



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 02:43 AM EDT

PDB ID : 4QQ8  
Title : Crystal structure of the formolase FLS in space group P 43 21 2  
Authors : Shen, B.W.; Siegel, J.B.; Stoddard, B.L.  
Deposited on : 2014-06-26  
Resolution : 2.88 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

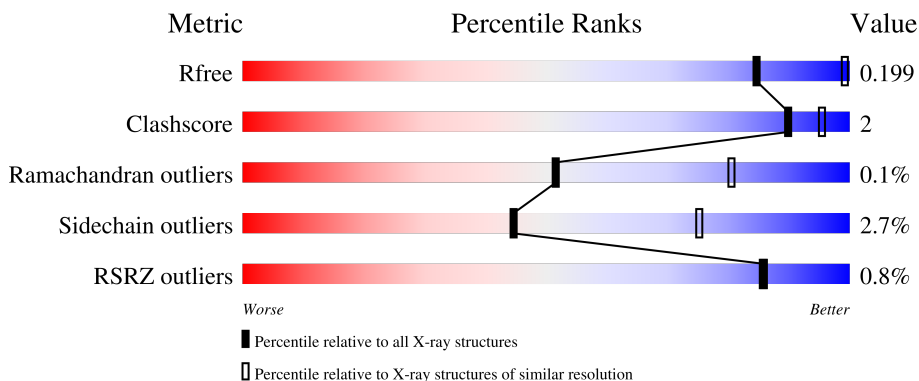
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

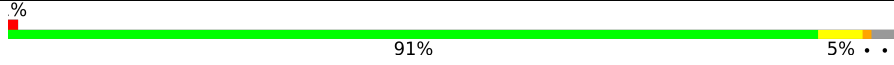
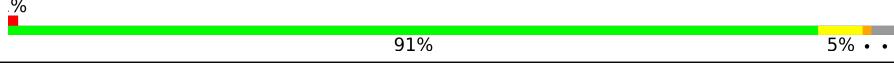
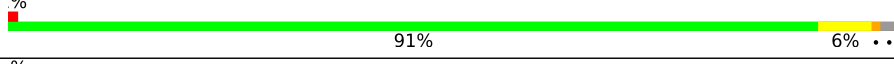
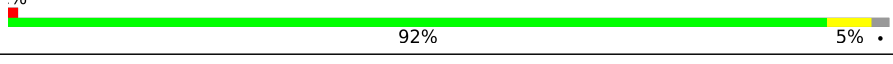
The reported resolution of this entry is 2.88 Å.

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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	583	 91% 5% . .
1	B	583	 91% 5% . .
1	C	583	 91% 6% . .
1	D	583	 92% 5% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	C	603	-	-	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 16915 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 Formolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	563	4163	2629	739	778	17	0	1	0
1	B	563	4163	2629	739	778	17	0	1	0
1	C	569	4202	2654	742	789	17	0	0	0
1	D	569	4213	2660	746	790	17	0	1	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ILE	ALA	conflict	UNP Q9F4L3
A	89	ARG	TRP	conflict	UNP Q9F4L3
A	90	THR	LEU	conflict	UNP Q9F4L3
A	188	HIS	ARG	conflict	UNP Q9F4L3
A	394	GLY	ALA	conflict	UNP Q9F4L3
A	419	ASN	GLY	conflict	UNP Q9F4L3
A	480	TRP	ALA	conflict	UNP Q9F4L3
A	564	GLY	-	expression tag	UNP Q9F4L3
A	565	SER	-	expression tag	UNP Q9F4L3
A	566	THR	-	expression tag	UNP Q9F4L3
A	567	GLU	-	expression tag	UNP Q9F4L3
A	568	ASN	-	expression tag	UNP Q9F4L3
A	569	LEU	-	expression tag	UNP Q9F4L3
A	570	TYR	-	expression tag	UNP Q9F4L3
A	571	PHE	-	expression tag	UNP Q9F4L3
A	572	GLN	-	expression tag	UNP Q9F4L3
A	573	SER	-	expression tag	UNP Q9F4L3
A	574	GLY	-	expression tag	UNP Q9F4L3
A	575	ALA	-	expression tag	UNP Q9F4L3
A	576	LEU	-	expression tag	UNP Q9F4L3
A	577	GLU	-	expression tag	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	578	HIS	-	expression tag	UNP Q9F4L3
A	579	HIS	-	expression tag	UNP Q9F4L3
A	580	HIS	-	expression tag	UNP Q9F4L3
A	581	HIS	-	expression tag	UNP Q9F4L3
A	582	HIS	-	expression tag	UNP Q9F4L3
A	583	HIS	-	expression tag	UNP Q9F4L3
B	28	ILE	ALA	conflict	UNP Q9F4L3
B	89	ARG	TRP	conflict	UNP Q9F4L3
B	90	THR	LEU	conflict	UNP Q9F4L3
B	188	HIS	ARG	conflict	UNP Q9F4L3
B	394	GLY	ALA	conflict	UNP Q9F4L3
B	419	ASN	GLY	conflict	UNP Q9F4L3
B	480	TRP	ALA	conflict	UNP Q9F4L3
B	564	GLY	-	expression tag	UNP Q9F4L3
B	565	SER	-	expression tag	UNP Q9F4L3
B	566	THR	-	expression tag	UNP Q9F4L3
B	567	GLU	-	expression tag	UNP Q9F4L3
B	568	ASN	-	expression tag	UNP Q9F4L3
B	569	LEU	-	expression tag	UNP Q9F4L3
B	570	TYR	-	expression tag	UNP Q9F4L3
B	571	PHE	-	expression tag	UNP Q9F4L3
B	572	GLN	-	expression tag	UNP Q9F4L3
B	573	SER	-	expression tag	UNP Q9F4L3
B	574	GLY	-	expression tag	UNP Q9F4L3
B	575	ALA	-	expression tag	UNP Q9F4L3
B	576	LEU	-	expression tag	UNP Q9F4L3
B	577	GLU	-	expression tag	UNP Q9F4L3
B	578	HIS	-	expression tag	UNP Q9F4L3
B	579	HIS	-	expression tag	UNP Q9F4L3
B	580	HIS	-	expression tag	UNP Q9F4L3
B	581	HIS	-	expression tag	UNP Q9F4L3
B	582	HIS	-	expression tag	UNP Q9F4L3
B	583	HIS	-	expression tag	UNP Q9F4L3
C	28	ILE	ALA	conflict	UNP Q9F4L3
C	89	ARG	TRP	conflict	UNP Q9F4L3
C	90	THR	LEU	conflict	UNP Q9F4L3
C	188	HIS	ARG	conflict	UNP Q9F4L3
C	394	GLY	ALA	conflict	UNP Q9F4L3
C	419	ASN	GLY	conflict	UNP Q9F4L3
C	480	TRP	ALA	conflict	UNP Q9F4L3
C	564	GLY	-	expression tag	UNP Q9F4L3
C	565	SER	-	expression tag	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	566	THR	-	expression tag	UNP Q9F4L3
C	567	GLU	-	expression tag	UNP Q9F4L3
C	568	ASN	-	expression tag	UNP Q9F4L3
C	569	LEU	-	expression tag	UNP Q9F4L3
C	570	TYR	-	expression tag	UNP Q9F4L3
C	571	PHE	-	expression tag	UNP Q9F4L3
C	572	GLN	-	expression tag	UNP Q9F4L3
C	573	SER	-	expression tag	UNP Q9F4L3
C	574	GLY	-	expression tag	UNP Q9F4L3
C	575	ALA	-	expression tag	UNP Q9F4L3
C	576	LEU	-	expression tag	UNP Q9F4L3
C	577	GLU	-	expression tag	UNP Q9F4L3
C	578	HIS	-	expression tag	UNP Q9F4L3
C	579	HIS	-	expression tag	UNP Q9F4L3
C	580	HIS	-	expression tag	UNP Q9F4L3
C	581	HIS	-	expression tag	UNP Q9F4L3
C	582	HIS	-	expression tag	UNP Q9F4L3
C	583	HIS	-	expression tag	UNP Q9F4L3
D	28	ILE	ALA	conflict	UNP Q9F4L3
D	89	ARG	TRP	conflict	UNP Q9F4L3
D	90	THR	LEU	conflict	UNP Q9F4L3
D	188	HIS	ARG	conflict	UNP Q9F4L3
D	394	GLY	ALA	conflict	UNP Q9F4L3
D	419	ASN	GLY	conflict	UNP Q9F4L3
D	480	TRP	ALA	conflict	UNP Q9F4L3
D	564	GLY	-	expression tag	UNP Q9F4L3
D	565	SER	-	expression tag	UNP Q9F4L3
D	566	THR	-	expression tag	UNP Q9F4L3
D	567	GLU	-	expression tag	UNP Q9F4L3
D	568	ASN	-	expression tag	UNP Q9F4L3
D	569	LEU	-	expression tag	UNP Q9F4L3
D	570	TYR	-	expression tag	UNP Q9F4L3
D	571	PHE	-	expression tag	UNP Q9F4L3
D	572	GLN	-	expression tag	UNP Q9F4L3
D	573	SER	-	expression tag	UNP Q9F4L3
D	574	GLY	-	expression tag	UNP Q9F4L3
D	575	ALA	-	expression tag	UNP Q9F4L3
D	576	LEU	-	expression tag	UNP Q9F4L3
D	577	GLU	-	expression tag	UNP Q9F4L3
D	578	HIS	-	expression tag	UNP Q9F4L3
D	579	HIS	-	expression tag	UNP Q9F4L3
D	580	HIS	-	expression tag	UNP Q9F4L3

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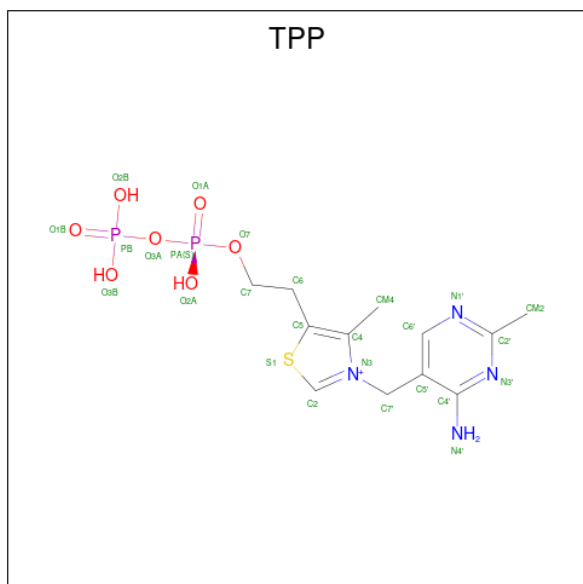
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Chain	Residue	Modelled	Actual	Comment	Reference
D	581	HIS	-	expression tag	UNP Q9F4L3
D	582	HIS	-	expression tag	UNP Q9F4L3
D	583	HIS	-	expression tag	UNP Q9F4L3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

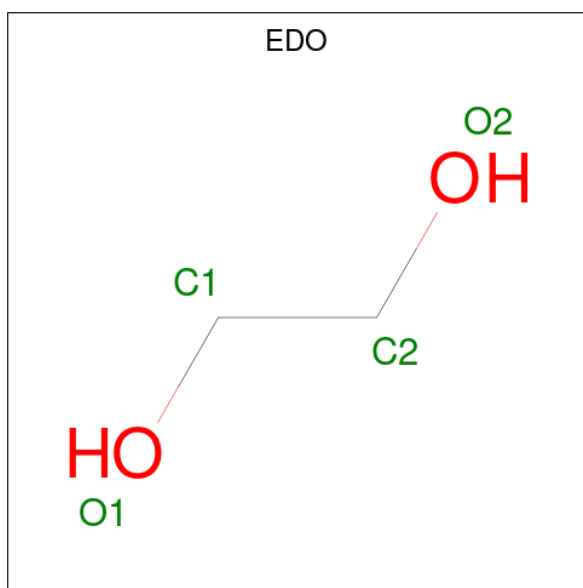
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	33	Total O 33 33	0	0
5	B	4	Total O 4 4	0	0
5	C	9	Total O 9 9	0	0
5	D	4	Total O 4 4	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.74Å 144.74Å 269.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.52 – 2.88 45.77 – 2.88	Depositor EDS
% Data completeness (in resolution range)	97.8 (127.52-2.88) 97.9 (45.77-2.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0071	Depositor
R, $R_{free}$	0.169 , 0.199 0.173 , 0.199	Depositor DCC
$R_{free}$ test set	3185 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtrriage
Anisotropy	0.142	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 17.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: MG, TPP, EDO

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	0.61	0/4249	0.73	0/5794
1	B	0.58	0/4249	0.73	1/5794 (0.0%)
1	C	0.63	0/4289	0.75	2/5850 (0.0%)
1	D	0.60	0/4300	0.74	1/5864 (0.0%)
All	All	0.61	0/17087	0.74	4/23302 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	LEU	CB-CG-CD2	5.92	121.06	111.00
1	C	335	GLN	CB-CA-C	-5.39	99.62	110.40
1	B	3	MET	CG-SD-CE	5.20	108.53	100.20
1	D	569	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4163	0	4148	15	0
1	B	4163	0	4148	18	0
1	C	4202	0	4180	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4213	0	4192	13	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	26	0	16	1	0
3	B	26	0	16	0	0
3	C	26	0	16	0	0
3	D	26	0	16	0	0
4	A	8	0	12	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
5	A	33	0	0	0	0
5	B	4	0	0	1	0
5	C	9	0	0	0	0
5	D	4	0	0	1	0
All	All	16915	0	16756	60	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 (60) 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:371:HIS:HD2	1:B:373:PHE:H	1.29	0.77
1:B:9:LEU:HD11	1:B:170:ILE:HD11	1.69	0.72
1:D:9:LEU:HD11	1:D:170:ILE:HD11	1.71	0.71
1:A:9:LEU:HD11	1:A:170:ILE:HD11	1.71	0.71
1:C:329:LEU:O	1:C:333:THR:HB	1.94	0.68
1:B:329:LEU:O	1:B:333:THR:HB	1.94	0.67
1:A:329:LEU:O	1:A:333:THR:HB	1.95	0.66
1:B:360:ILE:HD11	1:B:551:PRO:HG2	1.77	0.66
1:D:329:LEU:O	1:D:333:THR:HB	1.96	0.64
1:A:38:LEU:HD13	1:B:495:THR:HG21	1.80	0.62
1:B:371:HIS:CD2	1:B:373:PHE:H	2.19	0.55
1:C:336:ASP:OD1	1:C:337:ALA:N	2.31	0.55
1:B:89[A]:ARG:HD2	5:B:701:HOH:O	2.07	0.55
1:B:366:SER:OG	1:B:374:HIS:HD2	1.92	0.53
1:C:62:ARG:NH2	1:C:240:GLU:OE2	2.42	0.52
1:A:366:SER:OG	1:A:374:HIS:HD2	1.93	0.51
1:D:89[A]:ARG:HD2	5:D:701:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:SER:OG	1:D:374:HIS:HD2	1.94	0.49
1:A:310:ARG:NH2	1:B:108:GLU:OE2	2.46	0.49
1:C:366:SER:OG	1:C:374:HIS:HD2	1.95	0.48
1:B:304:ASP:OD1	1:B:306:CYS:SG	2.71	0.48
1:D:21:HIS:HD2	1:D:60:TYR:OH	1.96	0.48
1:D:123:ALA:N	1:D:124:PRO:CD	2.78	0.46
1:D:557:ILE:O	1:D:569:LEU:CD1	2.63	0.46
1:A:304:ASP:OD1	1:A:306:CYS:SG	2.72	0.46
1:D:123:ALA:N	1:D:124:PRO:HD2	2.31	0.46
1:B:145:ALA:HB1	1:B:157:VAL:HG11	1.98	0.46
1:A:145:ALA:HB1	1:A:157:VAL:HG11	1.97	0.45
1:B:360:ILE:CD1	1:B:551:PRO:HG2	2.46	0.45
1:D:24:GLY:O	1:D:46:ASP:HA	2.17	0.45
1:A:24:GLY:O	1:A:46:ASP:HA	2.17	0.45
1:C:14:LEU:O	1:C:19:VAL:HG13	2.17	0.45
1:C:123:ALA:N	1:C:124:PRO:CD	2.79	0.45
1:D:145:ALA:HB1	1:D:157:VAL:HG11	1.99	0.45
1:C:123:ALA:N	1:C:124:PRO:HD2	2.32	0.44
1:A:482:LEU:O	1:A:486:GLN:HG2	2.18	0.44
1:B:123:ALA:N	1:B:124:PRO:HD2	2.32	0.44
1:B:275:MET:HE3	1:B:300:GLN:HG3	2.00	0.44
1:B:123:ALA:N	1:B:124:PRO:CD	2.80	0.43
1:B:24:GLY:O	1:B:46:ASP:HA	2.19	0.43
1:C:492:ASN:OD1	1:C:492:ASN:N	2.51	0.43
1:A:478:TRP:CE3	3:A:602:TPP:HM41	2.53	0.43
1:C:432:GLN:HE22	1:C:442:THR:H	1.67	0.43
1:C:24:GLY:O	1:C:46:ASP:HA	2.18	0.42
1:C:304:ASP:OD1	1:C:306:CYS:SG	2.73	0.42
1:D:547:ASP:N	1:D:548:PRO:CD	2.82	0.42
1:A:17:ALA:HB2	1:A:143:MET:CE	2.50	0.42
1:C:227:PHE:HA	1:C:333:THR:HG21	2.02	0.42
1:C:145:ALA:HB1	1:C:157:VAL:HG11	2.01	0.42
1:D:227:PHE:HA	1:D:333:THR:HG21	2.02	0.42
1:A:143:MET:HE3	1:A:146:ILE:HD12	2.01	0.42
1:C:547:ASP:N	1:C:548:PRO:CD	2.82	0.42
1:A:21:HIS:HD2	1:A:60:TYR:OH	2.02	0.41
1:B:17:ALA:HB2	1:B:143:MET:CE	2.51	0.41
1:B:227:PHE:HA	1:B:333:THR:HG21	2.02	0.41
1:A:227:PHE:HA	1:A:333:THR:HG21	2.02	0.41
1:C:143:MET:HE3	1:C:146:ILE:HD12	2.03	0.41
1:D:432:GLN:HE22	1:D:442:THR:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ALA:HB2	1:A:143:MET:HE1	2.03	0.40
1:C:17:ALA:HB2	1:C:143:MET:CE	2.51	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	562/583 (96%)	543 (97%)	19 (3%)	0	100	100
1	B	562/583 (96%)	544 (97%)	17 (3%)	1 (0%)	47	76
1	C	567/583 (97%)	552 (97%)	15 (3%)	0	100	100
1	D	568/583 (97%)	549 (97%)	18 (3%)	1 (0%)	47	76
All	All	2259/2332 (97%)	2188 (97%)	69 (3%)	2 (0%)	51	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	337	ALA
1	D	337	ALA

### 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	422/439 (96%)	411 (97%)	11 (3%)	46	76
1	B	422/439 (96%)	412 (98%)	10 (2%)	49	78
1	C	427/439 (97%)	416 (97%)	11 (3%)	46	76
1	D	428/439 (98%)	415 (97%)	13 (3%)	41	73
All	All	1699/1756 (97%)	1654 (97%)	45 (3%)	44	76

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	203	LYS
1	A	306	CYS
1	A	312	GLN
1	A	333	THR
1	A	397	TYR
1	A	406	ARG
1	A	419	ASN
1	A	425	PHE
1	A	500	GLU
1	A	532	LEU
1	B	46	ASP
1	B	306	CYS
1	B	331	GLN
1	B	333	THR
1	B	397	TYR
1	B	406	ARG
1	B	419	ASN
1	B	425	PHE
1	B	500	GLU
1	B	535	ASN
1	C	46	ASP
1	C	306	CYS
1	C	312	GLN
1	C	333	THR
1	C	397	TYR
1	C	406	ARG
1	C	419	ASN
1	C	425	PHE
1	C	500	GLU
1	C	535	ASN
1	C	569	LEU
1	D	46	ASP

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Mol	Chain	Res	Type
1	D	203	LYS
1	D	306	CYS
1	D	312	GLN
1	D	331	GLN
1	D	333	THR
1	D	397	TYR
1	D	406	ARG
1	D	419	ASN
1	D	425	PHE
1	D	500	GLU
1	D	522	GLU
1	D	569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	87	ASN
1	A	118	GLN
1	A	283	ASN
1	A	374	HIS
1	A	432	GLN
1	B	118	GLN
1	B	259	ASN
1	B	371	HIS
1	B	374	HIS
1	B	432	GLN
1	C	118	GLN
1	C	294	HIS
1	C	374	HIS
1	C	432	GLN
1	D	21	HIS
1	D	87	ASN
1	D	118	GLN
1	D	259	ASN
1	D	294	HIS
1	D	331	GLN
1	D	374	HIS
1	D	432	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 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	EDO	C	603	-	3,3,3	0.58	0	2,2,2	0.21	0
4	EDO	D	603	-	3,3,3	0.58	0	2,2,2	0.24	0
3	TPP	C	602	2	22,27,27	2.06	3 (13%)	29,40,40	1.75	8 (27%)
3	TPP	A	602	2	22,27,27	1.65	5 (22%)	29,40,40	2.07	13 (44%)
3	TPP	B	602	2	22,27,27	1.87	3 (13%)	29,40,40	2.19	9 (31%)
3	TPP	D	602	2	22,27,27	1.87	5 (22%)	29,40,40	1.91	10 (34%)
4	EDO	A	603	-	3,3,3	0.69	0	2,2,2	0.16	0
4	EDO	A	604	-	3,3,3	0.59	0	2,2,2	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	603	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	603	-	-	1/1/1/1	-
3	TPP	C	602	2	-	2/16/17/17	0/2/2/2
3	TPP	A	602	2	-	1/16/17/17	0/2/2/2
3	TPP	B	602	2	-	3/16/17/17	0/2/2/2
3	TPP	D	602	2	-	1/16/17/17	0/2/2/2
4	EDO	A	603	-	-	0/1/1/1	-
4	EDO	A	604	-	-	1/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	TPP	C6-C5	8.05	1.54	1.50
3	B	602	TPP	C6-C5	6.32	1.53	1.50
3	D	602	TPP	C6-C5	6.24	1.53	1.50
3	A	602	TPP	C6-C5	3.65	1.52	1.50
3	A	602	TPP	C4-N3	3.61	1.42	1.39
3	D	602	TPP	C7'-C5'	3.55	1.58	1.51
3	B	602	TPP	C7'-C5'	3.35	1.58	1.51
3	C	602	TPP	C7'-C5'	2.85	1.57	1.51
3	B	602	TPP	C4'-N4'	2.80	1.41	1.34
3	A	602	TPP	C7'-C5'	2.77	1.57	1.51
3	A	602	TPP	C4'-N4'	2.63	1.40	1.34
3	A	602	TPP	C2'-N1'	-2.49	1.30	1.34
3	C	602	TPP	C4'-N4'	2.49	1.40	1.34
3	D	602	TPP	C6'-C5'	2.33	1.42	1.37
3	D	602	TPP	C4'-N4'	2.29	1.39	1.34
3	D	602	TPP	C4-N3	2.12	1.41	1.39

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	TPP	C6-C5-C4	4.68	131.19	127.43
3	A	602	TPP	CM4-C4-C5	-4.49	117.79	127.60
3	B	602	TPP	C6'-N1'-C2'	4.13	122.98	115.96
3	B	602	TPP	PA-O3A-PB	-4.11	118.73	132.83
3	B	602	TPP	C5-C4-N3	3.98	115.53	107.57
3	B	602	TPP	CM2-C2'-N1'	3.96	121.50	117.14
3	B	602	TPP	N1'-C2'-N3'	-3.85	118.91	125.54
3	D	602	TPP	C5-C4-N3	3.85	115.27	107.57
3	A	602	TPP	C5-C4-N3	3.77	115.12	107.57
3	A	602	TPP	CM4-C4-N3	3.57	127.09	122.53
3	D	602	TPP	CM2-C2'-N1'	3.54	121.03	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	TPP	C5'-C6'-N1'	-3.49	118.01	123.82
3	C	602	TPP	C5-C4-N3	3.43	114.43	107.57
3	D	602	TPP	C6-C5-C4	3.32	130.10	127.43
3	A	602	TPP	C6'-N1'-C2'	3.17	121.35	115.96
3	C	602	TPP	PA-O3A-PB	-3.12	122.12	132.83
3	D	602	TPP	C6'-N1'-C2'	3.11	121.25	115.96
3	D	602	TPP	CM4-C4-C5	-2.92	121.23	127.60
3	C	602	TPP	C6'-N1'-C2'	2.86	120.82	115.96
3	A	602	TPP	C6-C5-C4	2.83	129.70	127.43
3	B	602	TPP	C2'-N3'-C4'	2.75	122.37	118.08
3	B	602	TPP	CM4-C4-C5	-2.73	121.62	127.60
3	C	602	TPP	C6-C5-C4	2.73	129.63	127.43
3	A	602	TPP	N1'-C2'-N3'	-2.73	120.84	125.54
3	D	602	TPP	PA-O3A-PB	-2.71	123.52	132.83
3	A	602	TPP	C7'-N3-C2	-2.69	120.50	125.35
3	D	602	TPP	N1'-C2'-N3'	-2.67	120.95	125.54
3	A	602	TPP	C2'-N3'-C4'	2.65	122.22	118.08
3	A	602	TPP	PA-O3A-PB	-2.56	124.05	132.83
3	D	602	TPP	O3B-PB-O3A	2.55	113.18	104.64
3	B	602	TPP	C5'-C6'-N1'	-2.49	119.67	123.82
3	C	602	TPP	O2B-PB-O3A	2.40	112.69	104.64
3	C	602	TPP	C7'-N3-C2	-2.36	121.08	125.35
3	D	602	TPP	C5'-C6'-N1'	-2.28	120.02	123.82
3	A	602	TPP	CM2-C2'-N1'	2.27	119.64	117.14
3	A	602	TPP	N4'-C4'-N3'	2.25	120.22	117.03
3	D	602	TPP	C2'-N3'-C4'	2.25	121.59	118.08
3	C	602	TPP	CM4-C4-C5	-2.18	122.83	127.60
3	A	602	TPP	C5'-C6'-N1'	-2.08	120.35	123.82
3	A	602	TPP	C5'-C4'-N4'	-2.07	119.25	122.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	TPP	PA-O3A-PB-O3B
4	D	603	EDO	O1-C1-C2-O2
3	C	602	TPP	PB-O3A-PA-O7
3	D	602	TPP	PB-O3A-PA-O7
3	B	602	TPP	PA-O3A-PB-O2B
3	C	602	TPP	PA-O3A-PB-O1B
4	A	604	EDO	O1-C1-C2-O2
3	A	602	TPP	PA-O3A-PB-O2B

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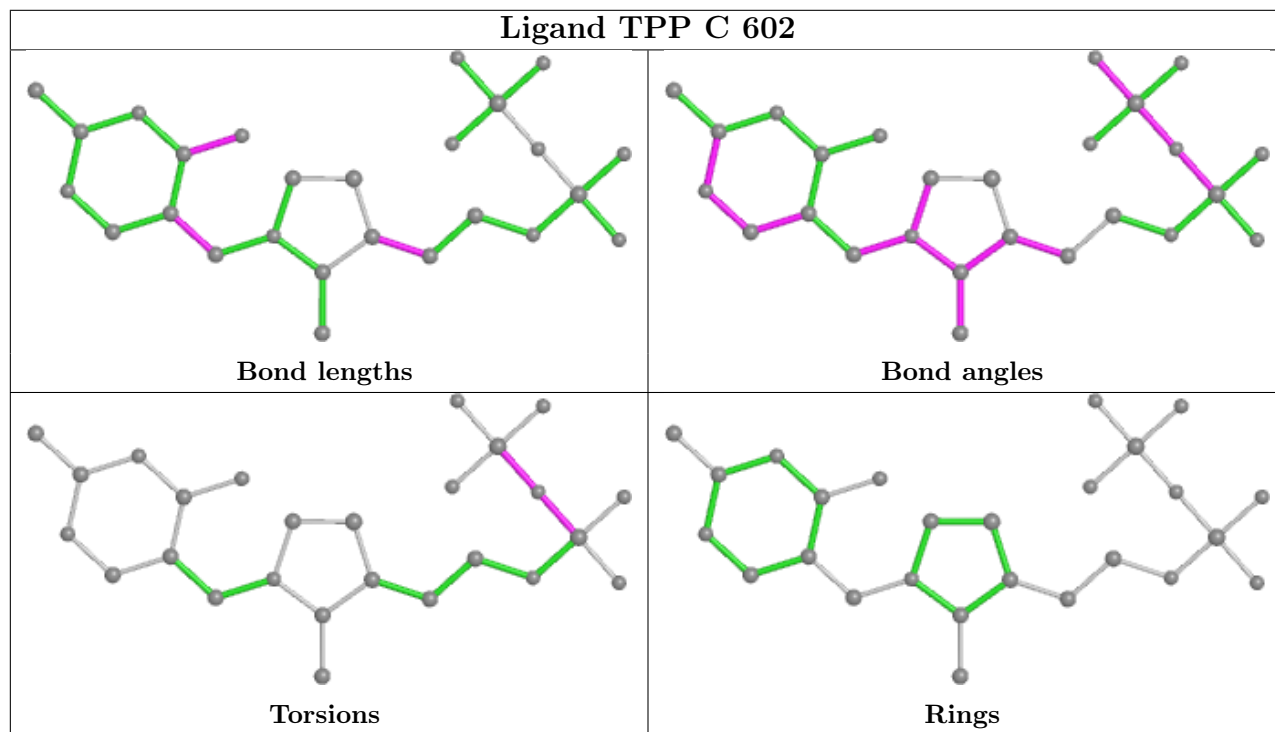
Mol	Chain	Res	Type	Atoms
3	B	602	TPP	PA-O3A-PB-O1B

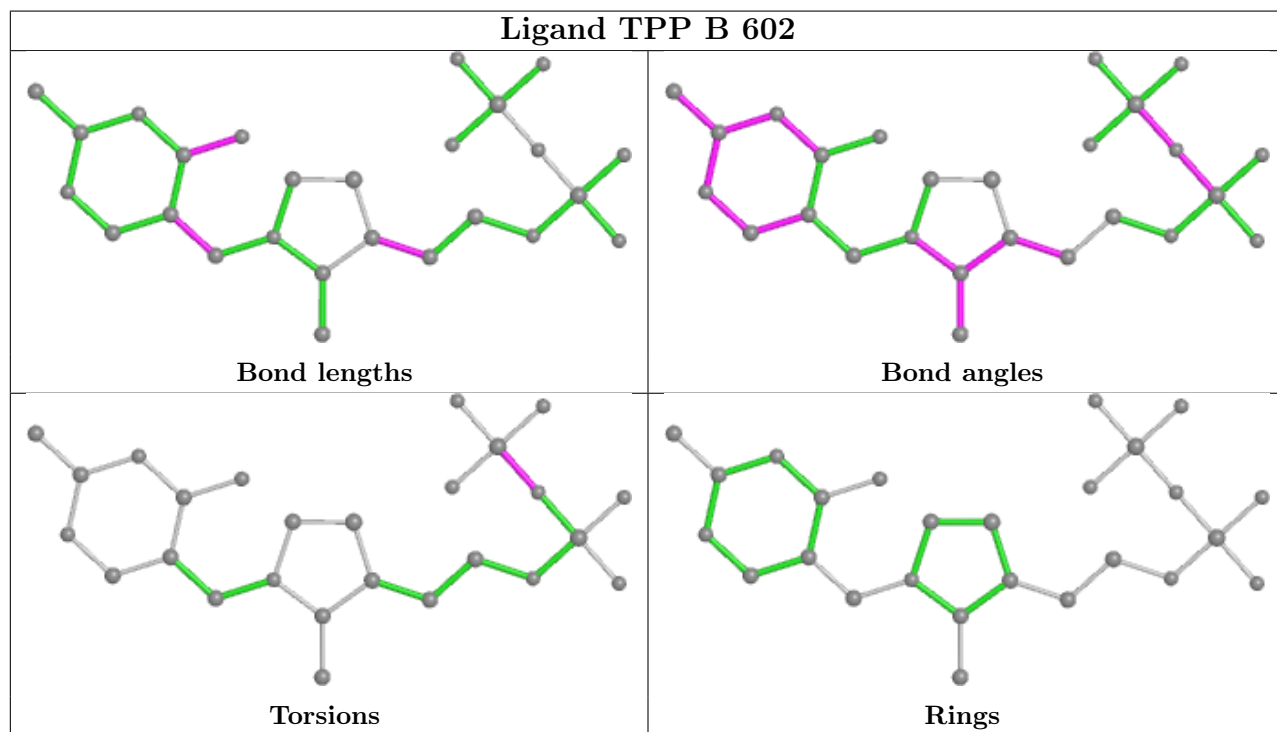
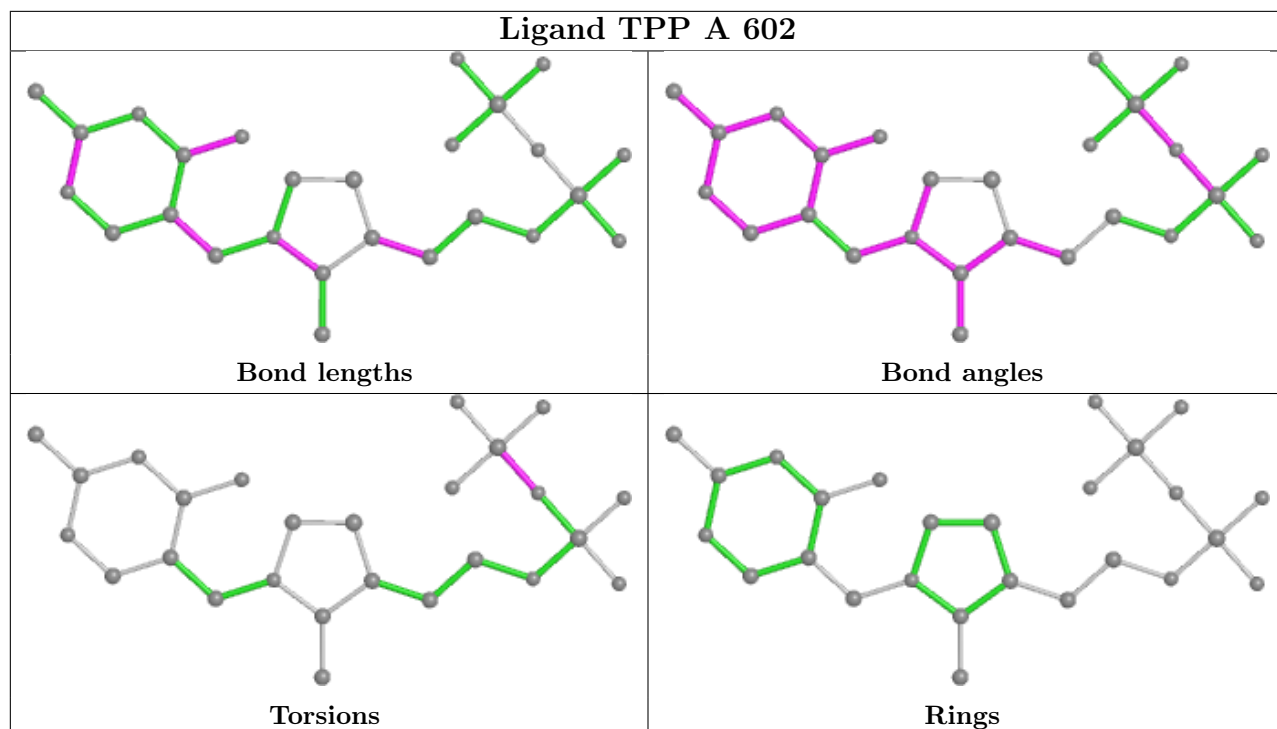
There are no ring outliers.

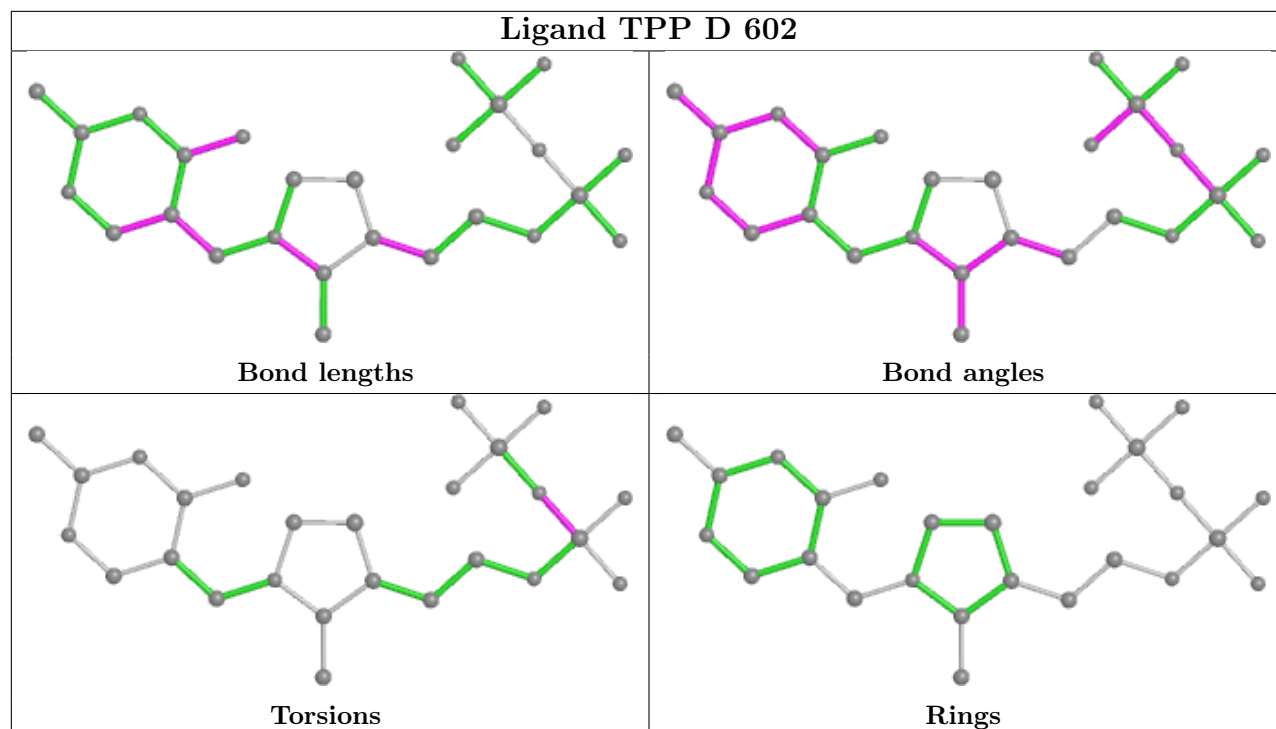
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	TPP	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.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	563/583 (96%)	-0.51	3 (0%) 91 90	32, 49, 73, 114	0
1	B	563/583 (96%)	-0.41	5 (0%) 84 84	38, 57, 81, 130	0
1	C	569/583 (97%)	-0.57	5 (0%) 84 84	31, 46, 66, 136	0
1	D	569/583 (97%)	-0.54	5 (0%) 84 84	33, 55, 82, 130	0
All	All	2264/2332 (97%)	-0.51	18 (0%) 86 86	31, 51, 78, 136	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	564	GLY	9.4
1	A	564	GLY	6.1
1	C	564	GLY	4.7
1	D	565	SER	4.0
1	C	565	SER	3.9
1	D	566	THR	3.7
1	A	563	ALA	3.5
1	C	566	THR	3.1
1	C	570	TYR	2.8
1	B	562	PHE	2.6
1	B	368	HIS	2.5
1	D	564	GLY	2.4
1	B	563	ALA	2.4
1	D	570	TYR	2.3
1	A	559	MET	2.2
1	B	337	ALA	2.1
1	D	563	ALA	2.0
1	C	563	ALA	2.0



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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

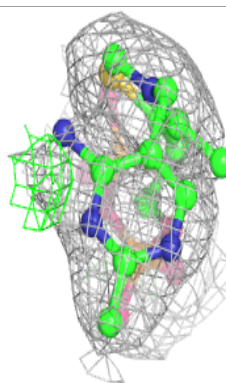
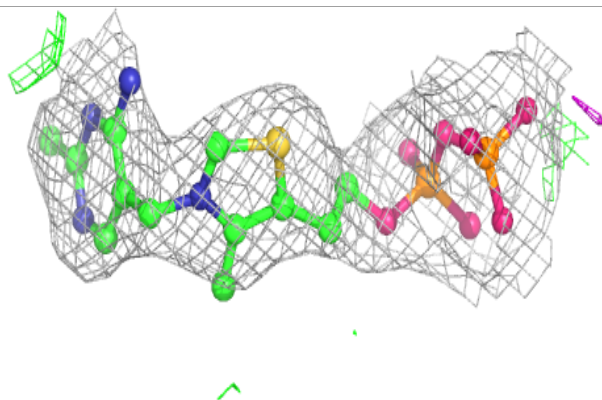
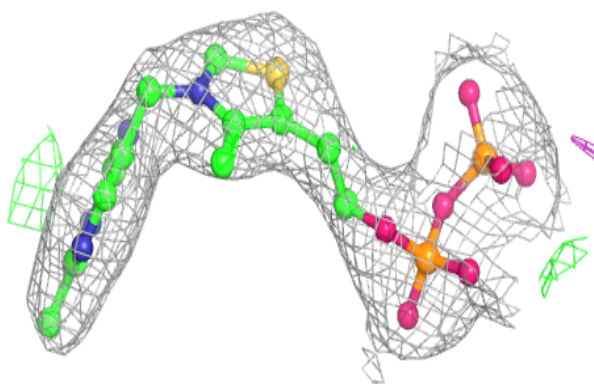
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	EDO	A	604	4/4	0.72	0.26	73,77,80,81	0
4	EDO	C	603	4/4	0.75	0.54	75,75,86,87	0
4	EDO	D	603	4/4	0.85	0.20	62,62,67,69	0
4	EDO	A	603	4/4	0.86	0.21	52,64,66,69	0
2	MG	B	601	1/1	0.96	0.12	34,34,34,34	0
2	MG	D	601	1/1	0.98	0.08	37,37,37,37	0
3	TPP	B	602	26/26	0.98	0.11	43,48,59,60	0
3	TPP	D	602	26/26	0.99	0.12	40,52,54,57	0
2	MG	A	601	1/1	0.99	0.08	39,39,39,39	0
3	TPP	A	602	26/26	0.99	0.12	40,47,52,54	0
2	MG	C	601	1/1	0.99	0.09	33,33,33,33	0
3	TPP	C	602	26/26	0.99	0.11	35,48,52,55	0

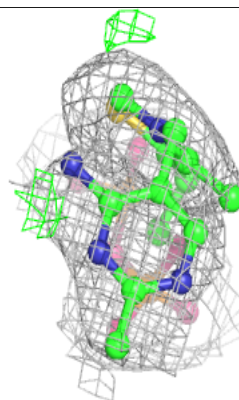
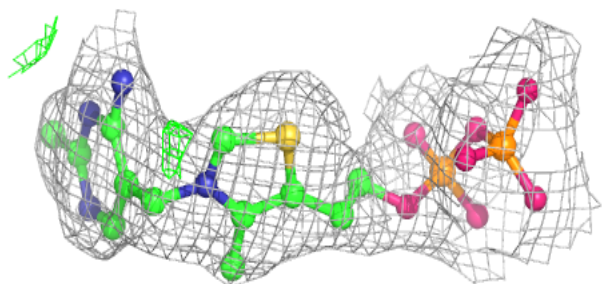
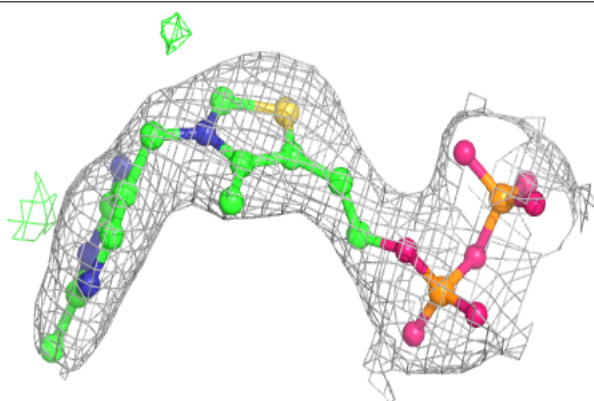
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPP 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)

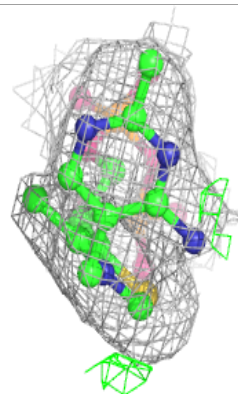
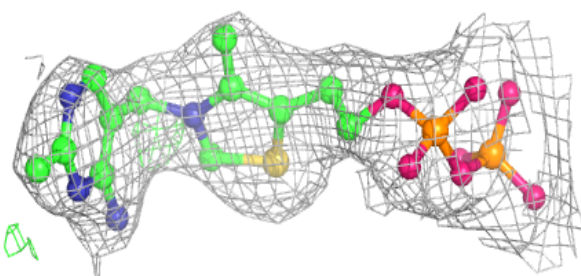
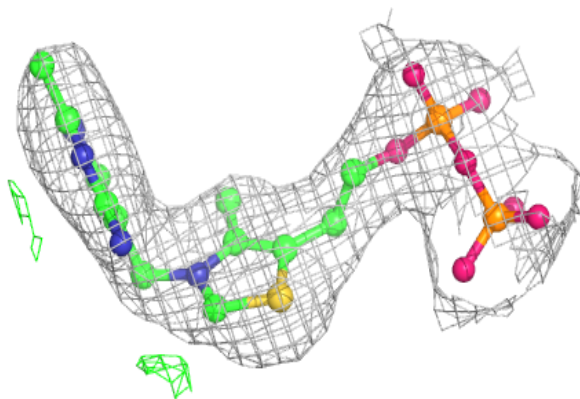
**Electron density around TPP D 602:**

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

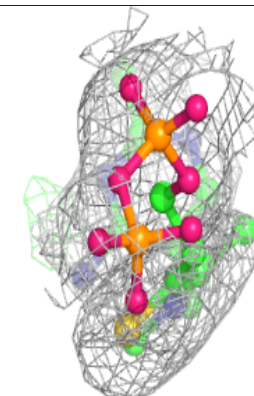
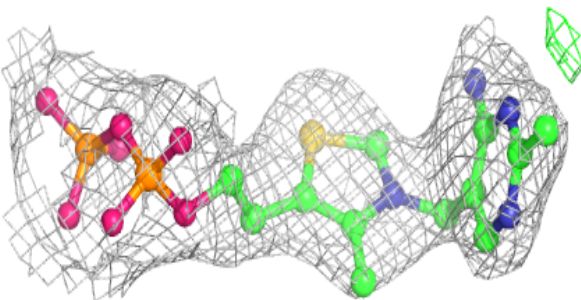
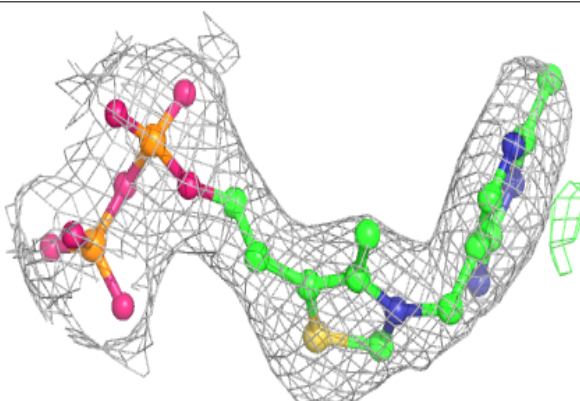


**Electron density around TPP A 602:**

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

**Electron density around TPP C 602:**

$2mF_o-DF_c$  (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.