



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:20 PM UTC

PDB ID : 8VZD / pdb\_00008vzd  
Title : Crystal Structure of 2-Hydroxyacyl-CoA lyase/synthase TbHACS from Thermoflexaceae bacterium in the Complex with THDP, Formyl-CoA and ADP  
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Deposited on : 2024-02-11  
Resolution : 2.20 Å(reported)

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<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>.

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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

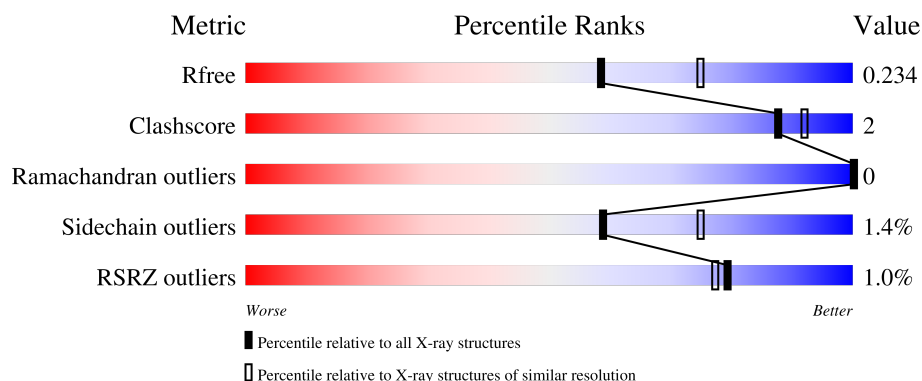
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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  $\geq 3$ , 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	550	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	B	550	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

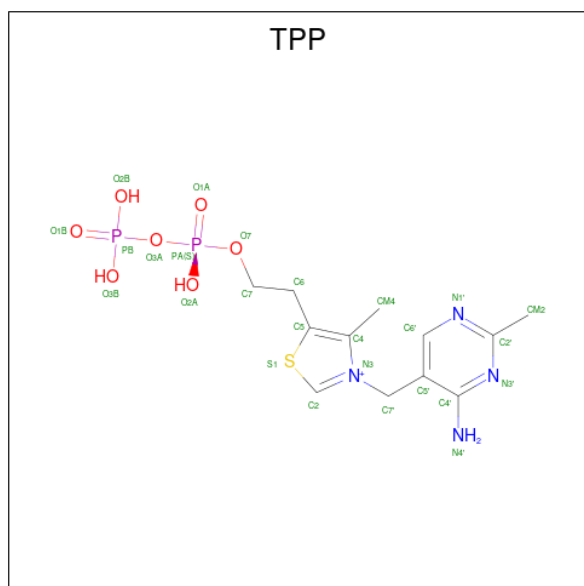
There are 8 unique types of molecules in this entry. The entry contains 9071 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-Hydroxyacyl-CoA Lyase/Synthase TbHACS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	2	0
			4173	2645	725	782	21			
1	B	548	Total	C	N	O	S	0	1	0
			4140	2626	716	778	20			

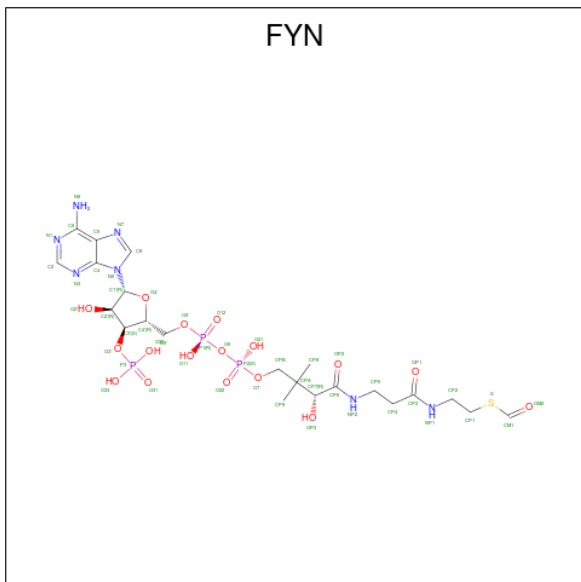
- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is S-{(9R,13S,15R)-17-[(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-4-HYDROXY-3-(PHOSPHONOXY)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-DIPHO

SPHAHEPTADEC-1-YL} THIOFORMATE (CCD ID: FYN) (formula:  $C_{22}H_{36}N_7O_{17}P_3S$ ) (labeled as "Ligand of Interest" by depositor).

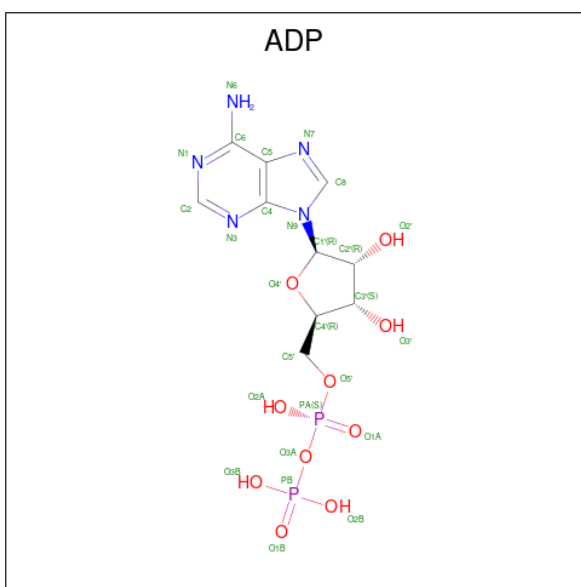


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			49	22	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			49	22	7	16	3	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

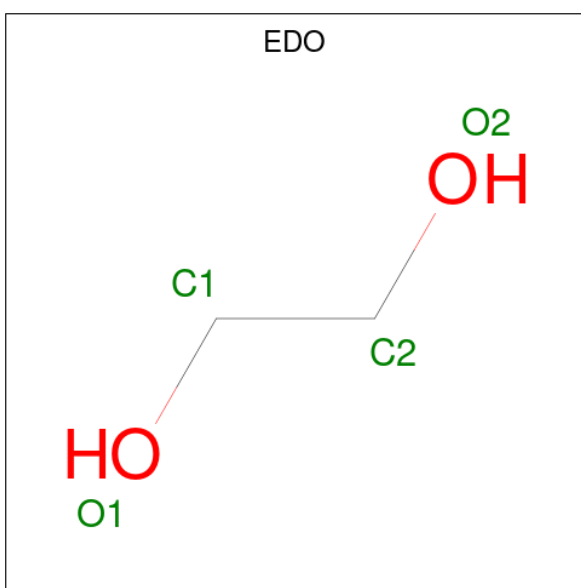
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



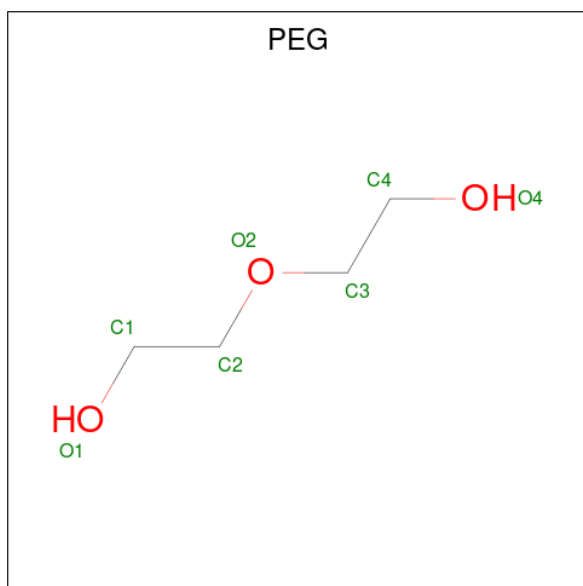
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



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

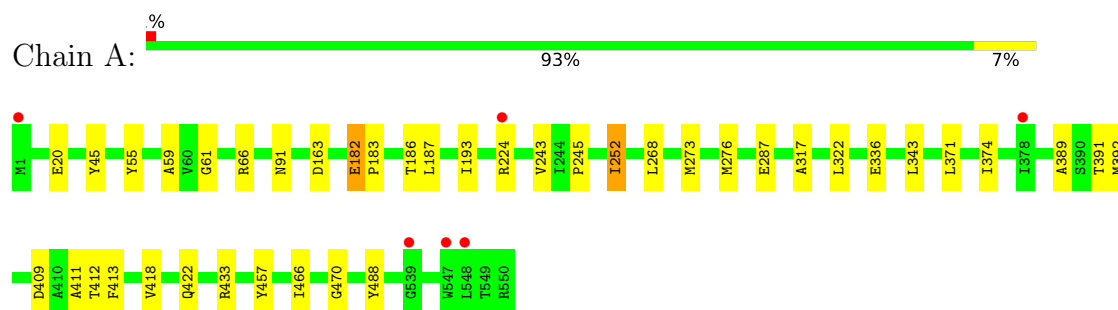
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	266	Total	O	0	0
			266	266		
8	B	247	Total	O	0	0
			247	247		

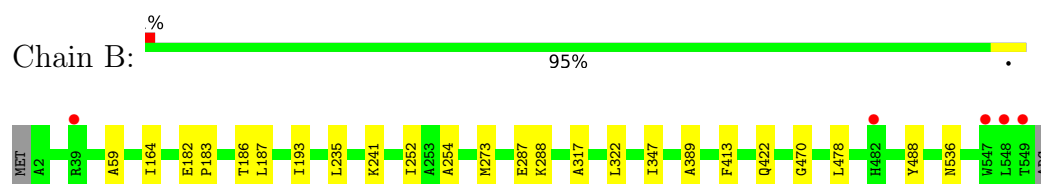
### 3 Residue-property plots [i](#)

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: 2-Hydroxyacyl-CoA Lyase/Synthase TbHACS



- Molecule 1: 2-Hydroxyacyl-CoA Lyase/Synthase TbHACS



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.17Å 182.51Å 123.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.38 – 2.20 37.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (37.38-2.20) 98.1 (37.38-2.20)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.198 , 0.234 0.197 , 0.234	Depositor DCC
$R_{free}$ test set	2797 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 21.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9071	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, ADP, TPP, FYN, CA, PEG

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	0.08	0/4274	0.25	0/5819
1	B	0.09	0/4241	0.25	0/5777
All	All	0.08	0/8515	0.25	0/11596

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	4173	0	4123	20	0
1	B	4140	0	4085	11	0
2	A	26	0	16	3	0
2	B	26	0	16	2	0
3	A	49	0	31	2	0
3	B	49	0	31	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	A	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	16	0	24	1	0
7	A	7	0	10	0	0
8	A	266	0	0	1	0
8	B	247	0	0	0	0
All	All	9071	0	8384	34	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 (34) 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:287:GLU:HG3	1:B:288:LYS:HG3	1.87	0.56
1:A:433:ARG:NH2	8:A:706:HOH:O	2.39	0.55
1:A:268:LEU:HD11	1:A:273:MET:HE2	1.88	0.54
1:A:252:ILE:HG21	1:A:343:LEU:HD13	1.89	0.53
1:B:59:ALA:HB2	1:B:422:GLN:HG2	1.91	0.52
1:A:470:GLY:HA2	1:A:488:TYR:CD2	2.46	0.50
1:A:391:THR:HG23	1:A:466:ILE:HD12	1.93	0.50
1:A:193:ILE:HG23	1:A:322:LEU:HD23	1.94	0.50
1:A:55:TYR:CG	1:A:418:VAL:HG12	2.48	0.49
1:B:182:GLU:HG3	1:B:183:PRO:HD2	1.95	0.49
1:A:182:GLU:HG3	1:A:183:PRO:HD2	1.95	0.48
1:A:371:LEU:HD23	1:A:374:ILE:HD12	1.97	0.47
1:B:536:ASN:H	6:B:608:EDO:H21	1.78	0.46
1:A:59:ALA:HB2	1:A:422:GLN:HG2	1.96	0.46
1:A:389:ALA:HB3	2:A:601:TPP:O3B	2.15	0.46
1:B:193:ILE:HG23	1:B:322:LEU:HD23	1.98	0.45
1:B:470:GLY:HA2	1:B:488:TYR:CD2	2.51	0.45
2:B:601:TPP:H2	3:B:602:FYN:S	2.56	0.45
1:A:224[A]:ARG:NE	1:A:243:VAL:O	2.49	0.45
2:A:601:TPP:H2	3:A:602:FYN:S	2.56	0.45
1:A:61:GLY:HA2	1:A:66:ARG:O	2.17	0.45
1:A:163:ASP:OD1	1:A:163:ASP:N	2.48	0.45
1:B:235:LEU:HB2	1:B:252:ILE:HD11	1.99	0.44
1:B:389:ALA:HB3	2:B:601:TPP:O3B	2.18	0.44
1:A:187:LEU:HD23	1:A:317:ALA:HB1	2.00	0.44
1:B:254:ALA:HB3	1:B:347:ILE:HG23	1.99	0.43
1:A:91:ASN:OD1	1:A:411:ALA:HB1	2.18	0.42
1:A:392:MET:SD	1:A:409:ASP:HB2	2.60	0.41
1:A:224[A]:ARG:CZ	1:A:245:PRO:HD3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LEU:HD23	1:B:317:ALA:HB1	2.02	0.41
1:A:276:MET:HE3	1:A:412:THR:HA	2.02	0.41
2:A:601:TPP:H2	3:A:602:FYN:CM1	2.51	0.41
1:B:478:LEU:HD23	1:B:478:LEU:HA	1.90	0.40
1:A:45:TYR:HA	1:A:457:TYR:CZ	2.56	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	550/550 (100%)	538 (98%)	12 (2%)	0	100	100
1	B	547/550 (100%)	535 (98%)	12 (2%)	0	100	100
All	All	1097/1100 (100%)	1073 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	425/423 (100%)	418 (98%)	7 (2%)	55	71
1	B	422/423 (100%)	417 (99%)	5 (1%)	63	78
All	All	847/846 (100%)	835 (99%)	12 (1%)	59	75

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	182	GLU
1	A	186	THR
1	A	252	ILE
1	A	287	GLU
1	A	336	GLU
1	A	413	PHE
1	B	164	ILE
1	B	186	THR
1	B	241	LYS
1	B	273	MET
1	B	413	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	143	GLN
1	A	422	GLN
1	B	143	GLN
1	B	422	GLN
1	B	491	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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$
7	PEG	A	607	-	6,6,6	0.12	0	5,5,5	0.09	0
6	EDO	A	608	-	3,3,3	0.43	0	2,2,2	0.35	0
6	EDO	B	605	-	3,3,3	0.42	0	2,2,2	0.35	0
3	FYN	B	602	-	49,51,52	0.85	3 (6%)	71,76,77	1.42	8 (11%)
3	FYN	A	602	-	49,51,52	0.86	4 (8%)	71,76,77	1.41	9 (12%)
6	EDO	B	607	-	3,3,3	0.42	0	2,2,2	0.39	0
6	EDO	A	606	-	3,3,3	0.44	0	2,2,2	0.28	0
2	TPP	A	601	4	26,27,27	0.31	0	38,40,40	0.33	0
6	EDO	A	609	-	3,3,3	0.43	0	2,2,2	0.38	0
2	TPP	B	601	4	26,27,27	0.28	0	38,40,40	0.33	0
6	EDO	B	606	-	3,3,3	0.43	0	2,2,2	0.37	0
6	EDO	B	608	-	3,3,3	0.42	0	2,2,2	0.44	0
5	ADP	A	604	-	28,29,29	1.41	4 (14%)	43,45,45	1.81	9 (20%)
5	ADP	B	604	-	28,29,29	1.41	4 (14%)	43,45,45	1.81	9 (20%)
6	EDO	A	605	-	3,3,3	0.45	0	2,2,2	0.31	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
7	PEG	A	607	-	-	2/4/4/4	-
6	EDO	A	608	-	-	0/1/1/1	-
6	EDO	B	605	-	-	0/1/1/1	-
3	FYN	B	602	-	-	3/49/65/66	0/3/3/3
3	FYN	A	602	-	-	2/49/65/66	0/3/3/3
6	EDO	B	607	-	-	1/1/1/1	-
6	EDO	A	606	-	-	0/1/1/1	-
2	TPP	A	601	4	-	2/17/17/17	0/2/2/2
6	EDO	A	609	-	-	0/1/1/1	-
2	TPP	B	601	4	-	3/17/17/17	0/2/2/2
6	EDO	B	606	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	608	-	-	1/1/1/1	-
5	ADP	A	604	-	-	4/16/32/32	0/3/3/3
5	ADP	B	604	-	-	6/16/32/32	0/3/3/3
6	EDO	A	605	-	-	1/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	ADP	C5-C4	4.64	1.47	1.39
5	B	604	ADP	C5-C4	4.60	1.47	1.39
5	B	604	ADP	C5-C6	2.78	1.48	1.41
5	A	604	ADP	C5-C6	2.76	1.48	1.41
5	A	604	ADP	C8-N7	2.43	1.36	1.31
5	B	604	ADP	C8-N7	2.42	1.36	1.31
5	A	604	ADP	C5-N7	-2.20	1.35	1.39
3	A	602	FYN	C8-N7	2.17	1.35	1.31
3	A	602	FYN	P1-O6	2.15	1.61	1.59
3	B	602	FYN	C8-N7	2.14	1.35	1.31
5	B	604	ADP	C5-N7	-2.13	1.35	1.39
3	A	602	FYN	P2-O6	2.10	1.61	1.59
3	B	602	FYN	C5-N7	-2.05	1.35	1.39
3	B	602	FYN	P1-O6	2.04	1.61	1.59
3	A	602	FYN	C5-N7	-2.02	1.35	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	ADP	C5-C4-N3	-5.59	119.02	126.72
5	B	604	ADP	C5-C4-N3	-5.50	119.14	126.72
3	B	602	FYN	C5-C4-N3	-5.11	119.69	126.72
3	A	602	FYN	C5-C4-N3	-5.04	119.77	126.72
3	A	602	FYN	N1-C2-N3	-4.94	121.11	128.58
3	B	602	FYN	N1-C2-N3	-4.90	121.16	128.58
5	A	604	ADP	N3-C4-N9	4.31	134.50	127.17
5	B	604	ADP	N3-C4-N9	4.25	134.39	127.17
5	B	604	ADP	C4-C5-N7	-3.67	106.38	110.58
5	B	604	ADP	C2-N3-C4	3.65	120.74	111.83
5	A	604	ADP	C2-N3-C4	3.65	120.73	111.83
5	A	604	ADP	C4-C5-N7	-3.63	106.43	110.58
3	A	602	FYN	N9-C8-N7	-3.62	108.80	113.94
3	B	602	FYN	N9-C8-N7	-3.60	108.83	113.94
3	B	602	FYN	C2-N3-C4	3.46	120.27	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	FYN	C2-N3-C4	3.45	120.26	111.83
5	B	604	ADP	N3-C2-N1	-3.29	123.60	128.58
5	A	604	ADP	N3-C2-N1	-3.25	123.66	128.58
3	B	602	FYN	N3-C4-N9	3.21	132.63	127.17
3	A	602	FYN	N3-C4-N9	3.15	132.52	127.17
5	B	604	ADP	C4-N9-C8	2.86	108.74	105.74
3	B	602	FYN	C4-C5-N7	-2.81	107.36	110.58
3	A	602	FYN	C4-C5-N7	-2.79	107.39	110.58
5	A	604	ADP	C4-N9-C8	2.72	108.59	105.74
5	B	604	ADP	C5-N7-C8	2.66	107.63	103.45
3	B	602	FYN	C5-N7-C8	2.65	107.62	103.45
3	A	602	FYN	C4-N9-C8	2.65	108.52	105.74
3	A	602	FYN	C5-N7-C8	2.63	107.58	103.45
3	B	602	FYN	C4-N9-C8	2.63	108.50	105.74
5	A	604	ADP	C5-N7-C8	2.61	107.55	103.45
5	B	604	ADP	C6-C5-N7	2.38	136.68	132.09
5	A	604	ADP	C6-C5-N7	2.30	136.52	132.09
5	B	604	ADP	N9-C8-N7	-2.23	110.78	113.94
5	A	604	ADP	N9-C8-N7	-2.11	110.94	113.94
3	A	602	FYN	CM1-S-CP1	2.01	110.73	100.32

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	TPP	PA-O3A-PB-O2B
2	B	601	TPP	PA-O3A-PB-O2B
5	B	604	ADP	PA-O3A-PB-O2B
6	A	605	EDO	O1-C1-C2-O2
5	A	604	ADP	O4'-C4'-C5'-O5'
5	A	604	ADP	C3'-C4'-C5'-O5'
5	B	604	ADP	O4'-C4'-C5'-O5'
5	A	604	ADP	C2'-C1'-N9-C8
5	B	604	ADP	C2'-C1'-N9-C8
3	A	602	FYN	P2-O6-P1-O11
3	B	602	FYN	P2-O6-P1-O11
3	A	602	FYN	CP2-CP1-S-CM1
7	A	607	PEG	O2-C3-C4-O4
5	B	604	ADP	PA-O3A-PB-O1B
5	B	604	ADP	C3'-C4'-C5'-O5'
6	B	608	EDO	O1-C1-C2-O2
3	B	602	FYN	CP2-CP1-S-CM1

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Mol	Chain	Res	Type	Atoms
7	A	607	PEG	C4-C3-O2-C2
6	B	607	EDO	O1-C1-C2-O2
2	A	601	TPP	PA-O3A-PB-O1B
2	B	601	TPP	PA-O3A-PB-O1B
2	B	601	TPP	PA-O3A-PB-O3B
5	B	604	ADP	O4'-C1'-N9-C8
3	B	602	FYN	NP2-CP6-CP7-CPA
5	A	604	ADP	O4'-C1'-N9-C8

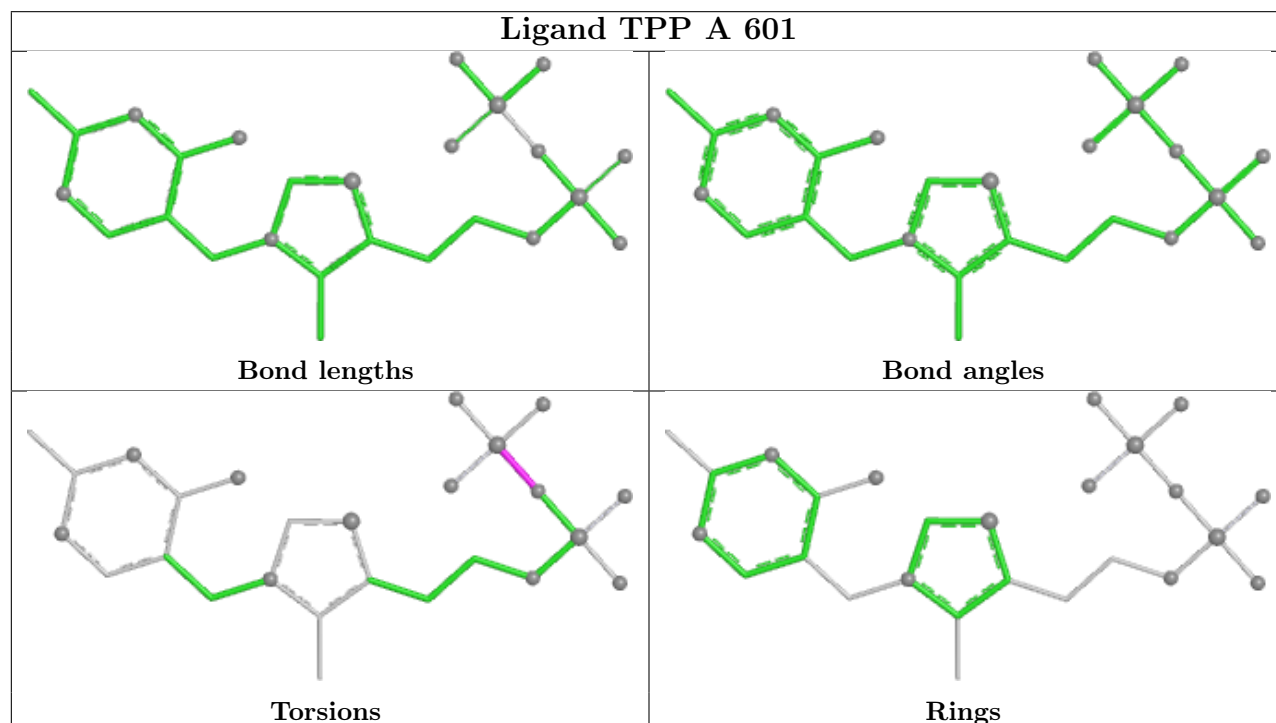
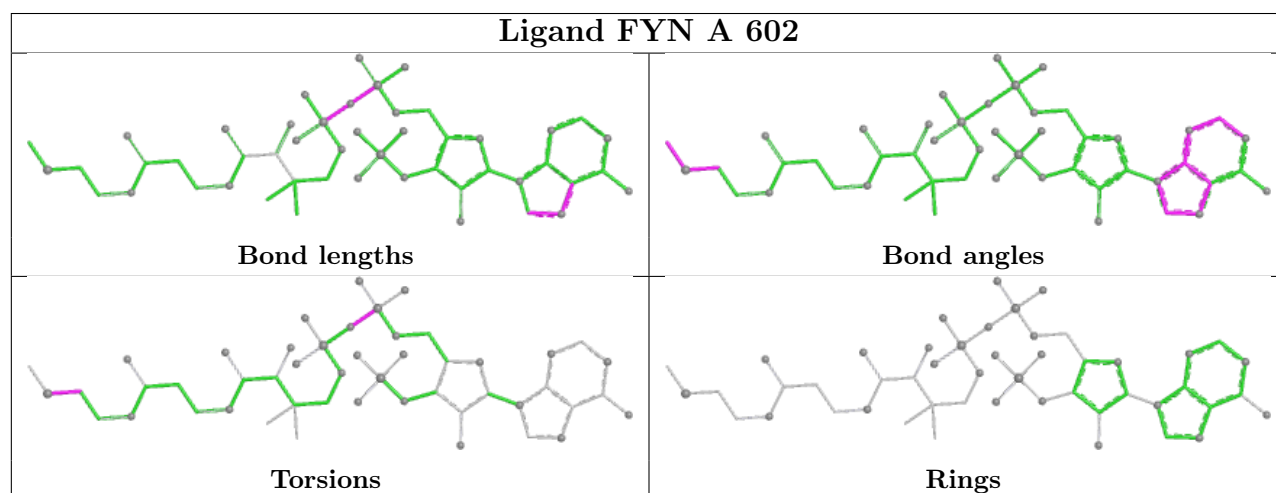
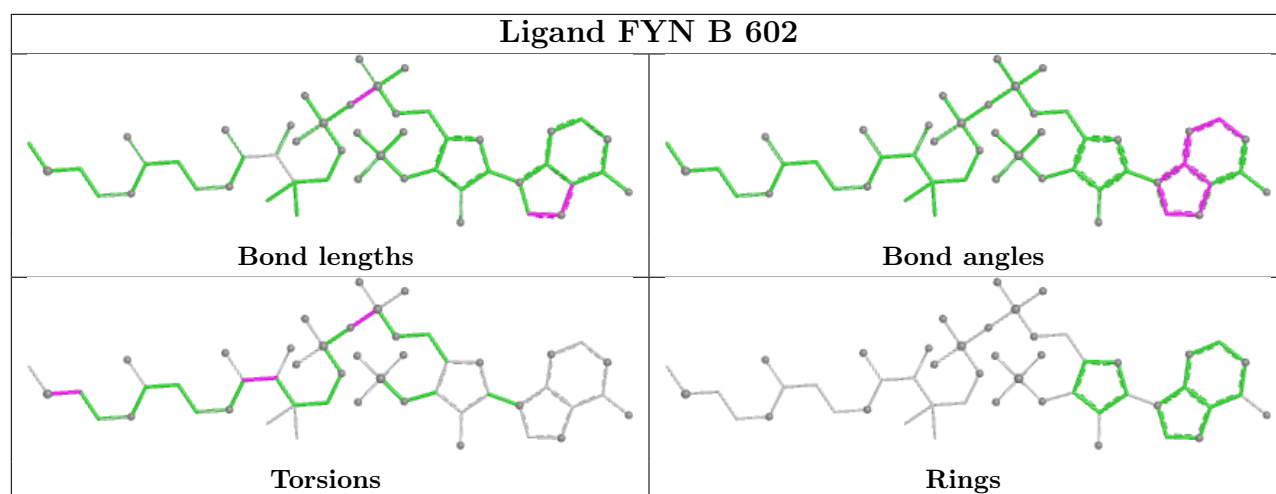
There are no ring outliers.

5 monomers are involved in 6 short contacts:

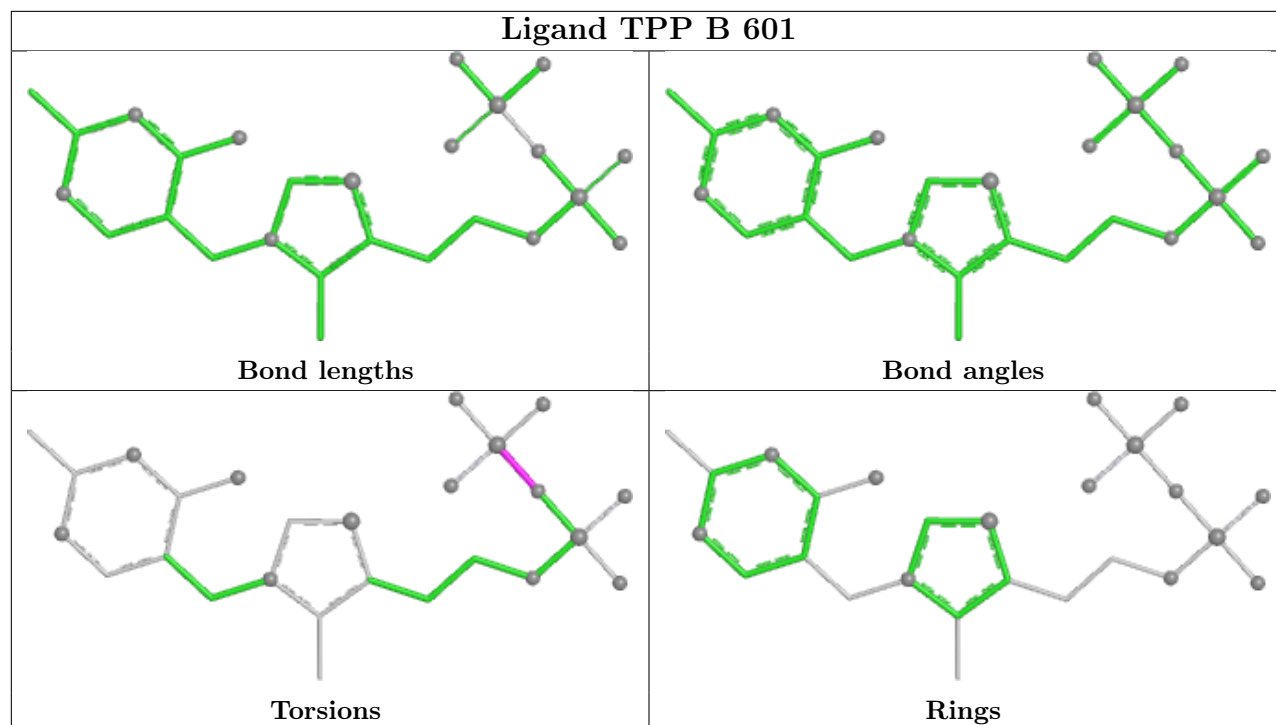
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	FYN	1	0
3	A	602	FYN	2	0
2	A	601	TPP	3	0
2	B	601	TPP	2	0
6	B	608	EDO	1	0

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.

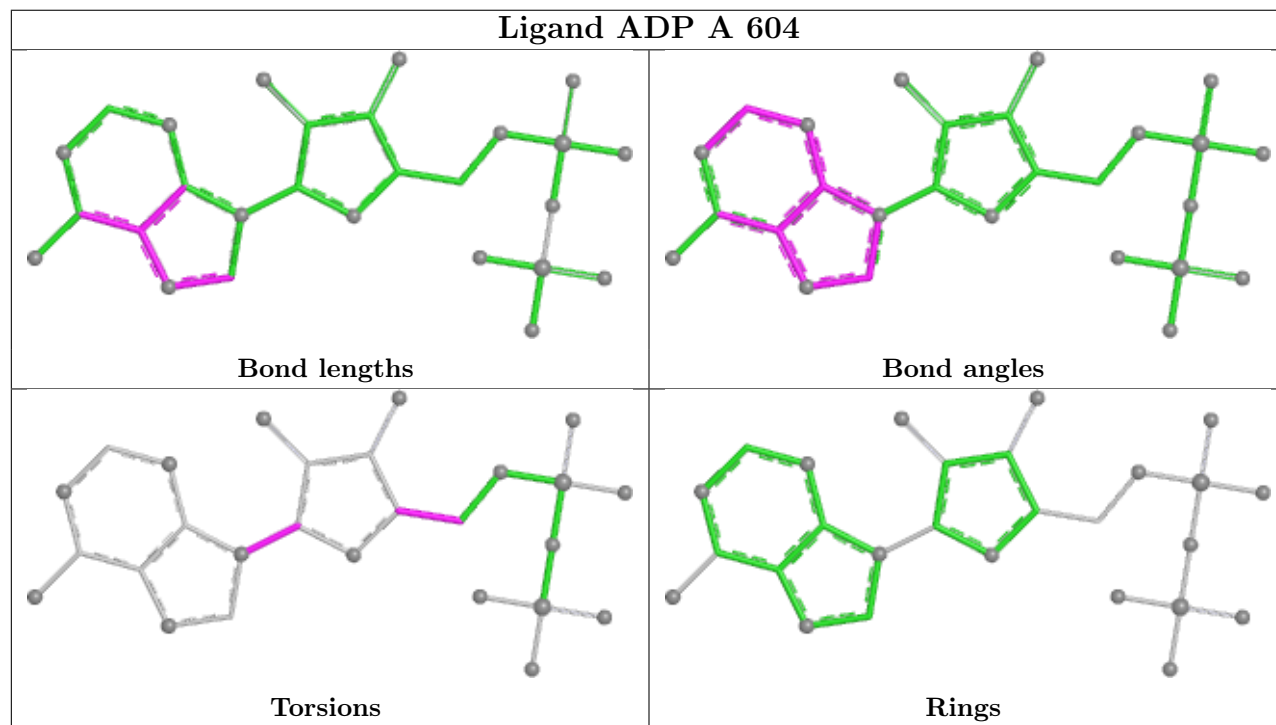


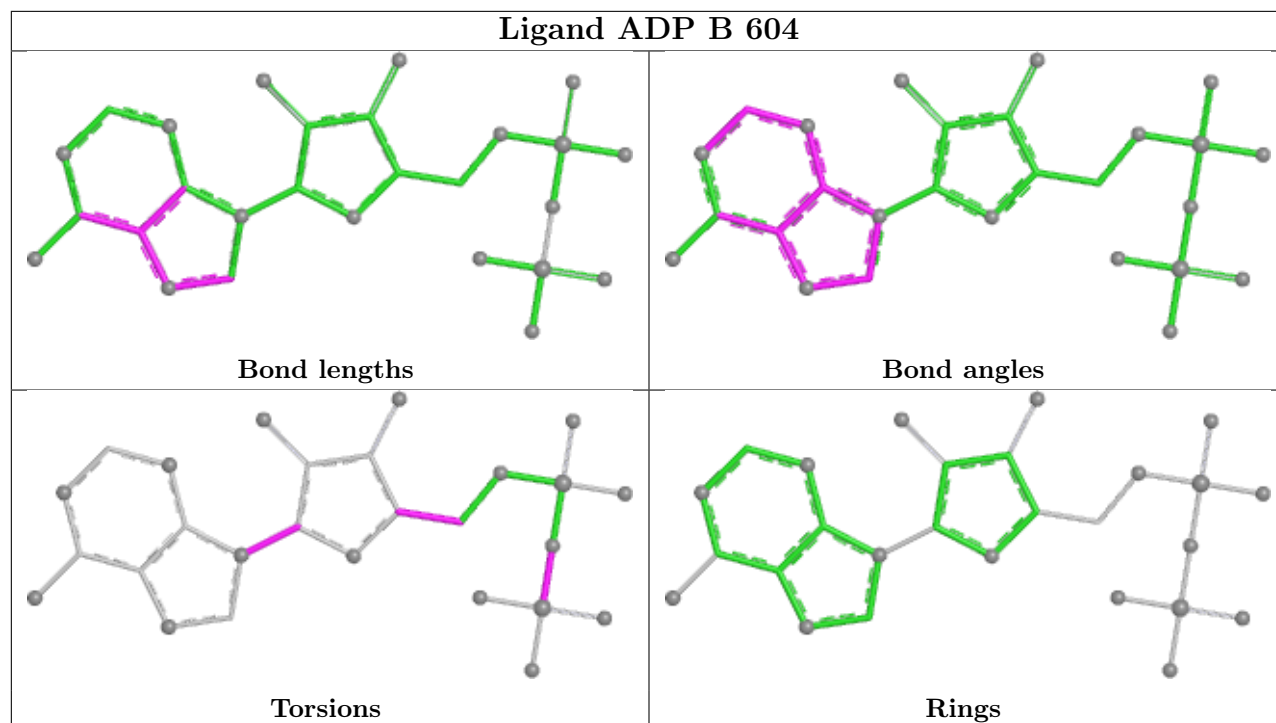


## Ligand TPP B 601



## Ligand ADP A 604





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	550/550 (100%)	-0.14	6 (1%) 78 76	12, 21, 32, 66	2 (0%)
1	B	548/550 (99%)	-0.10	5 (0%) 81 79	13, 22, 34, 52	1 (0%)
All	All	1098/1100 (99%)	-0.12	11 (1%) 79 77	12, 21, 34, 66	3 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.2
1	A	539	GLY	2.5
1	B	482	HIS	2.3
1	B	39	ARG	2.3
1	B	549	THR	2.2
1	A	378	ILE	2.1
1	B	547	TRP	2.1
1	A	224[A]	ARG	2.1
1	A	548	LEU	2.1
1	B	548	LEU	2.1
1	A	547	TRP	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 ⓘ

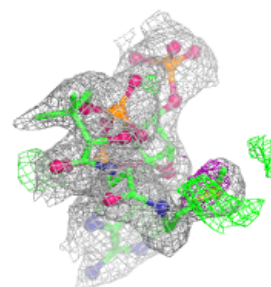
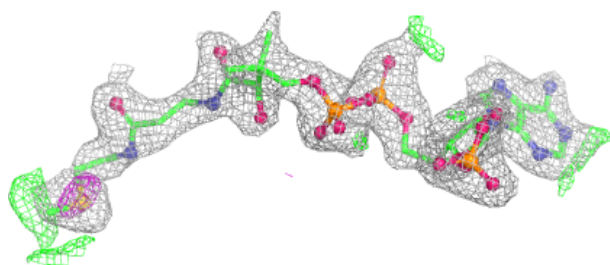
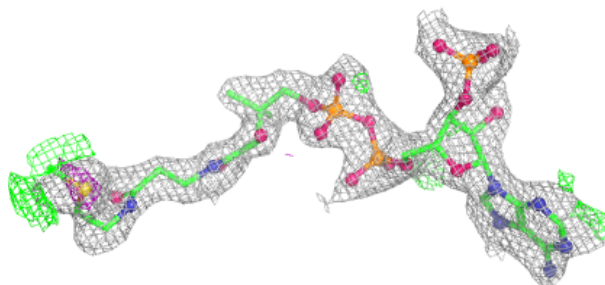
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	A	605	4/4	0.75	0.16	22,22,22,23	0
6	EDO	B	608	4/4	0.79	0.18	25,26,26,29	0
7	PEG	A	607	7/7	0.81	0.14	24,26,27,27	0
6	EDO	B	607	4/4	0.86	0.13	23,25,25,26	0
3	FYN	B	602	49/50	0.90	0.11	21,26,30,31	49
6	EDO	A	608	4/4	0.91	0.12	25,27,28,28	0
6	EDO	B	606	4/4	0.92	0.11	22,23,24,25	0
3	FYN	A	602	49/50	0.92	0.10	23,28,30,31	1
6	EDO	A	606	4/4	0.93	0.09	19,19,20,20	0
6	EDO	B	605	4/4	0.93	0.09	21,22,22,24	0
6	EDO	A	609	4/4	0.95	0.09	22,22,23,24	0
2	TPP	B	601	26/26	0.95	0.08	17,19,20,21	0
2	TPP	A	601	26/26	0.95	0.08	18,19,21,22	0
4	CA	B	603	1/1	0.97	0.10	18,18,18,18	0
5	ADP	A	604	27/27	0.97	0.06	17,19,20,20	0
5	ADP	B	604	27/27	0.97	0.07	17,19,20,21	0
4	CA	A	603	1/1	0.99	0.11	18,18,18,18	0

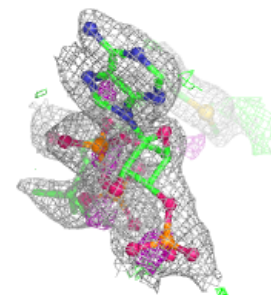
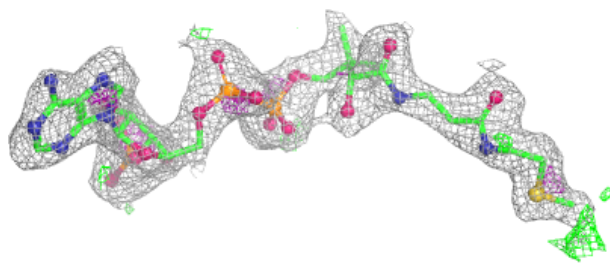
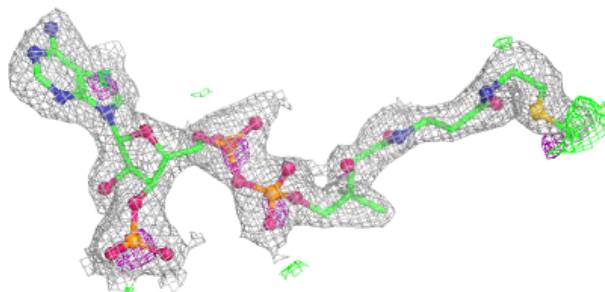
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FYN B 602:**

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

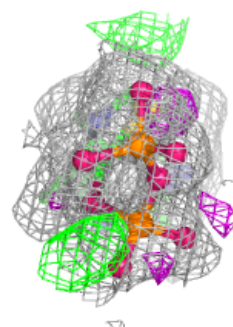
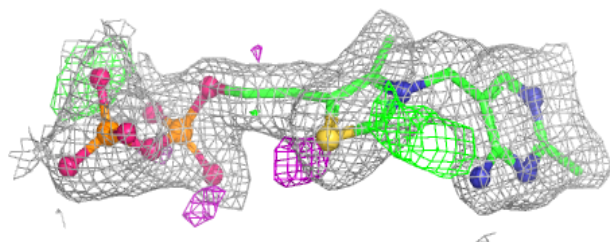
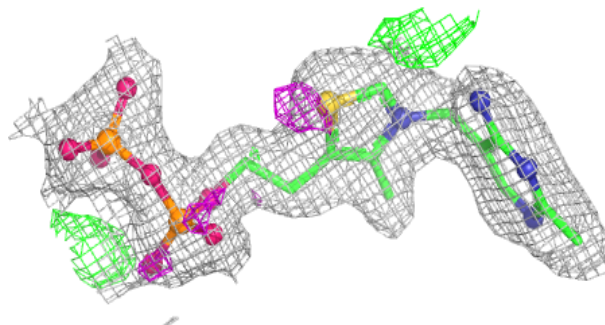
**Electron density around FYN A 602:**

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

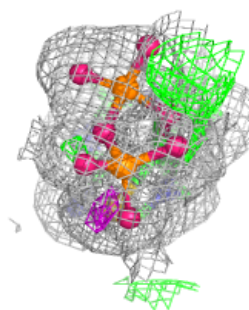
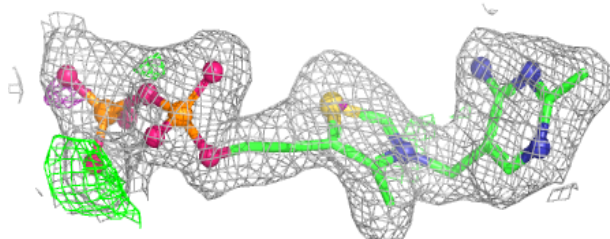
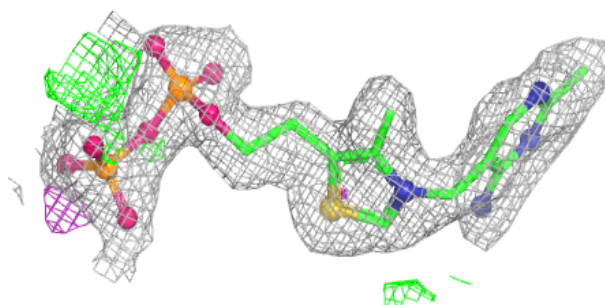


**Electron density around TPP B 601:**

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

**Electron density around TPP A 601:**

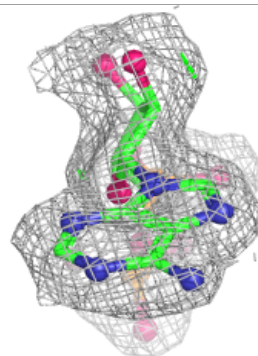
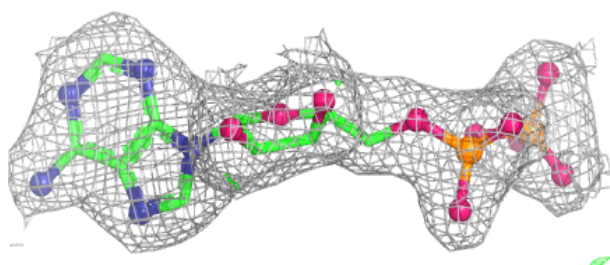
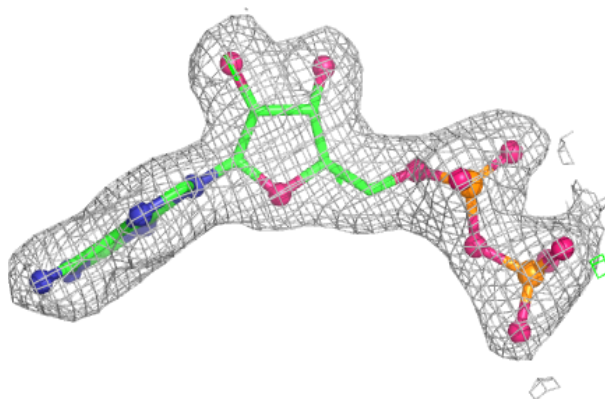
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



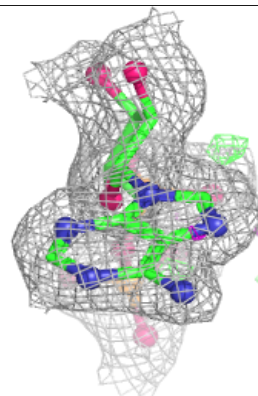
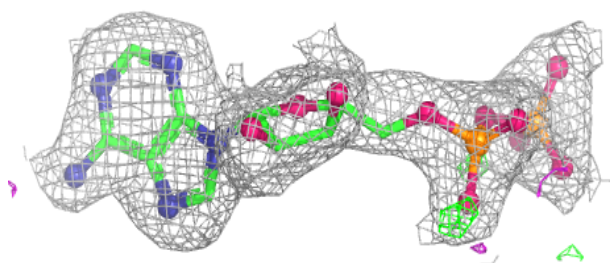
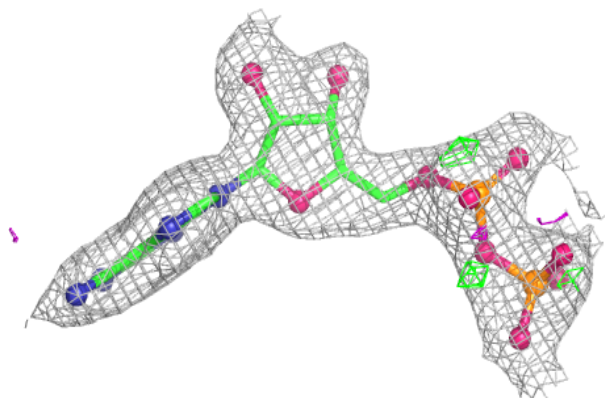


**Electron density around ADP A 604:**

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

**Electron density around ADP B 604:**

$2mF_o-DF_c$  (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.