Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 09:51 am GMT

PDB ID	:	2JI8
Title	:	X-ray structure of Oxalyl-CoA decarboxylase in complex with Formyl- CoA
Authors	:	Berthold, C.L.; Toyota, C.G.; Moussatche, P.; Wood, M.D.; Leeper, F.; Richards, N.G.J.; Lindqvist, Y.
Deposited on	:	2007-02-26
Resolution	:	2.15 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 (i) 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 (i)) were used in the production of this report:

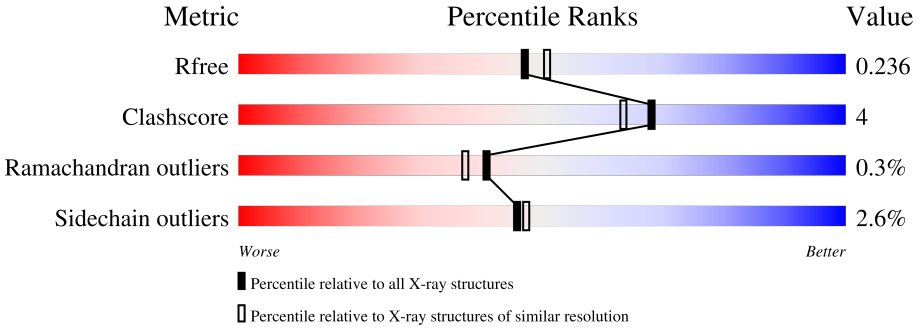
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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%

Mol	Chain	Length	Quality of chain
1	A	568	90% 8% • •
1	B	568	89% 8% • •

2 Entry composition (i)

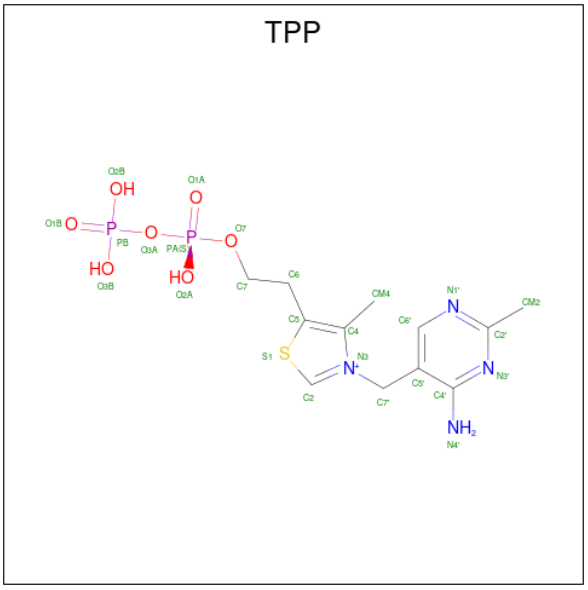
There are 7 unique types of molecules in this entry. The entry contains 9206 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OXALYL-COA DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	4194	2641	727	789	37	0	4	0
1	B	556	4170	2625	723	786	36	0	4	0

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).

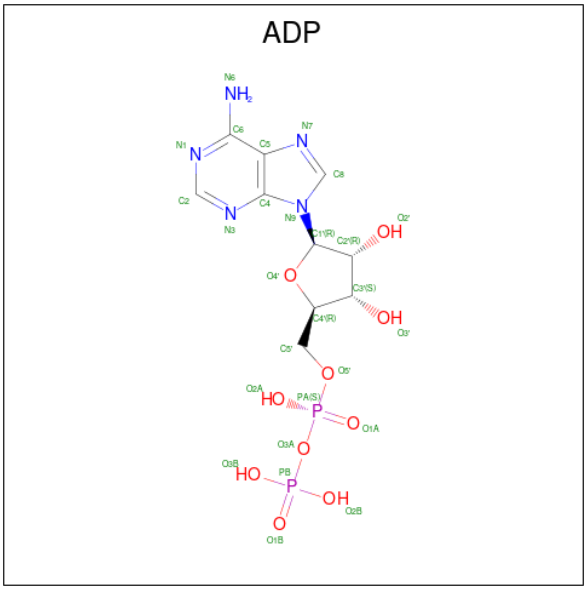


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	26	12	4	7	2	1	0	0
2	B	1	26	12	4	7	2	1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

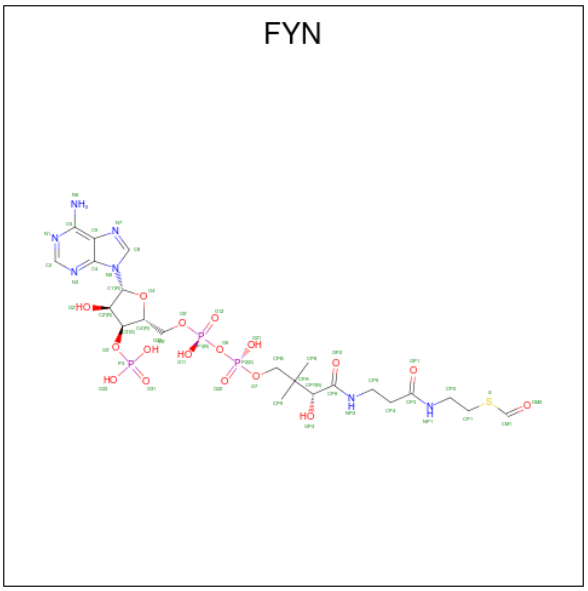
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
			Total	Mg		
3	B	1	1	1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



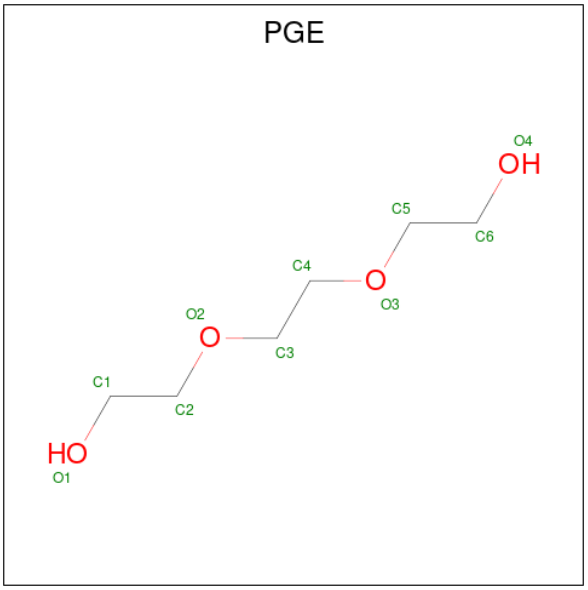
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
4	B	1	27	10	5	10	2	0	0

- Molecule 5 is S-{(9R,13S,15R)-17-[(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-4-HYDROXY-3-(PHOSPHONOOXY)TETRAHYDROFURAN-2-YL]-9,13,15-TRIHYDROXY-10,10-DIMETHYL-13,15-DIOXIDO-4,8-DIOXO-12,14,16-TRIOXA-3,7-DIAZA-13,15-DIPHOSPHAHEPTADEC-1-YL} THIOFORMATE (three-letter code: FYN) (formula: $C_{22}H_{36}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	A	1	50	22	7	17	3	1	0	0
			Total	C	N	O	P	S		
5	B	1	50	22	7	17	3	1	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 7 is water.

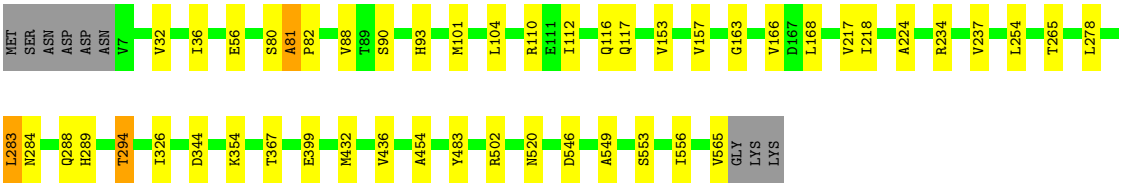
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	316	316	316	0	0
			Total	O		
7	B	298	298	298	0	0

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. 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. 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.

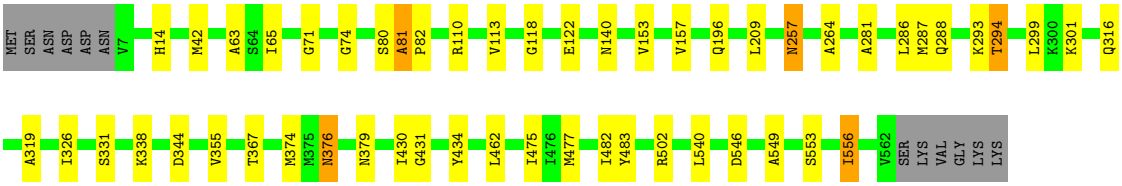
• Molecule 1: OXALYL-COA DECARBOXYLASE

Chain A:



• Molecule 1: OXALYL-COA DECARBOXYLASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.57Å 127.57Å 152.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.15 46.06 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (25.00-2.15) 98.6 (46.06-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.231 0.193 , 0.236	Depositor DCC
R_{free} test set	3662 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	1.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9206	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, TPP, FYN, PGE

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	0.46	0/4280	0.60	0/5793
1	B	0.45	0/4256	0.61	0/5762
All	All	0.46	0/8536	0.60	0/11555

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4194	0	4246	30	0
1	B	4170	0	4215	36	0
2	A	26	0	16	0	0
2	B	26	0	16	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	1	0
5	A	50	0	32	1	0
5	B	50	0	32	2	0
6	A	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	10	0	14	1	0
7	A	316	0	0	2	0
7	B	298	0	0	1	0
All	All	9206	0	8609	65	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 4.

All (65) 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:153:VAL:O	1:B:157:VAL:HG22	1.89	0.73
1:B:288:GLN:HG2	1:B:294:THR:HG21	1.72	0.71
1:B:113:VAL:HG22	1:B:122:GLU:HG3	1.79	0.64
1:B:14:HIS:CE1	1:B:42:MET:CE	2.81	0.63
1:A:153:VAL:O	1:A:157:VAL:HG22	1.99	0.63
1:B:376:ASN:HD22	1:B:376:ASN:C	2.03	0.62
1:B:81:ALA:HB3	1:B:82:PRO:CD	2.30	0.61
1:B:299:LEU:HD13	1:B:316:GLN:NE2	2.15	0.61
1:A:278:LEU:CD1	1:A:283:LEU:HD13	2.34	0.57
1:A:556:ILE:HD11	5:A:1569:FYN:S	2.44	0.57
1:A:283:LEU:O	1:A:289:HIS:HA	2.04	0.57
1:B:376:ASN:HD21	1:B:379:ASN:H	1.53	0.57
1:A:81:ALA:HB3	1:A:82:PRO:CD	2.36	0.55
1:B:556:ILE:HD11	5:B:1566:FYN:S	2.48	0.54
1:B:140:ASN:ND2	7:B:2110:HOH:O	2.40	0.54
1:B:257:ASN:C	1:B:257:ASN:HD22	2.12	0.53
1:B:81:ALA:CB	1:B:82:PRO:CD	2.87	0.52
1:A:112:ILE:HG23	1:A:117:GLN:HB2	1.90	0.52
1:A:56:GLU:OE2	2:B:1563:TPP:N1'	2.45	0.50
1:B:63:ALA:O	1:B:74:GLY:HA3	2.11	0.50
1:B:430:ILE:HD12	1:B:431:GLY:N	2.26	0.50
1:A:104:LEU:HD23	1:A:166:VAL:HB	1.93	0.49
1:A:278:LEU:HD11	1:A:283:LEU:HD13	1.93	0.49
1:B:326:ILE:HG13	4:B:1565:ADP:C2	2.46	0.49
1:A:104:LEU:HD22	1:A:168:LEU:HD11	1.95	0.49
1:B:209:LEU:HD21	1:B:301:LYS:HD3	1.95	0.49
1:B:546:ASP:HB3	1:B:549:ALA:HB2	1.92	0.49
1:A:288:GLN:OE1	1:A:294:THR:HG21	2.12	0.49
1:A:81:ALA:HB3	1:A:82:PRO:HD3	1.95	0.48
1:B:81:ALA:HB3	1:B:82:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:GLN:HG2	1:B:294:THR:CG2	2.41	0.47
1:A:483:TYR:CE1	1:A:553:SER:HA	2.49	0.47
1:B:14:HIS:CE1	1:B:42:MET:HE1	2.48	0.47
1:B:376:ASN:ND2	1:B:379:ASN:H	2.12	0.47
1:A:278:LEU:HD13	1:A:283:LEU:HD13	1.97	0.47
1:B:264:ALA:HB3	1:B:355:VAL:HG13	1.96	0.46
1:A:546:ASP:HB3	1:A:549:ALA:HB2	1.96	0.46
1:B:14:HIS:CE1	1:B:42:MET:HE3	2.50	0.46
1:B:430:ILE:HD12	1:B:430:ILE:C	2.36	0.46
1:A:278:LEU:HD11	1:A:283:LEU:CD1	2.46	0.45
1:A:432:MET:O	1:A:436:VAL:HG23	2.17	0.45
1:A:224:ALA:HA	1:A:326:ILE:HD13	1.98	0.45
1:A:116:GLN:NE2	7:A:2059:HOH:O	2.49	0.45
1:B:475:ILE:HG22	1:B:477:MET:CE	2.46	0.45
1:A:32:VAL:HA	1:A:36:ILE:HD11	1.97	0.45
1:B:483:TYR:CE1	1:B:553:SER:HA	2.52	0.44
1:A:520:ASN:ND2	7:A:2285:HOH:O	2.51	0.44
1:A:218:ILE:HD12	1:A:237:VAL:HG22	1.99	0.44
1:A:565:VAL:O	1:A:565:VAL:HG12	2.18	0.43
1:A:234:ARG:HA	1:A:254:LEU:HD11	2.00	0.43
1:B:71:GLY:HA3	6:B:1567:PGE:H2	2.00	0.43
1:A:81:ALA:CB	1:A:82:PRO:CD	2.96	0.43
1:B:286:LEU:O	5:B:1566:FYN:HP83	2.18	0.43
1:B:209:LEU:HD11	1:B:319:ALA:HB3	1.99	0.43
1:B:540:LEU:C	1:B:540:LEU:HD23	2.39	0.43
1:B:196:GLN:HE21	1:B:196:GLN:HA	1.83	0.43
1:A:399:GLU:HG3	1:A:454:ALA:HB1	2.01	0.42
1:A:101:MET:O	1:A:163:GLY:HA2	2.20	0.42
1:B:281:ALA:HB1	1:B:287:MET:CE	2.50	0.41
1:A:90:SER:O	1:A:93:HIS:HB3	2.20	0.41
1:A:284:ASN:HB2	1:B:118:GLY:O	2.20	0.41
1:A:265:THR:HG23	1:A:265:THR:O	2.21	0.41
1:B:65:ILE:HD13	1:B:434:TYR:CZ	2.56	0.41
1:B:482:ILE:HG23	2:B:1563:TPP:H62	2.02	0.41
1:B:475:ILE:HG22	1:B:477:MET:HE2	2.03	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	561/568 (99%)	540 (96%)	20 (4%)	1 (0%)	47	46
1	B	558/568 (98%)	541 (97%)	15 (3%)	2 (0%)	34	29
All	All	1119/1136 (98%)	1081 (97%)	35 (3%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ALA
1	B	81	ALA
1	B	556	ILE

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	441/445 (99%)	431 (98%)	10 (2%)	50	53
1	B	438/445 (98%)	424 (97%)	14 (3%)	39	38
All	All	879/890 (99%)	855 (97%)	24 (3%)	46	46

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	88	VAL
1	A	110	ARG

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Mol	Chain	Res	Type
1	A	217	VAL
1	A	283	LEU
1	A	294	THR
1	A	344	ASP
1	A	354	LYS
1	A	367	THR
1	A	502	ARG
1	B	80	SER
1	B	110	ARG
1	B	257	ASN
1	B	293	LYS
1	B	294	THR
1	B	331[A]	SER
1	B	331[B]	SER
1	B	338	LYS
1	B	344	ASP
1	B	367	THR
1	B	374	MET
1	B	376	ASN
1	B	462	LEU
1	B	502	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	228	GLN
1	A	520	ASN
1	B	140	ASN
1	B	183	ASN
1	B	196	GLN
1	B	228	GLN
1	B	257	ASN
1	B	304	GLN
1	B	316	GLN
1	B	376	ASN
1	B	491	GLN
1	B	520	ASN

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)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	ADP	A	1568	-	24,29,29	0.97	1 (4%)	29,45,45	1.38	6 (20%)
2	TPP	B	1563	3	22,27,27	1.54	5 (22%)	29,40,40	1.64	8 (27%)
4	ADP	B	1565	-	24,29,29	0.98	1 (4%)	29,45,45	1.34	5 (17%)
6	PGE	A	1570	-	9,9,9	0.54	0	8,8,8	0.30	0
2	TPP	A	1566	3	22,27,27	1.61	5 (22%)	29,40,40	1.59	9 (31%)
5	FYN	B	1566	-	43,52,52	1.04	1 (2%)	52,77,77	1.45	7 (13%)
6	PGE	B	1567	-	9,9,9	0.56	0	8,8,8	0.35	0
5	FYN	A	1569	-	43,52,52	1.04	1 (2%)	52,77,77	1.45	6 (11%)

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	ADP	A	1568	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	B	1563	3	-	5/16/17/17	0/2/2/2
4	ADP	B	1565	-	-	2/12/32/32	0/3/3/3
6	PGE	A	1570	-	-	4/7/7/7	-
2	TPP	A	1566	3	-	3/16/17/17	0/2/2/2
5	FYN	B	1566	-	-	3/45/66/66	0/3/3/3
6	PGE	B	1567	-	-	4/7/7/7	-
5	FYN	A	1569	-	-	3/45/66/66	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1569	FYN	CP1-S	-5.33	1.74	1.81
5	B	1566	FYN	CP1-S	-5.18	1.75	1.81
2	A	1566	TPP	C4-N3	-4.58	1.35	1.39
2	B	1563	TPP	C4-N3	-3.81	1.36	1.39
4	A	1568	ADP	C5-C4	2.58	1.47	1.40
2	A	1566	TPP	C4'-N3'	2.54	1.38	1.35
2	A	1566	TPP	C7'-N3	-2.52	1.44	1.48
2	A	1566	TPP	C2'-N1'	2.50	1.38	1.34
2	A	1566	TPP	C2'-N3'	2.49	1.38	1.34
4	B	1565	ADP	C5-C4	2.42	1.47	1.40
2	B	1563	TPP	C4'-N3'	2.33	1.38	1.35
2	B	1563	TPP	C2'-N1'	2.28	1.38	1.34
2	B	1563	TPP	C6'-N1'	2.11	1.38	1.34
2	B	1563	TPP	C7'-N3	-2.00	1.45	1.48

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1569	FYN	N3-C2-N1	-4.99	120.89	128.68
5	B	1566	FYN	N3-C2-N1	-4.79	121.19	128.68
5	A	1569	FYN	CP1-CP2-NP1	-4.51	102.94	112.42
5	B	1566	FYN	CP1-CP2-NP1	-4.15	103.69	112.42
5	B	1566	FYN	CP4-CP5-NP2	-3.93	103.97	111.90
2	B	1563	TPP	CM4-C4-N3	3.80	127.38	122.53
4	B	1565	ADP	N3-C2-N1	-3.77	122.78	128.68
5	A	1569	FYN	CP2-NP1-CP3	3.48	129.31	122.84
4	A	1568	ADP	N3-C2-N1	-3.45	123.29	128.68
5	B	1566	FYN	CP2-NP1-CP3	3.28	128.92	122.84
5	A	1569	FYN	CP4-CP5-NP2	-3.19	105.46	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1566	TPP	C6'-C5'-C4'	3.19	120.06	115.72
2	B	1563	TPP	N1'-C2'-N3'	-2.97	120.43	125.54
2	A	1566	TPP	N1'-C2'-N3'	-2.82	120.69	125.54
4	A	1568	ADP	C4-C5-N7	-2.81	106.47	109.40
2	A	1566	TPP	CM4-C4-N3	2.78	126.07	122.53
2	B	1563	TPP	CM2-C2'-N1'	2.74	120.15	117.14
2	B	1563	TPP	C6'-C5'-C4'	2.67	119.35	115.72
2	B	1563	TPP	PA-O3A-PB	-2.55	124.07	132.83
2	A	1566	TPP	O3B-PB-O3A	2.49	112.97	104.64
4	B	1565	ADP	C4-C5-N7	-2.47	106.82	109.40
5	B	1566	FYN	CP5-NP2-CP6	2.42	126.91	122.59
4	A	1568	ADP	C1'-N9-C4	-2.41	122.40	126.64
5	A	1569	FYN	CP5-NP2-CP6	2.35	126.78	122.59
4	A	1568	ADP	O3B-PB-O2B	2.28	116.33	107.64
2	A	1566	TPP	C5'-C6'-N1'	-2.27	120.03	123.82
5	B	1566	FYN	C1'-N9-C4	-2.26	122.67	126.64
2	B	1563	TPP	CM4-C4-C5	-2.25	122.67	127.60
2	A	1566	TPP	C6'-N1'-C2'	2.24	119.78	115.96
4	A	1568	ADP	C2-N1-C6	2.23	122.58	118.75
5	B	1566	FYN	C4-C5-N7	-2.20	107.10	109.40
2	A	1566	TPP	N4'-C4'-N3'	2.20	120.14	117.03
4	B	1565	ADP	PA-O3A-PB	-2.12	125.56	132.83
2	A	1566	TPP	CM2-C2'-N3'	2.11	120.45	117.15
4	B	1565	ADP	C1'-N9-C4	-2.10	122.95	126.64
4	B	1565	ADP	C2-N1-C6	2.07	122.29	118.75
2	A	1566	TPP	PA-O3A-PB	-2.07	125.73	132.83
4	A	1568	ADP	PA-O3A-PB	-2.06	125.76	132.83
2	B	1563	TPP	C6'-N1'-C2'	2.03	119.42	115.96
5	A	1569	FYN	C1'-N9-C4	-2.02	123.08	126.64
2	B	1563	TPP	C5'-C6'-N1'	-2.01	120.47	123.82

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1566	TPP	PA-O3A-PB-O2B
2	A	1566	TPP	PA-O3A-PB-O3B
2	B	1563	TPP	PA-O3A-PB-O3B
4	A	1568	ADP	O4'-C4'-C5'-O5'
4	B	1565	ADP	O4'-C4'-C5'-O5'
4	A	1568	ADP	C3'-C4'-C5'-O5'
4	B	1565	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
6	A	1570	PGE	O1-C1-C2-O2
6	B	1567	PGE	C6-C5-O3-C4
6	B	1567	PGE	O3-C5-C6-O4
6	B	1567	PGE	O2-C3-C4-O3
5	B	1566	FYN	P2-O6-P1-O12
5	A	1569	FYN	CP2-CP1-S-CM1
6	A	1570	PGE	C6-C5-O3-C4
5	A	1569	FYN	P2-O6-P1-O11
5	B	1566	FYN	P2-O6-P1-O11
2	A	1566	TPP	C4-C5-C6-C7
2	B	1563	TPP	C4-C5-C6-C7
6	B	1567	PGE	C4-C3-O2-C2
6	A	1570	PGE	C1-C2-O2-C3
5	B	1566	FYN	CP2-CP1-S-CM1
2	B	1563	TPP	PA-O3A-PB-O2B
5	A	1569	FYN	P2-O6-P1-O12
6	A	1570	PGE	O3-C5-C6-O4
2	B	1563	TPP	PA-O3A-PB-O1B
2	B	1563	TPP	C6-C7-O7-PA

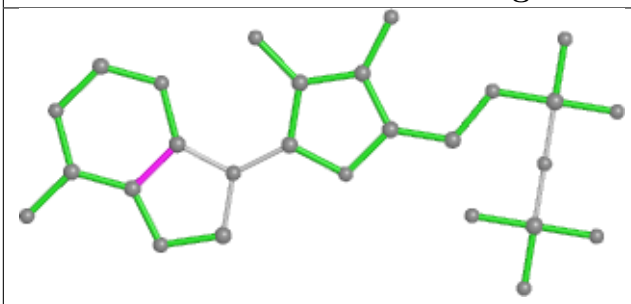
There are no ring outliers.

5 monomers are involved in 7 short contacts:

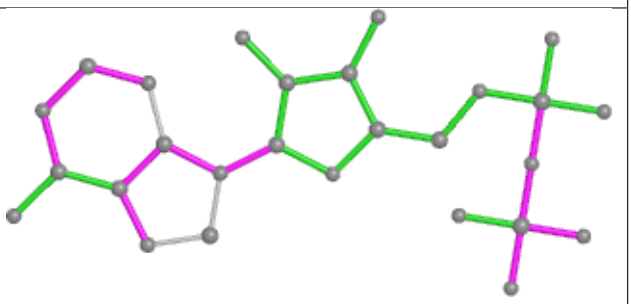
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1563	TPP	2	0
4	B	1565	ADP	1	0
5	B	1566	FYN	2	0
6	B	1567	PGE	1	0
5	A	1569	FYN	1	0

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 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.

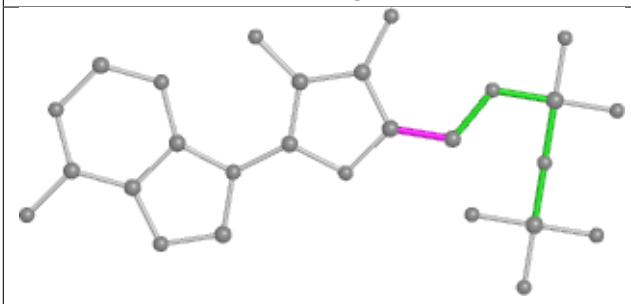
Ligand ADP A 1568



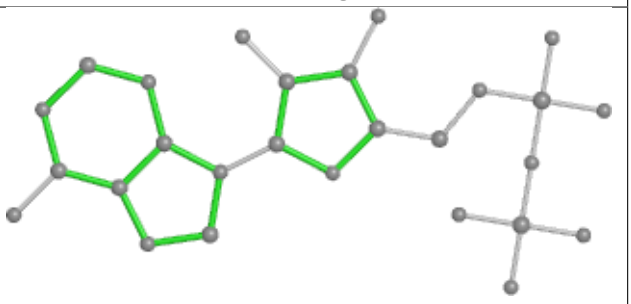
Bond lengths



Bond angles

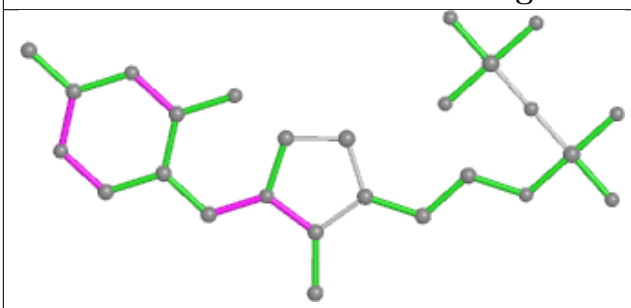


Torsions

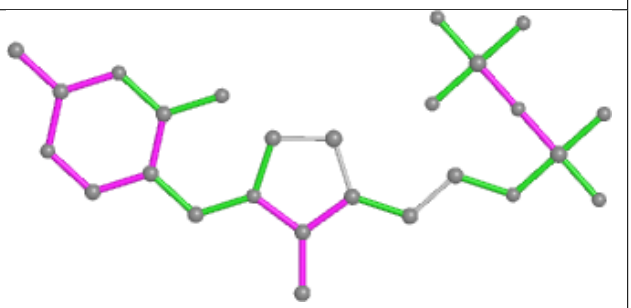


Rings

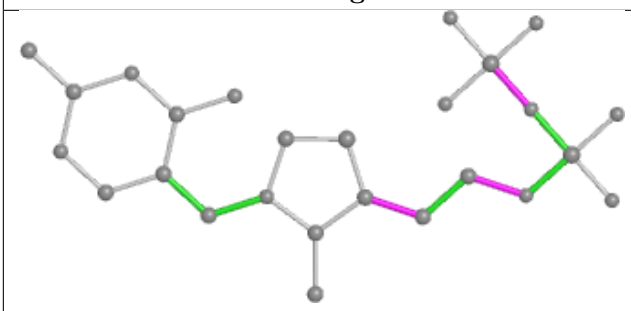
Ligand TPP B 1563



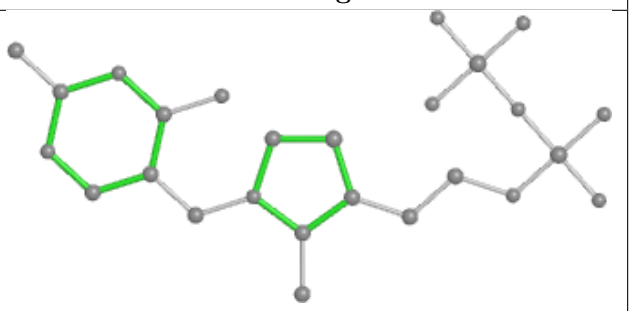
Bond lengths



Bond angles

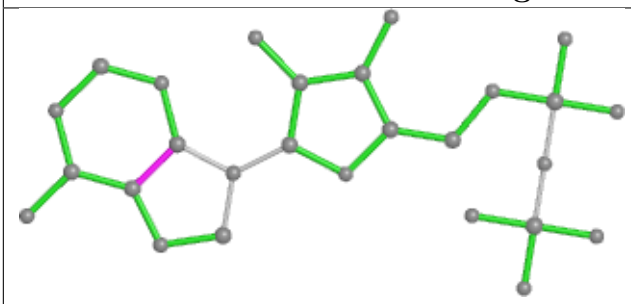


Torsions

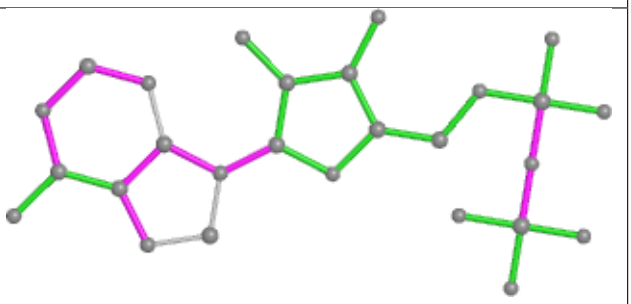


Rings

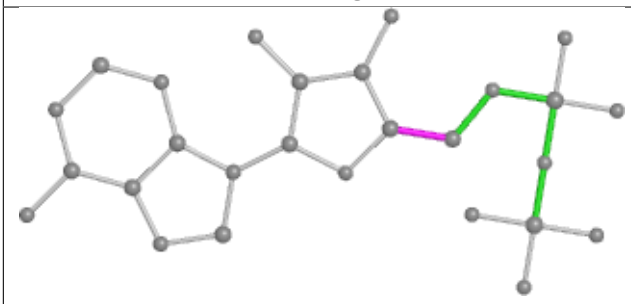
Ligand ADP B 1565



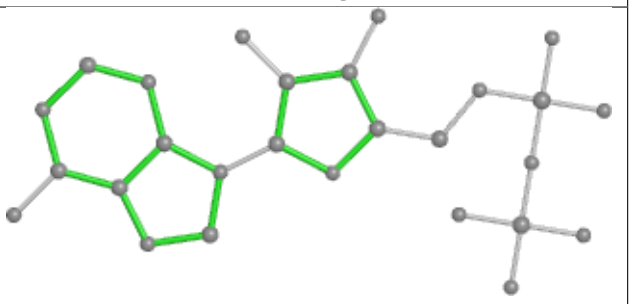
Bond lengths



Bond angles

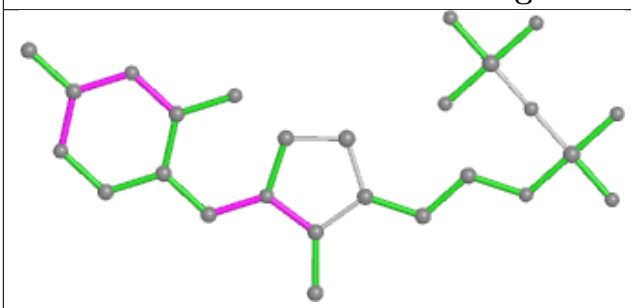


Torsions

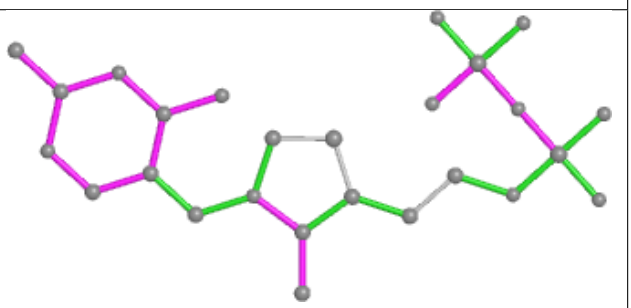


Rings

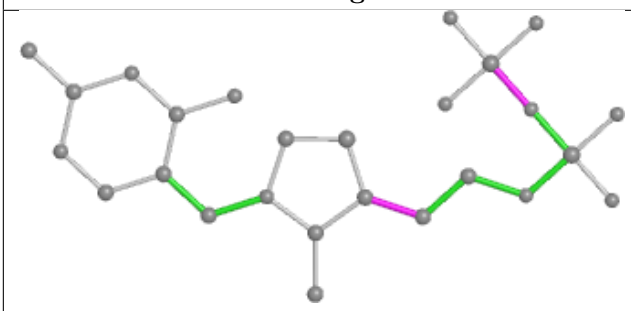
Ligand TPP A 1566



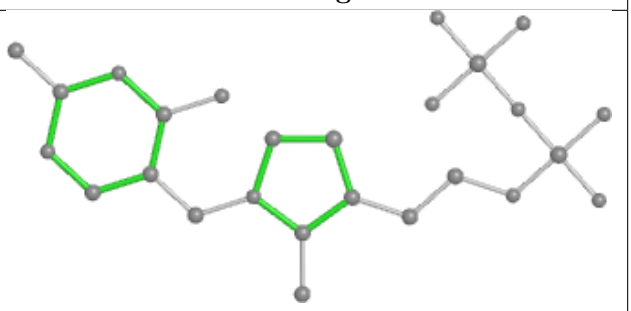
Bond lengths



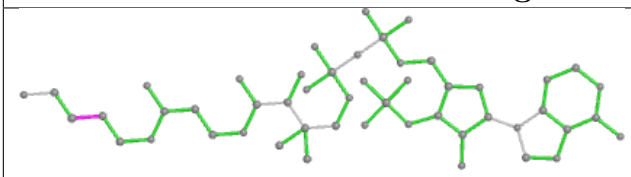
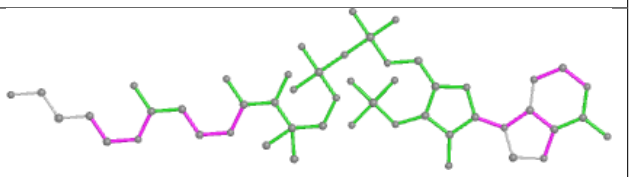
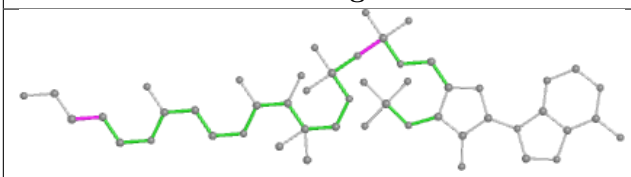
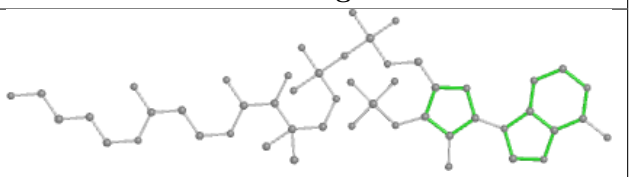
Bond angles

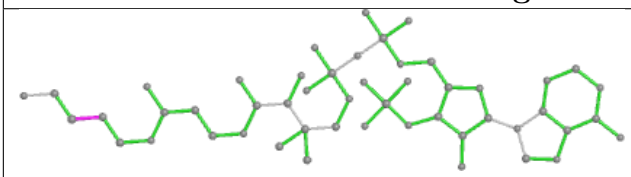
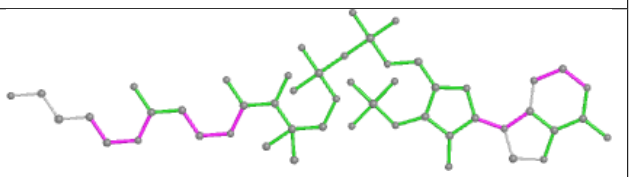
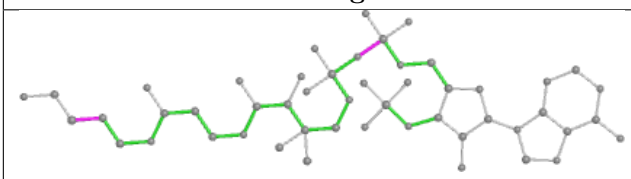
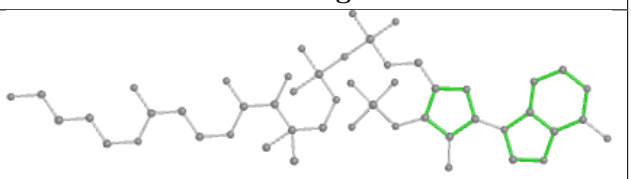


Torsions



Rings

Ligand FYN B 1566	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FYN A 1569	
 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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

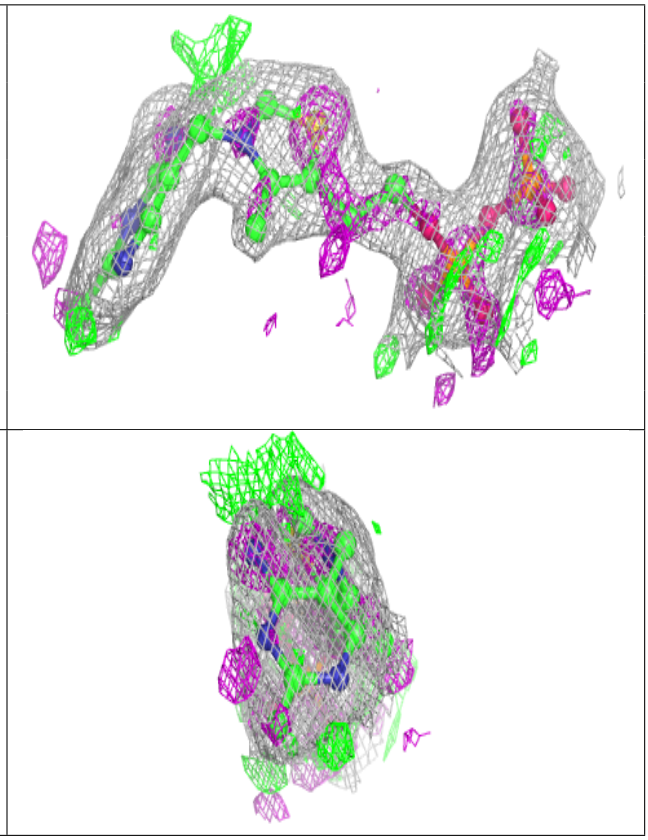
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

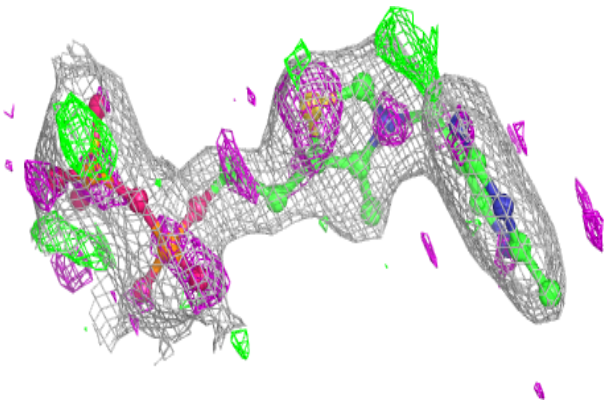
Electron density around TPP A 1566:

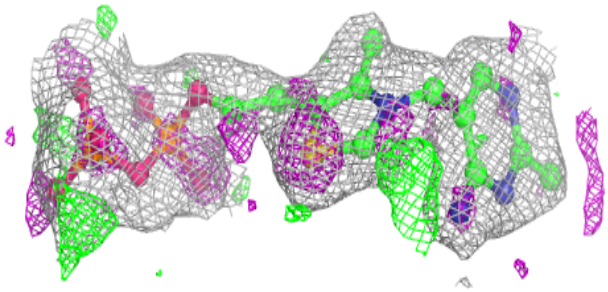
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

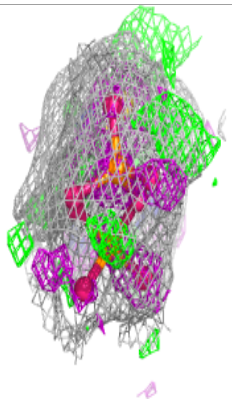


Electron density around TPP B 1563:

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

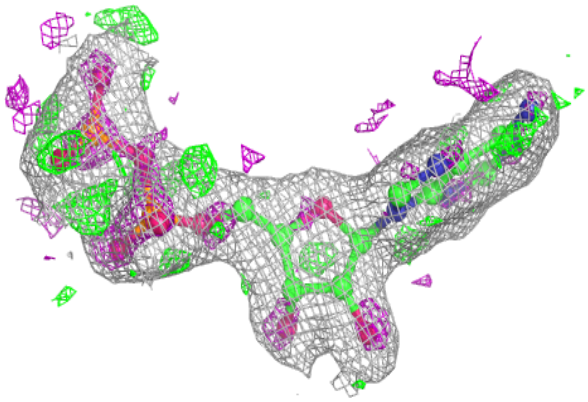


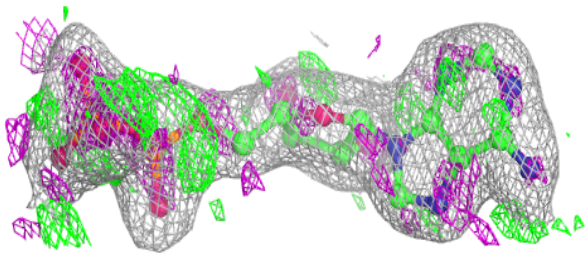


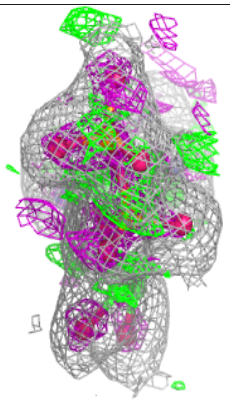


Electron density around ADP A 1568:

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

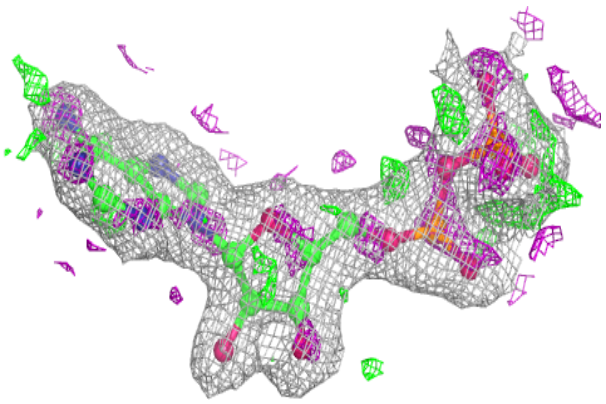


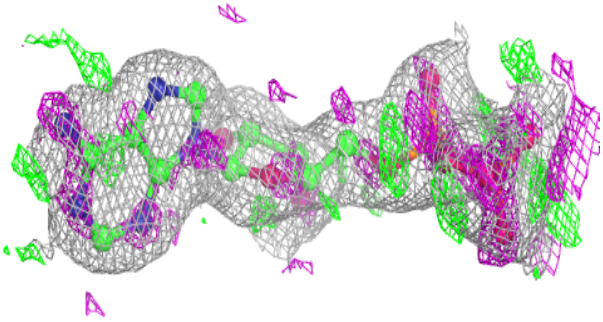


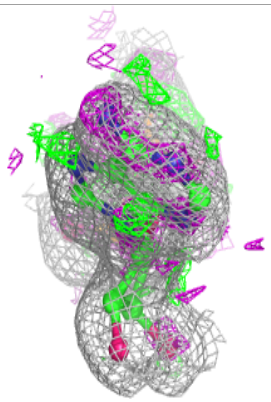


Electron density around ADP B 1565:

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

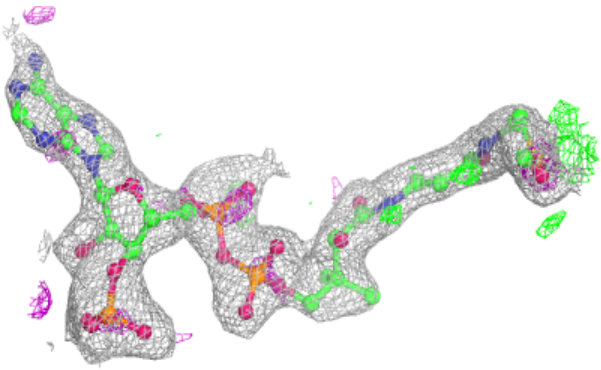


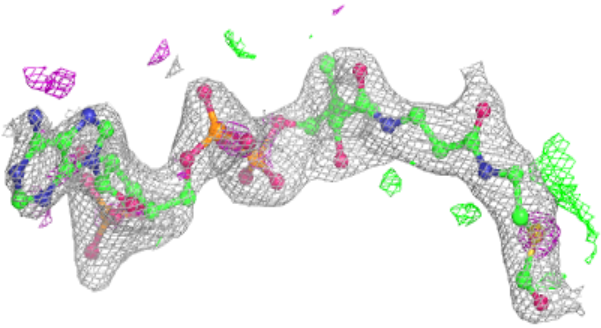


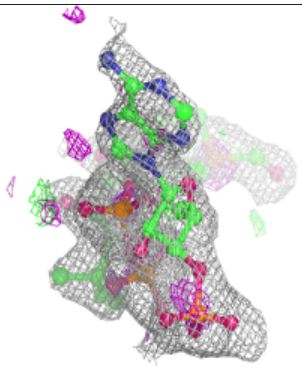


Electron density around FYN A 1569:

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

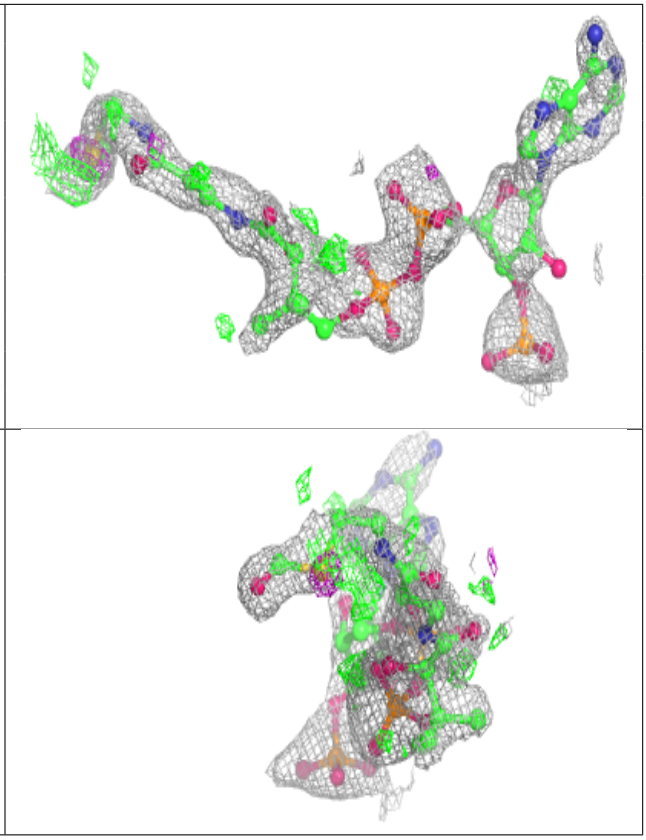






Electron density around FYN B 1566:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.