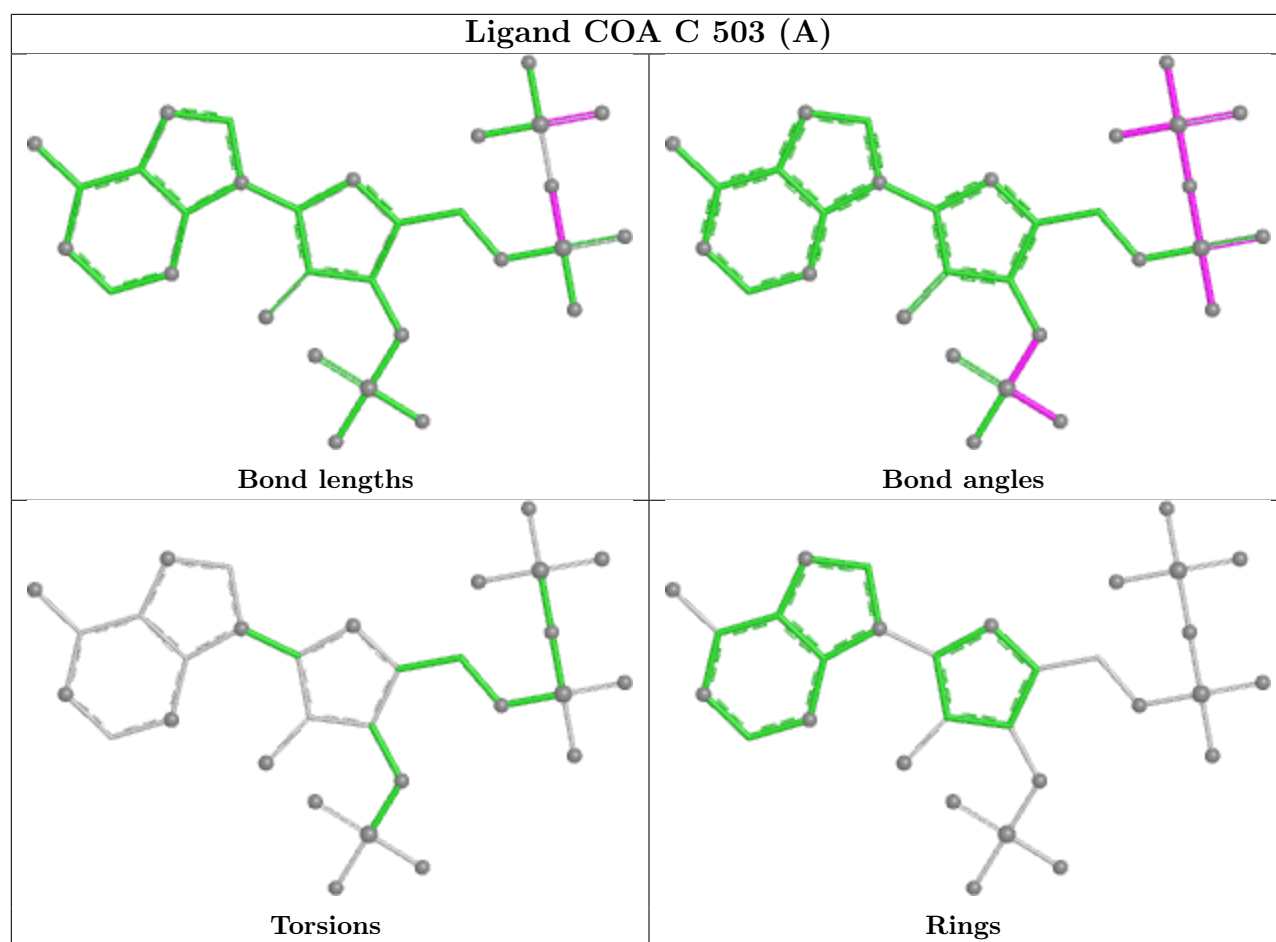


Ligand COA A 504 (A)



Ligand ADP A 502 (A)





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, 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	418/436 (95%)	-0.30	7 (1%) 69 66	23, 44, 81, 124	9 (2%)
1	B	408/436 (93%)	-0.03	9 (2%) 62 59	28, 53, 107, 128	7 (1%)
1	C	419/436 (96%)	-0.05	8 (1%) 66 63	28, 56, 96, 119	4 (0%)
1	D	411/436 (94%)	-0.15	12 (2%) 53 50	27, 47, 94, 122	2 (0%)
All	All	1656/1744 (94%)	-0.13	36 (2%) 62 59	23, 50, 97, 128	22 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	433	ASP	5.5
1	D	92	SER	4.3
1	B	365	THR	3.5
1	C	382	SER	3.4
1	B	93	SER	3.3
1	A	421	SER	3.2
1	A	425	ALA	3.2
1	B	371	GLU	3.1
1	A	368	ASN	3.0
1	D	368	ASN	2.8
1	D	369	GLN	2.8
1	D	421	SER	2.7
1	A	434	ASN	2.7
1	D	2	SER	2.7
1	B	400	LEU	2.5
1	C	385	ASN	2.5
1	A	398[A]	ARG	2.4
1	A	426	VAL	2.4
1	C	383	THR	2.3
1	C	0	GLY	2.3
1	B	351[A]	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	378	LEU	2.3
1	B	336	LYS	2.3
1	D	373	ILE	2.2
1	A	419	PRO	2.2
1	D	311	GLY	2.2
1	C	53	ILE	2.2
1	B	426	VAL	2.1
1	D	420	GLN	2.1
1	D	363	LEU	2.1
1	D	383	THR	2.1
1	D	433	ASP	2.1
1	B	97	THR	2.1
1	C	279	GLU	2.0
1	C	381	LEU	2.0
1	D	365	THR	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 oligosaccharides 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, 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
9	EDO	D	506	4/4	0.73	0.18	76,78,78,78	0
10	PEG	D	504	7/7	0.73	0.23	63,65,73,74	0
9	EDO	C	508	4/4	0.75	0.16	68,68,68,68	0
9	EDO	B	506	4/4	0.78	0.17	59,62,63,64	0
9	EDO	C	510	4/4	0.81	0.14	58,59,59,60	0
9	EDO	B	504	4/4	0.82	0.19	74,74,74,76	0
8	SO4	A	511	5/5	0.83	0.15	53,53,56,58	5
9	EDO	D	507	4/4	0.85	0.13	50,51,51,52	0

Continued on next page...

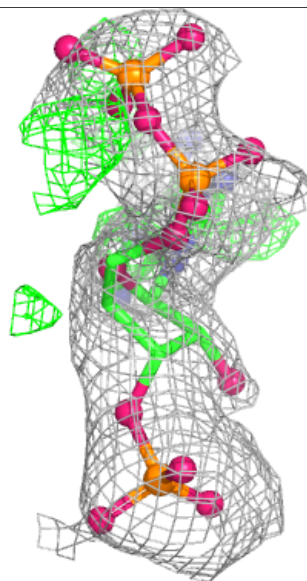
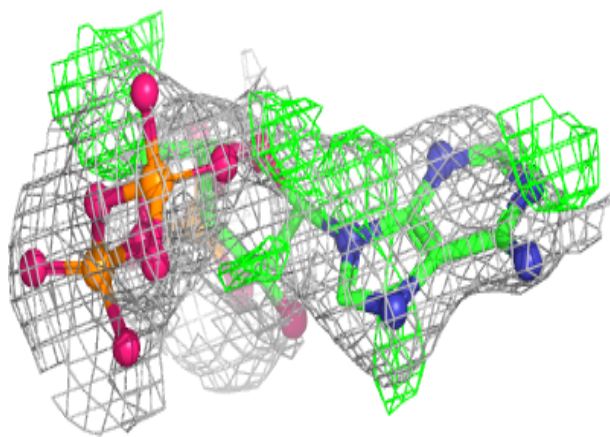
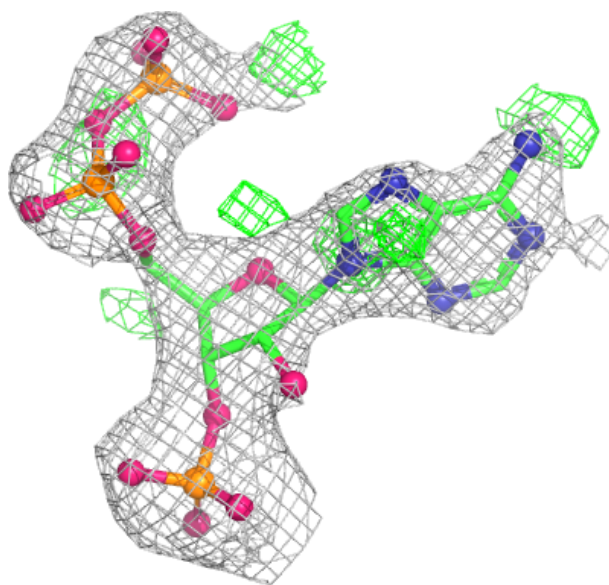
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	EDO	B	505	4/4	0.87	0.16	55,55,58,60	0
9	EDO	A	512	4/4	0.87	0.15	59,59,59,60	0
8	SO4	C	507	5/5	0.87	0.14	49,50,51,52	5
9	EDO	C	509	4/4	0.87	0.13	63,65,66,68	0
9	EDO	A	513	4/4	0.88	0.12	69,70,71,74	0
5	COA	A	504[A]	31/48	0.89	0.13	37,45,59,61	31
8	SO4	B	503	5/5	0.89	0.12	43,43,44,45	5
3	ADP	D	502	27/27	0.90	0.09	31,43,80,83	0
8	SO4	D	505	5/5	0.91	0.10	78,79,80,81	0
3	ADP	A	502[A]	27/27	0.92	0.10	38,52,55,55	27
3	ADP	B	502	27/27	0.92	0.09	41,54,85,86	0
5	COA	C	503[A]	31/48	0.92	0.11	23,35,42,43	31
7	PGE	A	508	10/10	0.92	0.16	64,75,78,78	0
8	SO4	A	509[B]	5/5	0.92	0.10	102,102,102,102	5
8	SO4	C	506[B]	5/5	0.93	0.13	126,126,126,126	5
4	AMP	C	502	23/23	0.94	0.07	37,45,53,61	0
9	EDO	A	514	4/4	0.94	0.13	61,61,62,63	0
9	EDO	A	515	4/4	0.94	0.10	31,36,38,41	0
2	ZN	B	501	1/1	0.96	0.05	48,48,48,48	0
6	K	A	507	1/1	0.97	0.06	43,43,43,43	0
6	K	D	503	1/1	0.97	0.08	37,37,37,37	0
8	SO4	A	510	5/5	0.97	0.05	53,54,58,60	0
4	AMP	A	503[B]	23/23	0.98	0.04	13,21,24,25	23
6	K	C	505	1/1	0.98	0.05	42,42,42,42	0
2	ZN	C	501	1/1	0.98	0.04	65,65,65,65	0
2	ZN	D	501	1/1	0.99	0.04	47,47,47,47	0
6	K	C	504	1/1	0.99	0.11	45,45,45,45	0
2	ZN	A	501	1/1	0.99	0.02	47,47,47,47	0
6	K	A	505	1/1	0.99	0.06	40,40,40,40	0
6	K	A	506	1/1	0.99	0.07	32,32,32,32	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.

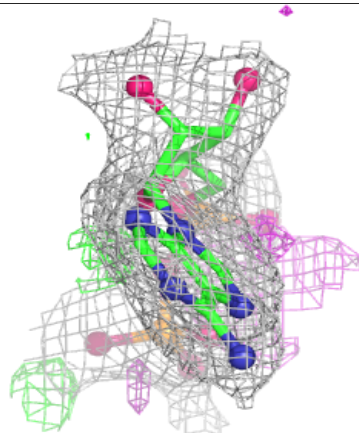
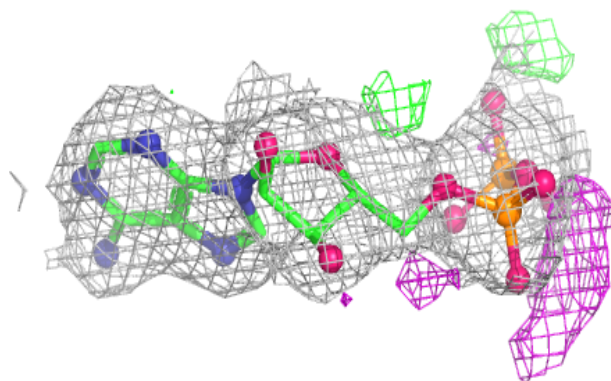
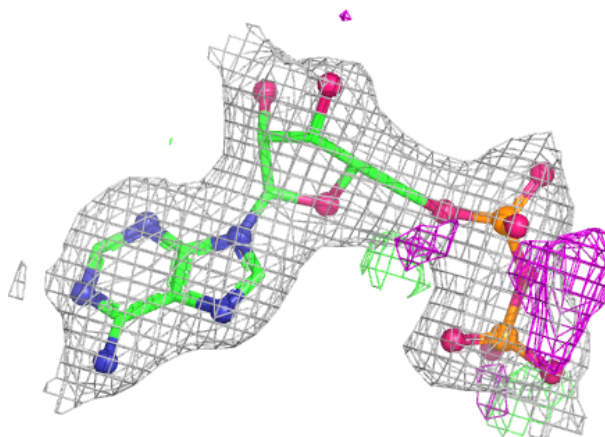
Electron density around COA A 504 (A):

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



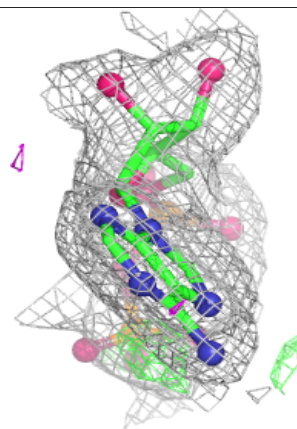
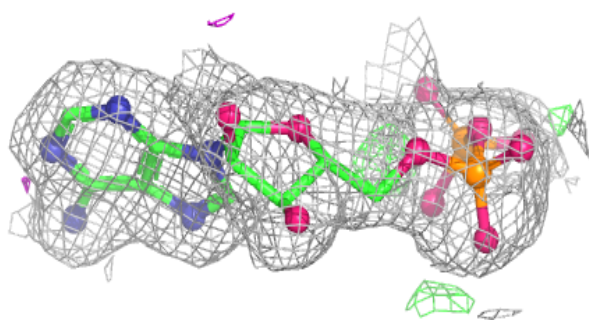
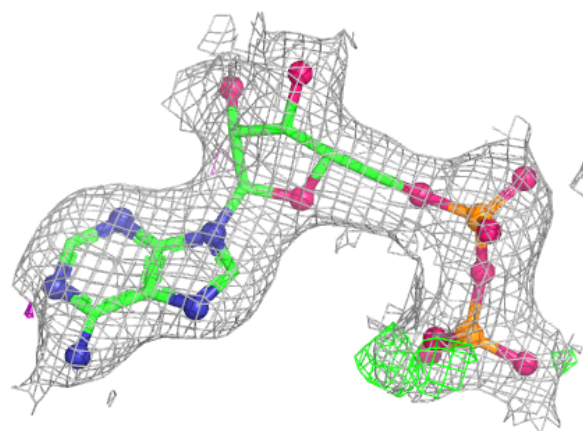
Electron density around ADP D 502:

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



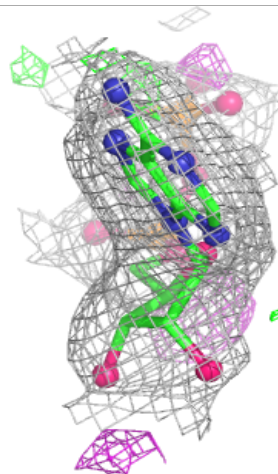
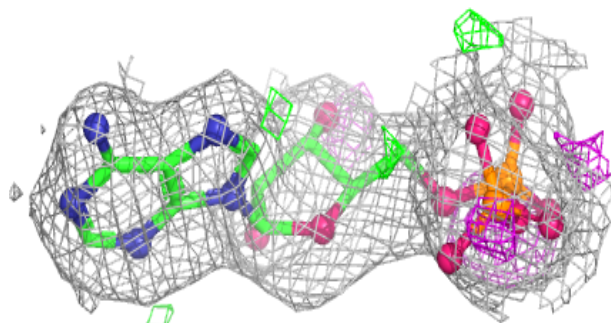
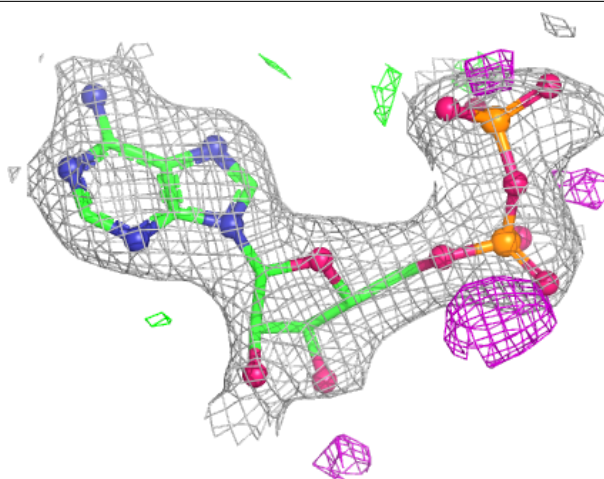
Electron density around ADP A 502 (A):

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



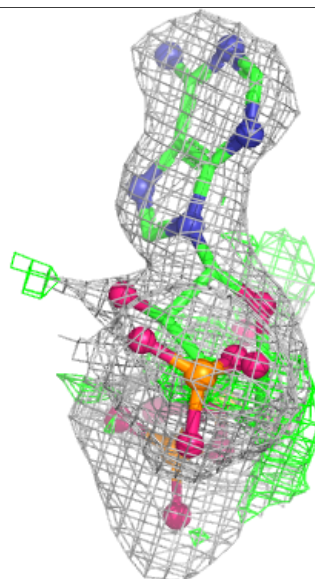
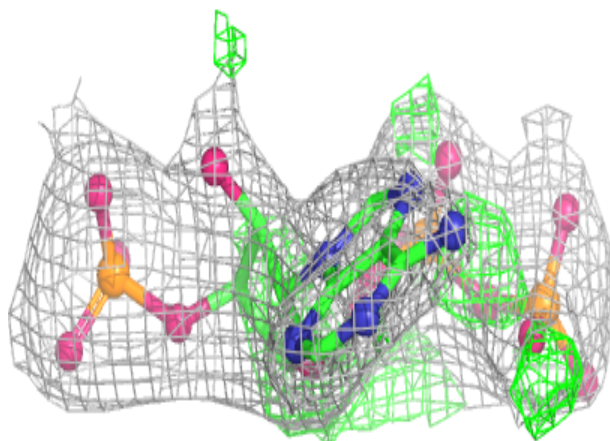
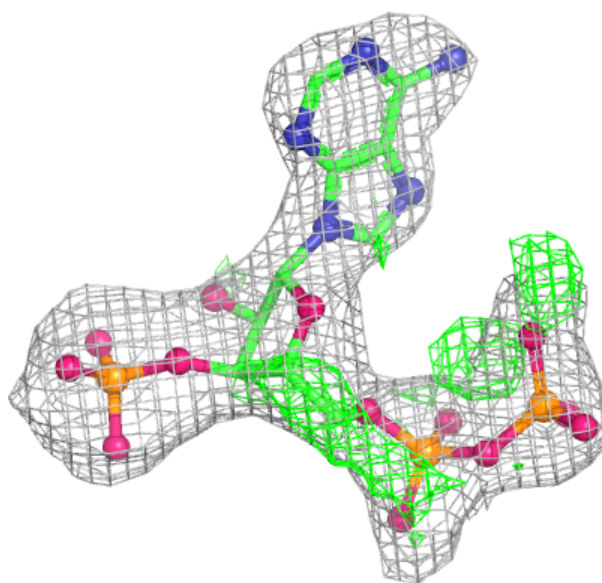
Electron density around ADP B 502:

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



Electron density around COA C 503 (A):

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.