



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2022 – 07:26 AM JST

PDB ID : 7WRR  
Title : X-ray structure of Thermus thermophilus HB8 transketorase in complex with TPP and MES  
Authors : Kamitori, S.; Yoshihara, A.  
Deposited on : 2022-01-27  
Resolution : 2.01 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 : 2.31.3  
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) : 2.31.3

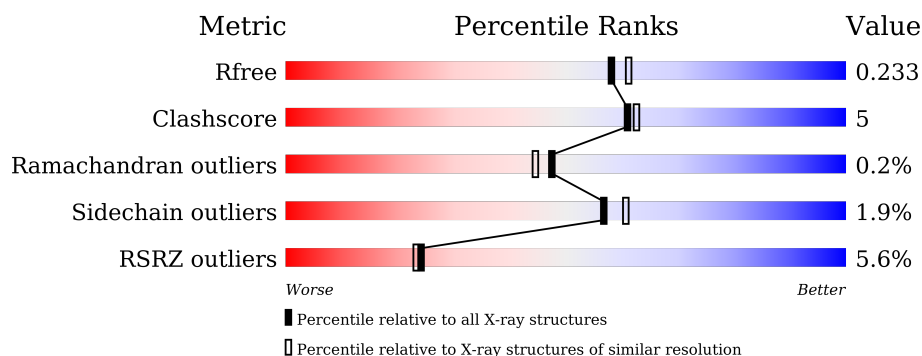
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	672	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="width: 90%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">90%</span> </div> <div style="width: 6%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">6%</span> </div> <div style="width: 4%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">.</span> </div> </div>
1	B	672	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="width: 88%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">88%</span> </div> <div style="width: 8%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">8%</span> </div> <div style="width: 4%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">..</span> </div> </div>
1	C	672	<div> <div style="width: 3%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">3%</span> </div> <div style="width: 85%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">85%</span> </div> <div style="width: 11%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">11%</span> </div> <div style="width: 1%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">.</span> </div> </div>
1	D	672	<div> <div style="width: 16%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">16%</span> </div> <div style="width: 78%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">78%</span> </div> <div style="width: 18%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">18%</span> </div> <div style="width: 8%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">..</span> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MES	A	703	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20961 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 Transketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	0	0
			5070	3236	902	917	15			
1	B	650	Total	C	N	O	S	0	0	0
			5070	3236	902	917	15			
1	C	650	Total	C	N	O	S	0	0	0
			5070	3236	902	917	15			
1	D	650	Total	C	N	O	S	0	0	0
			5070	3236	902	917	15			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q5SM35
A	-19	GLY	-	expression tag	UNP Q5SM35
A	-18	SER	-	expression tag	UNP Q5SM35
A	-17	SER	-	expression tag	UNP Q5SM35
A	-16	HIS	-	expression tag	UNP Q5SM35
A	-15	HIS	-	expression tag	UNP Q5SM35
A	-14	HIS	-	expression tag	UNP Q5SM35
A	-13	HIS	-	expression tag	UNP Q5SM35
A	-12	HIS	-	expression tag	UNP Q5SM35
A	-11	HIS	-	expression tag	UNP Q5SM35
A	-10	SER	-	expression tag	UNP Q5SM35
A	-9	SER	-	expression tag	UNP Q5SM35
A	-8	GLY	-	expression tag	UNP Q5SM35
A	-7	LEU	-	expression tag	UNP Q5SM35
A	-6	VAL	-	expression tag	UNP Q5SM35
A	-5	PRO	-	expression tag	UNP Q5SM35
A	-4	ARG	-	expression tag	UNP Q5SM35
A	-3	GLY	-	expression tag	UNP Q5SM35
A	-2	SER	-	expression tag	UNP Q5SM35
A	-1	HIS	-	expression tag	UNP Q5SM35
A	0	SER	-	expression tag	UNP Q5SM35

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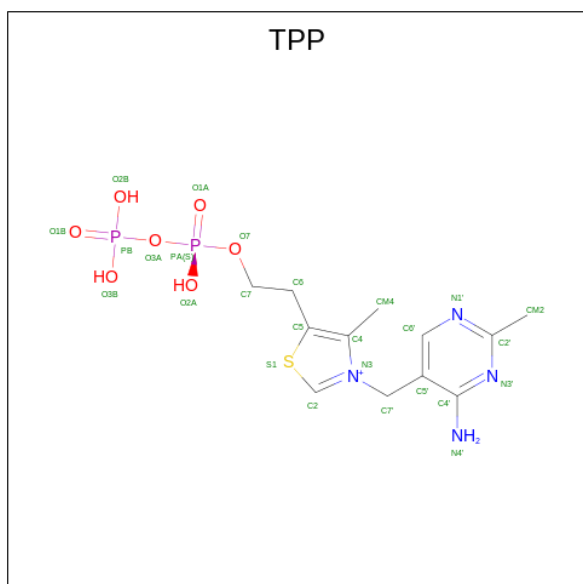
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP Q5SM35
B	-19	GLY	-	expression tag	UNP Q5SM35
B	-18	SER	-	expression tag	UNP Q5SM35
B	-17	SER	-	expression tag	UNP Q5SM35
B	-16	HIS	-	expression tag	UNP Q5SM35
B	-15	HIS	-	expression tag	UNP Q5SM35
B	-14	HIS	-	expression tag	UNP Q5SM35
B	-13	HIS	-	expression tag	UNP Q5SM35
B	-12	HIS	-	expression tag	UNP Q5SM35
B	-11	HIS	-	expression tag	UNP Q5SM35
B	-10	SER	-	expression tag	UNP Q5SM35
B	-9	SER	-	expression tag	UNP Q5SM35
B	-8	GLY	-	expression tag	UNP Q5SM35
B	-7	LEU	-	expression tag	UNP Q5SM35
B	-6	VAL	-	expression tag	UNP Q5SM35
B	-5	PRO	-	expression tag	UNP Q5SM35
B	-4	ARG	-	expression tag	UNP Q5SM35
B	-3	GLY	-	expression tag	UNP Q5SM35
B	-2	SER	-	expression tag	UNP Q5SM35
B	-1	HIS	-	expression tag	UNP Q5SM35
B	0	SER	-	expression tag	UNP Q5SM35
C	-20	MET	-	initiating methionine	UNP Q5SM35
C	-19	GLY	-	expression tag	UNP Q5SM35
C	-18	SER	-	expression tag	UNP Q5SM35
C	-17	SER	-	expression tag	UNP Q5SM35
C	-16	HIS	-	expression tag	UNP Q5SM35
C	-15	HIS	-	expression tag	UNP Q5SM35
C	-14	HIS	-	expression tag	UNP Q5SM35
C	-13	HIS	-	expression tag	UNP Q5SM35
C	-12	HIS	-	expression tag	UNP Q5SM35
C	-11	HIS	-	expression tag	UNP Q5SM35
C	-10	SER	-	expression tag	UNP Q5SM35
C	-9	SER	-	expression tag	UNP Q5SM35
C	-8	GLY	-	expression tag	UNP Q5SM35
C	-7	LEU	-	expression tag	UNP Q5SM35
C	-6	VAL	-	expression tag	UNP Q5SM35
C	-5	PRO	-	expression tag	UNP Q5SM35
C	-4	ARG	-	expression tag	UNP Q5SM35
C	-3	GLY	-	expression tag	UNP Q5SM35
C	-2	SER	-	expression tag	UNP Q5SM35
C	-1	HIS	-	expression tag	UNP Q5SM35
C	0	SER	-	expression tag	UNP Q5SM35

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP Q5SM35
D	-19	GLY	-	expression tag	UNP Q5SM35
D	-18	SER	-	expression tag	UNP Q5SM35
D	-17	SER	-	expression tag	UNP Q5SM35
D	-16	HIS	-	expression tag	UNP Q5SM35
D	-15	HIS	-	expression tag	UNP Q5SM35
D	-14	HIS	-	expression tag	UNP Q5SM35
D	-13	HIS	-	expression tag	UNP Q5SM35
D	-12	HIS	-	expression tag	UNP Q5SM35
D	-11	HIS	-	expression tag	UNP Q5SM35
D	-10	SER	-	expression tag	UNP Q5SM35
D	-9	SER	-	expression tag	UNP Q5SM35
D	-8	GLY	-	expression tag	UNP Q5SM35
D	-7	LEU	-	expression tag	UNP Q5SM35
D	-6	VAL	-	expression tag	UNP Q5SM35
D	-5	PRO	-	expression tag	UNP Q5SM35
D	-4	ARG	-	expression tag	UNP Q5SM35
D	-3	GLY	-	expression tag	UNP Q5SM35
D	-2	SER	-	expression tag	UNP Q5SM35
D	-1	HIS	-	expression tag	UNP Q5SM35
D	0	SER	-	expression tag	UNP Q5SM35

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

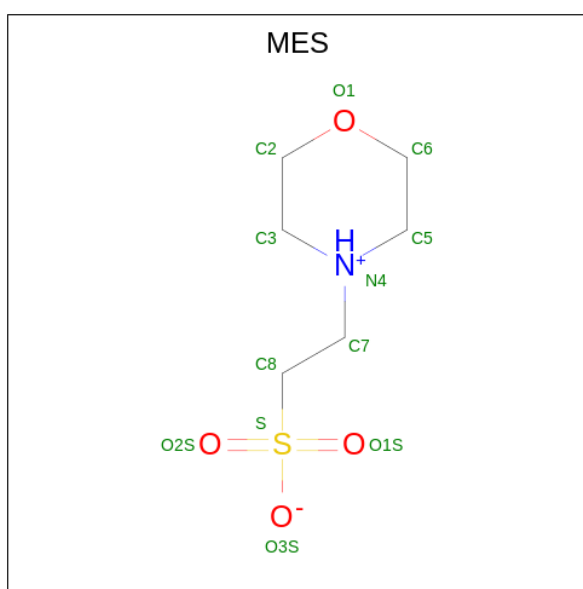


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
2	B	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
2	C	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
2	D	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S		
			12	6	1	4	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

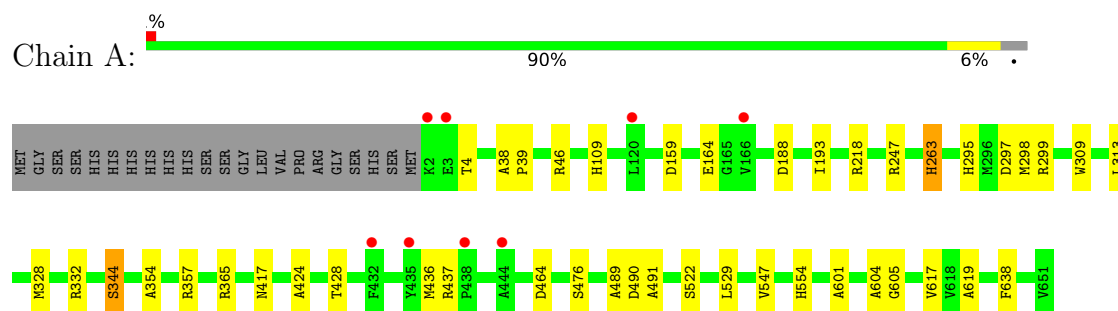
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total	O	0	0
			206	206		
5	B	179	Total	O	0	0
			179	179		
5	C	85	Total	O	0	0
			85	85		
5	D	55	Total	O	0	0
			55	55		

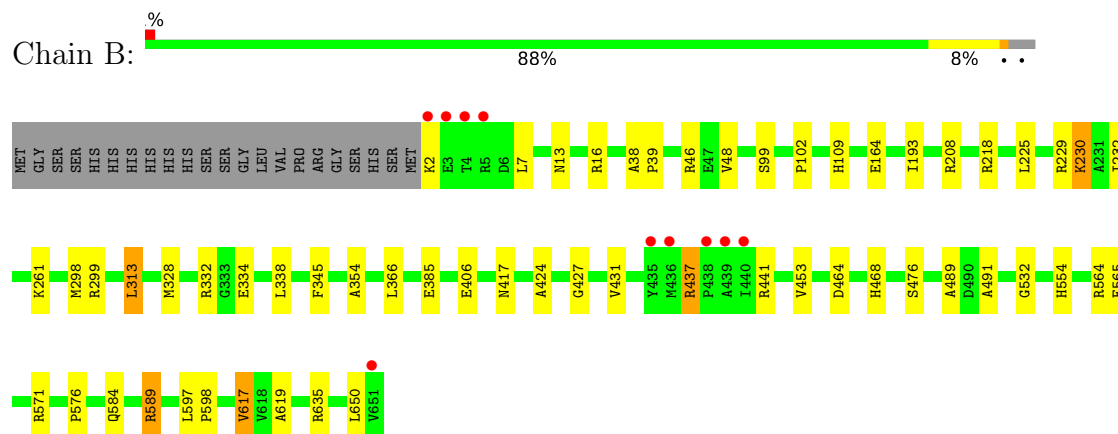
### 3 Residue-property plots [i](#)

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.

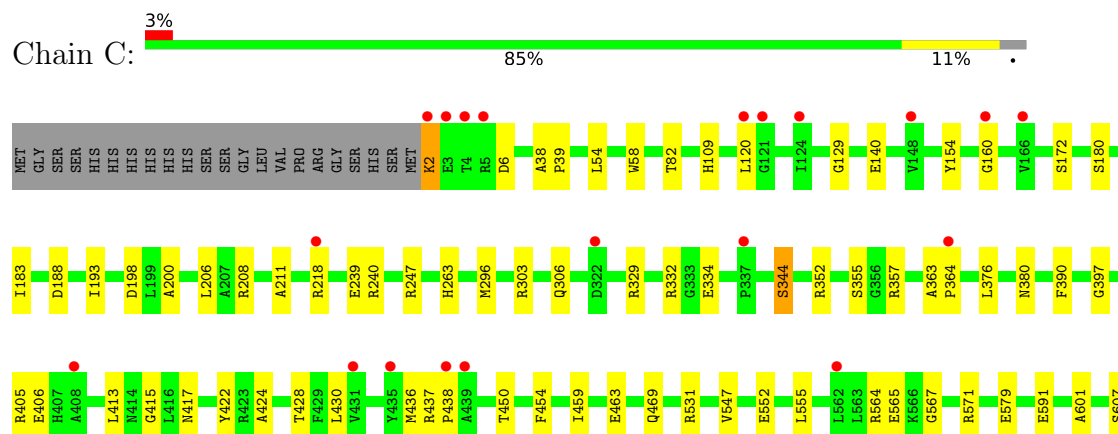
#### • Molecule 1: Transketolase



#### • Molecule 1: Transketolase

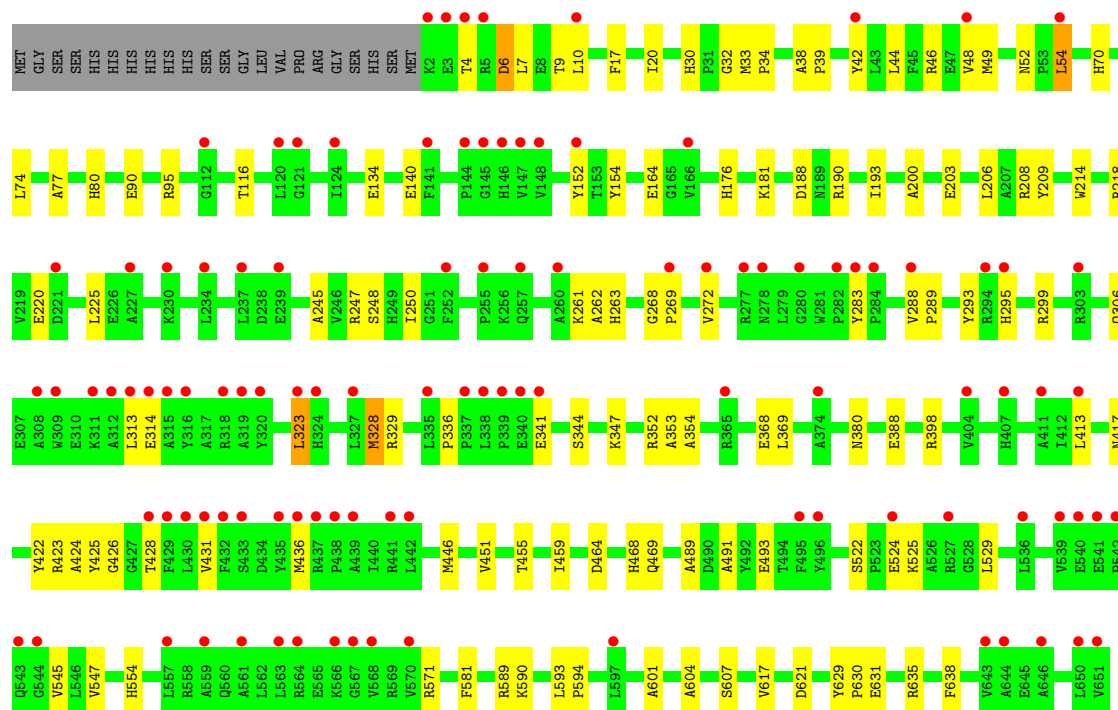
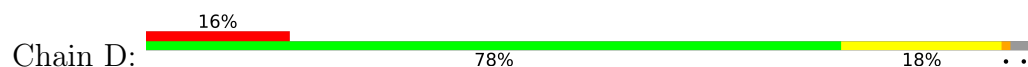


#### • Molecule 1: Transketolase





● Molecule 1: Transketolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.72Å 88.84Å 117.61Å 72.56° 88.74° 73.74°	Depositor
Resolution (Å)	46.67 – 2.01 46.67 – 2.01	Depositor EDS
% Data completeness (in resolution range)	97.8 (46.67-2.01) 97.8 (46.67-2.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.198 , 0.228 0.204 , 0.233	Depositor DCC
$R_{free}$ test set	8735 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20961	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: CA, MES, TPP

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	0.74	0/5205	0.87	0/7080
1	B	0.75	0/5205	0.89	5/7080 (0.1%)
1	C	0.71	0/5205	0.84	0/7080
1	D	0.72	0/5205	0.83	0/7080
All	All	0.73	0/20820	0.86	5/28320 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	437	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	B	635	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	B	208	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	441	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	589	ARG	NE-CZ-NH1	5.27	122.94	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	HIS	Peptide
1	B	650	LEU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5070	0	5041	31	0
1	B	5070	0	5041	41	0
1	C	5070	0	5041	41	0
1	D	5070	0	5041	70	0
2	A	26	0	16	7	0
2	B	26	0	16	4	0
2	C	26	0	16	2	0
2	D	26	0	16	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	13	6	0
4	B	12	0	13	5	0
4	C	12	0	13	0	0
4	D	12	0	13	2	0
5	A	206	0	0	2	0
5	B	179	0	0	5	0
5	C	85	0	0	2	0
5	D	55	0	0	0	0
All	All	20961	0	20280	184	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 5.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ARG:NH1	1:D:295:HIS:O	2.04	0.90
1:B:464:ASP:OD2	4:B:801:MES:H31	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASN:HD21	1:A:424:ALA:H	1.19	0.86
1:B:218:ARG:HB3	5:B:1074:HOH:O	1.75	0.86
1:B:417:ASN:HD21	1:B:424:ALA:H	1.19	0.86
1:D:631:GLU:OE2	1:D:635:ARG:NH1	2.07	0.85
1:B:230:LYS:HG3	5:B:1072:HOH:O	1.81	0.78
1:D:464:ASP:OD2	4:D:801:MES:H31	1.89	0.72
1:A:344:SER:O	1:A:357:ARG:NH1	2.23	0.70
1:D:522:SER:OG	1:D:525:LYS:HB2	1.93	0.69
1:C:571:ARG:NH1	1:C:591:GLU:O	2.25	0.69
4:A:703:MES:C6	1:B:193:ILE:HD11	2.23	0.68
1:C:417:ASN:HD21	1:C:424:ALA:H	1.43	0.67
1:D:629:TYR:CD2	1:D:630:PRO:HA	2.30	0.67
1:A:193:ILE:HD11	4:B:801:MES:C6	2.25	0.66
1:D:30:HIS:HB2	1:D:70:HIS:O	1.96	0.65
1:C:206:LEU:HD12	1:C:218:ARG:HD2	1.79	0.65
2:A:701:TPP:HN42	2:A:701:TPP:C2	2.10	0.64
1:B:489:ALA:O	1:B:554:HIS:HE1	1.80	0.64
1:D:428:THR:HG21	1:D:436:MET:CE	2.28	0.64
1:A:464:ASP:OD2	4:A:703:MES:H31	1.98	0.63
1:D:547:VAL:O	1:D:601:ALA:HA	1.97	0.63
4:A:703:MES:H61	1:B:193:ILE:HD11	1.81	0.62
1:A:193:ILE:HD11	4:B:801:MES:H61	1.81	0.62
1:D:52:ASN:ND2	1:D:306:GLN:OE1	2.34	0.61
1:D:6:ASP:O	1:D:10:LEU:HB2	2.01	0.61
2:A:701:TPP:HN42	2:A:701:TPP:H2	1.66	0.59
2:B:802:TPP:HN42	2:B:802:TPP:C2	2.15	0.59
1:C:109:HIS:HB2	5:C:882:HOH:O	2.02	0.59
2:C:701:TPP:C2	2:C:701:TPP:HN42	2.16	0.59
1:B:299:ARG:NH1	5:B:902:HOH:O	2.34	0.58
1:C:38:ALA:HB3	1:C:39:PRO:HD3	1.84	0.58
1:D:369:LEU:HA	1:D:423:ARG:O	2.04	0.57
1:D:323:LEU:HD23	1:D:323:LEU:N	2.20	0.57
1:B:109:HIS:HB2	5:B:1066:HOH:O	2.04	0.57
1:B:417:ASN:ND2	1:B:424:ALA:H	1.96	0.57
1:B:332:ARG:HD2	1:B:334:GLU:OE2	2.06	0.56
1:A:297:ASP:OD1	1:A:299:ARG:HD3	2.05	0.55
1:A:489:ALA:O	1:A:554:HIS:HE1	1.88	0.55
1:B:584:GLN:O	1:B:589:ARG:NH1	2.38	0.55
1:D:39:PRO:HB3	1:D:225:LEU:HD21	1.88	0.55
1:B:617:VAL:CG2	1:B:619:ALA:HB2	2.36	0.55
1:A:417:ASN:HD21	1:A:424:ALA:N	1.97	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:GLY:HA2	1:B:453:VAL:O	2.06	0.54
1:A:263:HIS:ND1	2:A:701:TPP:O1B	2.30	0.54
1:D:417:ASN:HD21	1:D:424:ALA:H	1.56	0.54
1:A:263:HIS:NE2	4:B:801:MES:H61	2.22	0.54
1:A:476:SER:HB2	1:B:476:SER:HB2	1.90	0.54
1:C:263:HIS:ND1	2:C:701:TPP:O1B	2.40	0.54
1:C:607:SER:HB2	1:C:617:VAL:HG21	1.90	0.54
1:D:34:PRO:HA	1:D:74:LEU:HD13	1.89	0.54
1:C:188:ASP:O	1:C:247:ARG:HD2	2.08	0.54
1:B:46:ARG:HD2	1:B:298:MET:CE	2.37	0.54
1:B:417:ASN:HD21	1:B:424:ALA:N	1.98	0.53
1:D:428:THR:HG21	1:D:436:MET:HE1	1.89	0.53
1:C:352:ARG:O	1:C:355:SER:HB3	2.08	0.53
1:D:368:GLU:HB2	1:D:422:TYR:HA	1.91	0.52
2:B:802:TPP:HN42	2:B:802:TPP:H2	1.75	0.52
1:D:607:SER:HB2	1:D:617:VAL:HG21	1.92	0.52
1:A:193:ILE:HD11	4:B:801:MES:H62	1.91	0.52
1:C:109:HIS:CD2	5:C:882:HOH:O	2.62	0.51
1:A:46:ARG:HD2	1:A:298:MET:CE	2.40	0.51
1:D:44:LEU:HB3	1:D:49:MET:HE2	1.93	0.51
1:D:328:MET:CE	1:D:328:MET:HA	2.42	0.50
1:A:309:TRP:CH2	1:A:313:LEU:HD11	2.46	0.50
1:C:198:ASP:O	1:D:176:HIS:HE1	1.95	0.50
1:C:180:SER:HA	1:C:240:ARG:O	2.11	0.50
1:C:428:THR:HG21	1:C:436:MET:HE3	1.94	0.50
1:C:193:ILE:HD11	4:D:801:MES:H61	1.94	0.49
1:C:459:ILE:HA	1:C:469:GLN:HG2	1.94	0.49
1:D:116:THR:OG1	1:D:446:MET:HG2	2.12	0.49
1:D:206:LEU:HD21	1:D:245:ALA:HB2	1.93	0.49
1:A:46:ARG:HE	1:A:295:HIS:CE1	2.31	0.48
1:D:459:ILE:HA	1:D:469:GLN:HG2	1.94	0.48
1:D:140:GLU:OE1	1:D:398:ARG:NH2	2.41	0.48
1:C:344:SER:O	1:C:357:ARG:NH1	2.46	0.48
1:D:6:ASP:HA	1:D:9:THR:HB	1.94	0.48
1:D:354:ALA:CB	1:D:491:ALA:HA	2.44	0.48
1:B:48:VAL:HG21	1:B:232:ILE:HD13	1.95	0.48
1:D:288:VAL:HB	1:D:293:TYR:CE2	2.49	0.47
1:A:428:THR:CG2	1:A:436:MET:HE3	2.44	0.47
1:C:547:VAL:O	1:C:601:ALA:HA	2.15	0.47
1:D:607:SER:OG	1:D:621:ASP:OD1	2.24	0.47
1:B:489:ALA:O	1:B:554:HIS:CE1	2.64	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ASP:O	1:D:247:ARG:HD2	2.14	0.47
1:D:32:GLY:HA3	1:D:262:ALA:O	2.14	0.46
1:B:431:VAL:HG11	1:B:468:HIS:HA	1.98	0.46
1:D:44:LEU:HB3	1:D:49:MET:CE	2.46	0.46
1:A:605:GLY:O	1:A:619:ALA:HB1	2.15	0.46
1:B:164:GLU:OE2	2:B:802:TPP:HM23	2.14	0.46
1:B:354:ALA:CB	1:B:491:ALA:HA	2.46	0.46
1:C:140:GLU:OE2	1:C:422:TYR:OH	2.28	0.46
1:D:380:ASN:HA	1:D:455:THR:HG21	1.96	0.46
1:D:604:ALA:HA	1:D:638:PHE:CZ	2.51	0.46
4:A:703:MES:H62	1:B:193:ILE:HD11	1.94	0.46
1:C:82:THR:HA	1:C:296:MET:O	2.16	0.46
2:D:802:TPP:C2	2:D:802:TPP:HN42	2.29	0.46
1:A:164:GLU:OE2	2:A:701:TPP:HM23	2.16	0.46
1:D:44:LEU:HA	1:D:48:VAL:HB	1.98	0.46
1:C:430:LEU:HA	1:C:454:PHE:HB3	1.97	0.45
1:B:532:GLY:O	1:B:576:PRO:HD2	2.16	0.45
1:D:268:GLY:O	1:D:272:VAL:HG23	2.17	0.45
1:D:188:ASP:O	1:D:247:ARG:CD	2.65	0.45
1:D:493:GLU:O	1:D:529:LEU:HD13	2.16	0.45
1:A:188:ASP:O	1:A:247:ARG:HD2	2.16	0.45
1:D:33:MET:N	1:D:34:PRO:HD2	2.31	0.44
1:B:38:ALA:HB3	1:B:39:PRO:HD3	1.99	0.44
1:C:58:TRP:CD1	1:C:306:GLN:HG3	2.52	0.44
1:C:332:ARG:NH1	1:C:334:GLU:OE1	2.45	0.44
1:D:428:THR:HG21	1:D:436:MET:HE3	1.99	0.44
1:B:46:ARG:HD2	1:B:298:MET:HE3	1.99	0.44
1:D:545:VAL:HG22	1:D:571:ARG:CG	2.47	0.44
1:A:354:ALA:CB	1:A:491:ALA:HA	2.47	0.44
1:B:7:LEU:HD12	1:B:7:LEU:HA	1.90	0.44
1:D:134:GLU:OE1	1:D:181:LYS:HD3	2.17	0.44
1:A:547:VAL:O	1:A:601:ALA:HA	2.18	0.44
1:A:46:ARG:HD2	1:A:298:MET:HE3	1.99	0.43
1:D:193:ILE:HG13	2:D:802:TPP:H71	2.00	0.43
1:D:545:VAL:HG22	1:D:571:ARG:HG3	2.00	0.43
4:A:703:MES:C6	1:B:193:ILE:CD1	2.95	0.43
1:D:38:ALA:HB3	1:D:39:PRO:HD3	2.00	0.43
1:D:431:VAL:HG11	1:D:468:HIS:HA	2.00	0.43
1:A:159:ASP:HB2	2:A:701:TPP:O1A	2.18	0.43
1:C:437:ARG:HB3	1:C:438:PRO:HD3	2.01	0.43
1:D:152:TYR:HB2	1:D:154:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:703:MES:H62	1:B:193:ILE:CD1	2.48	0.43
1:D:352:ARG:HG3	1:D:353:ALA:N	2.32	0.43
1:A:109:HIS:HE1	5:A:866:HOH:O	2.00	0.43
1:B:313:LEU:HD11	1:B:328:MET:CE	2.48	0.43
1:C:120:LEU:HD13	1:C:160:GLY:HA3	2.00	0.43
1:C:154:TYR:HA	1:C:183:ILE:O	2.18	0.43
1:A:328:MET:HB3	1:A:332:ARG:NH1	2.34	0.43
1:C:463:GLU:HB3	1:D:95:ARG:HD3	2.00	0.43
5:A:931:HOH:O	1:B:102:PRO:HA	2.19	0.43
1:D:188:ASP:OD2	1:D:218:ARG:NH2	2.43	0.43
1:A:46:ARG:HD2	1:A:298:MET:HE1	2.01	0.43
1:B:345:PHE:CE2	1:B:491:ALA:HB1	2.54	0.43
1:B:597:LEU:HA	1:B:598:PRO:HD2	1.81	0.43
1:C:129:GLY:HA3	1:C:415:GLY:HA3	2.01	0.43
1:D:54:LEU:HD21	1:D:299:ARG:HB3	2.00	0.43
1:D:425:TYR:HA	1:D:451:VAL:O	2.19	0.43
1:B:338:LEU:HD21	1:B:366:LEU:HD21	2.00	0.42
1:B:554:HIS:HD2	5:B:1079:HOH:O	2.01	0.42
1:D:17:PHE:HA	1:D:20:ILE:HD12	2.01	0.42
1:D:203:GLU:OE1	1:D:208:ARG:NE	2.38	0.42
1:D:283:TYR:CZ	1:D:289:PRO:HG3	2.54	0.42
1:B:13:ASN:OD1	1:B:16:ARG:NH2	2.50	0.42
1:D:209:TYR:O	1:D:214:TRP:HB2	2.18	0.42
1:C:329:ARG:NH1	1:C:334:GLU:O	2.53	0.42
1:D:4:THR:HA	1:D:7:LEU:HB3	2.00	0.42
1:C:198:ASP:O	1:D:176:HIS:CE1	2.73	0.42
1:D:590:LYS:O	1:D:594:PRO:HA	2.18	0.42
1:C:180:SER:HB3	1:C:239:GLU:C	2.40	0.42
1:C:376:LEU:HB2	1:C:380:ASN:ND2	2.34	0.42
1:A:38:ALA:HB3	1:A:39:PRO:HD3	2.01	0.42
1:A:428:THR:HG21	1:A:436:MET:CE	2.49	0.42
1:B:193:ILE:HG13	2:B:802:TPP:H71	2.02	0.42
1:C:2:LYS:O	1:C:2:LYS:HD2	2.20	0.42
1:C:555:LEU:HD11	1:C:639:THR:C	2.40	0.42
1:D:329:ARG:NH1	1:D:336:PRO:HD3	2.35	0.42
1:C:172:SER:OG	1:C:405:ARG:NH1	2.53	0.41
1:C:579:GLU:H	1:C:579:GLU:CD	2.23	0.41
1:A:604:ALA:HA	1:A:638:PHE:CZ	2.55	0.41
1:C:413:LEU:HB3	1:C:450:THR:HG23	2.02	0.41
1:C:390:PHE:HB2	1:C:397:GLY:O	2.20	0.41
1:D:413:LEU:HD11	1:D:426:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:581:PHE:CZ	1:D:589:ARG:HG2	2.56	0.41
2:A:701:TPP:N1'	1:B:406:GLU:OE2	2.54	0.41
1:D:188:ASP:CG	1:D:190:ARG:HH11	2.24	0.41
1:A:437:ARG:CD	1:B:437:ARG:HD3	2.51	0.41
1:C:208:ARG:O	1:C:211:ALA:HB3	2.21	0.41
1:C:406:GLU:OE1	1:D:164:GLU:OE2	2.39	0.41
1:C:564:ARG:O	1:C:567:GLY:N	2.48	0.41
1:D:489:ALA:O	1:D:554:HIS:HE1	2.03	0.41
1:B:225:LEU:O	1:B:229:ARG:HG3	2.21	0.41
1:B:46:ARG:HD2	1:B:298:MET:HE1	2.03	0.40
1:D:90:GLU:OE1	1:D:90:GLU:HA	2.21	0.40
1:A:529:LEU:HD23	1:A:529:LEU:C	2.42	0.40
1:C:363:ALA:N	1:C:364:PRO:CD	2.84	0.40
1:D:428:THR:CG2	1:D:436:MET:HE3	2.52	0.40
1:D:593:LEU:O	1:D:594:PRO:C	2.59	0.40
2:A:701:TPP:C2	2:A:701:TPP:N4'	2.83	0.40
1:D:42:TYR:O	1:D:46:ARG:HB3	2.20	0.40
1:D:250:ILE:HD11	1:D:263:HIS:HA	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	648/672 (96%)	636 (98%)	12 (2%)	0	100	100
1	B	648/672 (96%)	636 (98%)	12 (2%)	0	100	100
1	C	648/672 (96%)	622 (96%)	24 (4%)	2 (0%)	41	37
1	D	648/672 (96%)	602 (93%)	42 (6%)	4 (1%)	25	19
All	All	2592/2688 (96%)	2496 (96%)	90 (4%)	6 (0%)	47	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	565	GLU
1	D	269	PRO
1	D	200	ALA
1	C	200	ALA
1	D	77	ALA
1	D	80	HIS

### 5.3.2 Protein sidechains ⓘ

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	521/540 (96%)	514 (99%)	7 (1%)	69	74
1	B	521/540 (96%)	511 (98%)	10 (2%)	57	61
1	C	521/540 (96%)	513 (98%)	8 (2%)	65	69
1	D	521/540 (96%)	507 (97%)	14 (3%)	44	46
All	All	2084/2160 (96%)	2045 (98%)	39 (2%)	57	61

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	218	ARG
1	A	344	SER
1	A	365	ARG
1	A	490	ASP
1	A	522	SER
1	A	617	VAL
1	B	2	LYS
1	B	99	SER
1	B	230	LYS
1	B	261	LYS
1	B	313	LEU
1	B	385	GLU
1	B	564	ARG
1	B	565	GLU
1	B	571	ARG

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Mol	Chain	Res	Type
1	B	617	VAL
1	C	2	LYS
1	C	6	ASP
1	C	54	LEU
1	C	303	ARG
1	C	344	SER
1	C	531	ARG
1	C	552	GLU
1	C	642	ARG
1	D	6	ASP
1	D	54	LEU
1	D	220	GLU
1	D	248	SER
1	D	261	LYS
1	D	313	LEU
1	D	314	GLU
1	D	323	LEU
1	D	328	MET
1	D	341	GLU
1	D	344	SER
1	D	347	LYS
1	D	388	GLU
1	D	524	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	ASN
1	A	394	ASN
1	A	417	ASN
1	A	554	HIS
1	A	560	GLN
1	B	324	HIS
1	B	380	ASN
1	B	394	ASN
1	B	417	ASN
1	B	554	HIS
1	B	560	GLN
1	C	394	ASN
1	C	417	ASN
1	C	554	HIS
1	D	324	HIS

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Mol	Chain	Res	Type
1	D	380	ASN
1	D	417	ASN
1	D	554	HIS
1	D	560	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	$\# Z  > 2$
2	TPP	C	701	3	22,27,27	0.61	0	29,40,40	1.12	3 (10%)
2	TPP	B	802	3	22,27,27	0.78	0	29,40,40	1.07	2 (6%)
4	MES	B	801	-	12,12,12	0.74	0	14,16,16	1.12	2 (14%)
2	TPP	A	701	3	22,27,27	0.65	0	29,40,40	0.94	1 (3%)
2	TPP	D	802	3	22,27,27	0.68	0	29,40,40	0.87	0
4	MES	C	703	-	12,12,12	0.73	0	14,16,16	0.65	0
4	MES	D	801	-	12,12,12	0.72	0	14,16,16	0.57	0
4	MES	A	703	-	12,12,12	0.66	0	14,16,16	0.65	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
2	TPP	C	701	3	-	2/16/17/17	0/2/2/2
2	TPP	B	802	3	-	1/16/17/17	0/2/2/2
4	MES	B	801	-	-	1/6/14/14	0/1/1/1
2	TPP	A	701	3	-	6/16/17/17	0/2/2/2
2	TPP	D	802	3	-	1/16/17/17	0/2/2/2
4	MES	C	703	-	-	4/6/14/14	0/1/1/1
4	MES	D	801	-	-	4/6/14/14	0/1/1/1
4	MES	A	703	-	-	4/6/14/14	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	TPP	C6-C5-C4	-3.10	124.94	127.43
2	A	701	TPP	C6-C5-C4	-2.84	125.15	127.43
2	B	802	TPP	C6-C5-C4	-2.53	125.40	127.43
4	B	801	MES	C6-C5-N4	-2.20	106.77	110.10
2	C	701	TPP	O2A-PA-O1A	2.18	123.03	112.24
4	B	801	MES	O2S-S-C8	-2.18	104.29	106.92
2	B	802	TPP	O2B-PB-O3A	-2.16	97.38	104.64
2	C	701	TPP	C5-C4-N3	2.09	111.75	107.57

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TPP	C4-C5-C6-C7
2	A	701	TPP	PA-O3A-PB-O2B
2	A	701	TPP	PA-O3A-PB-O3B
2	B	802	TPP	C4-C5-C6-C7
2	C	701	TPP	C4-C5-C6-C7
2	D	802	TPP	C4-C5-C6-C7
4	A	703	MES	C7-C8-S-O2S
4	A	703	MES	C7-C8-S-O3S
4	B	801	MES	N4-C7-C8-S
4	C	703	MES	C7-C8-S-O3S

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Mol	Chain	Res	Type	Atoms
4	D	801	MES	N4-C7-C8-S
4	D	801	MES	C7-C8-S-O2S
4	D	801	MES	C7-C8-S-O3S
4	A	703	MES	N4-C7-C8-S
4	A	703	MES	C7-C8-S-O1S
4	C	703	MES	C7-C8-S-O1S
4	C	703	MES	C7-C8-S-O2S
4	D	801	MES	C7-C8-S-O1S
2	A	701	TPP	C4'-C5'-C7'-N3
2	C	701	TPP	C4'-C5'-C7'-N3
2	A	701	TPP	PA-O3A-PB-O1B
2	A	701	TPP	C6'-C5'-C7'-N3
4	C	703	MES	N4-C7-C8-S

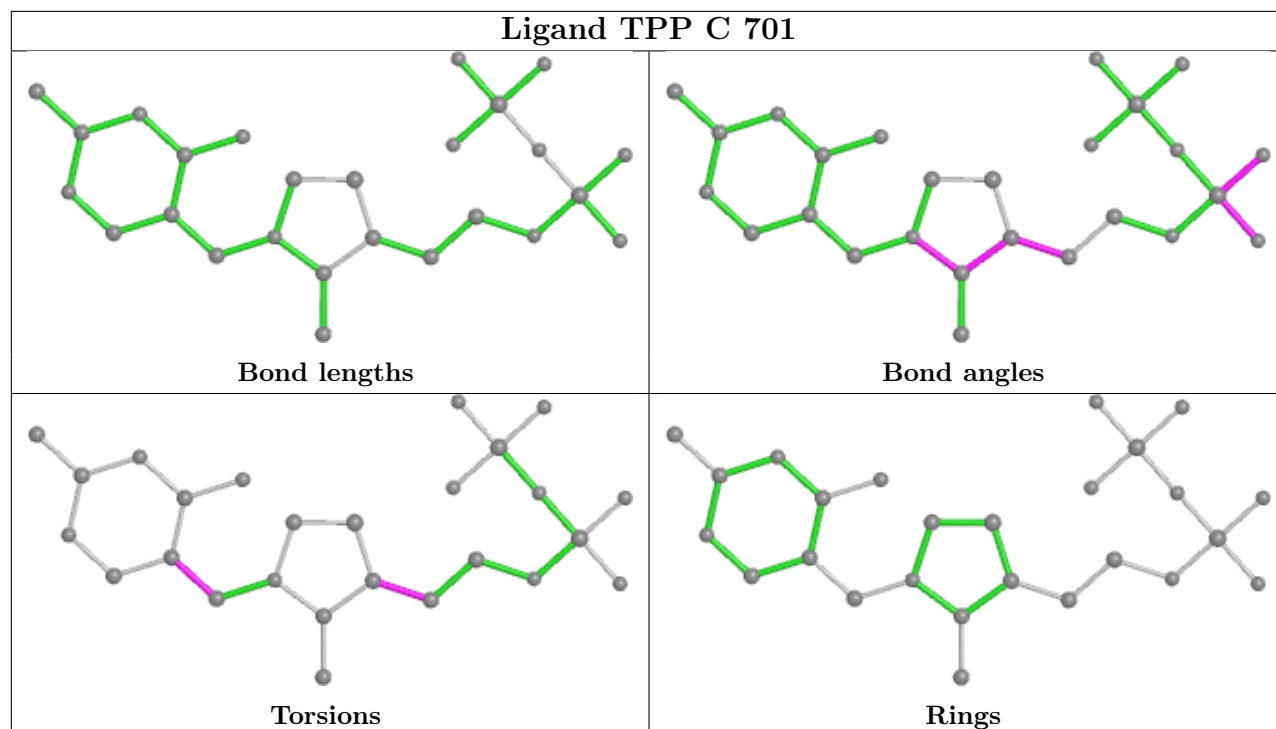
There are no ring outliers.

7 monomers are involved in 28 short contacts:

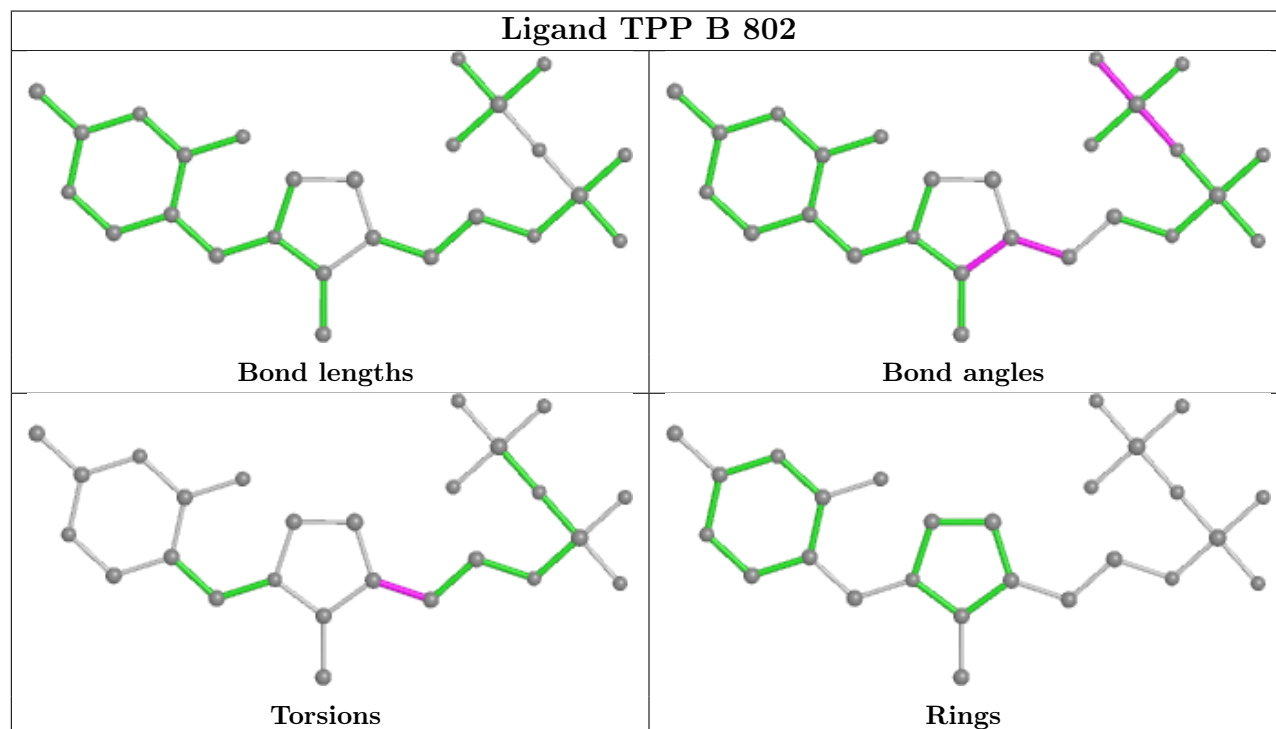
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	TPP	2	0
2	B	802	TPP	4	0
4	B	801	MES	5	0
2	A	701	TPP	7	0
2	D	802	TPP	2	0
4	D	801	MES	2	0
4	A	703	MES	6	0

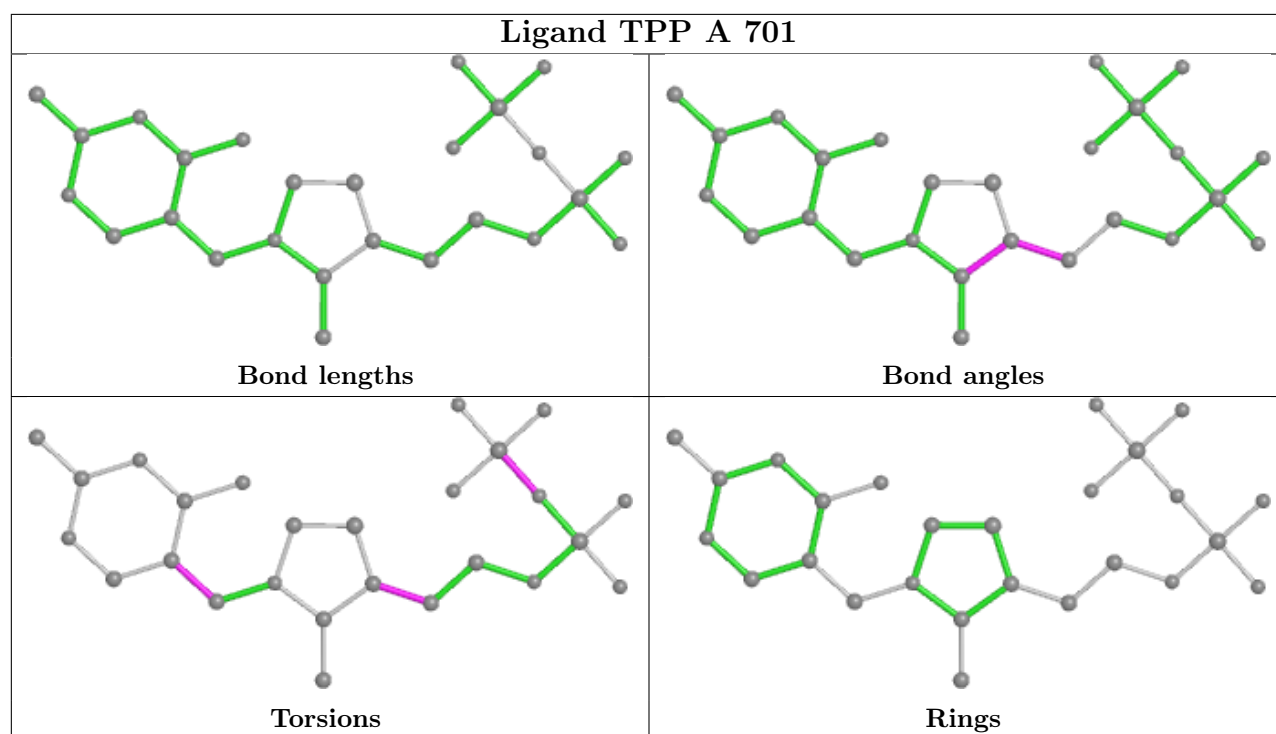
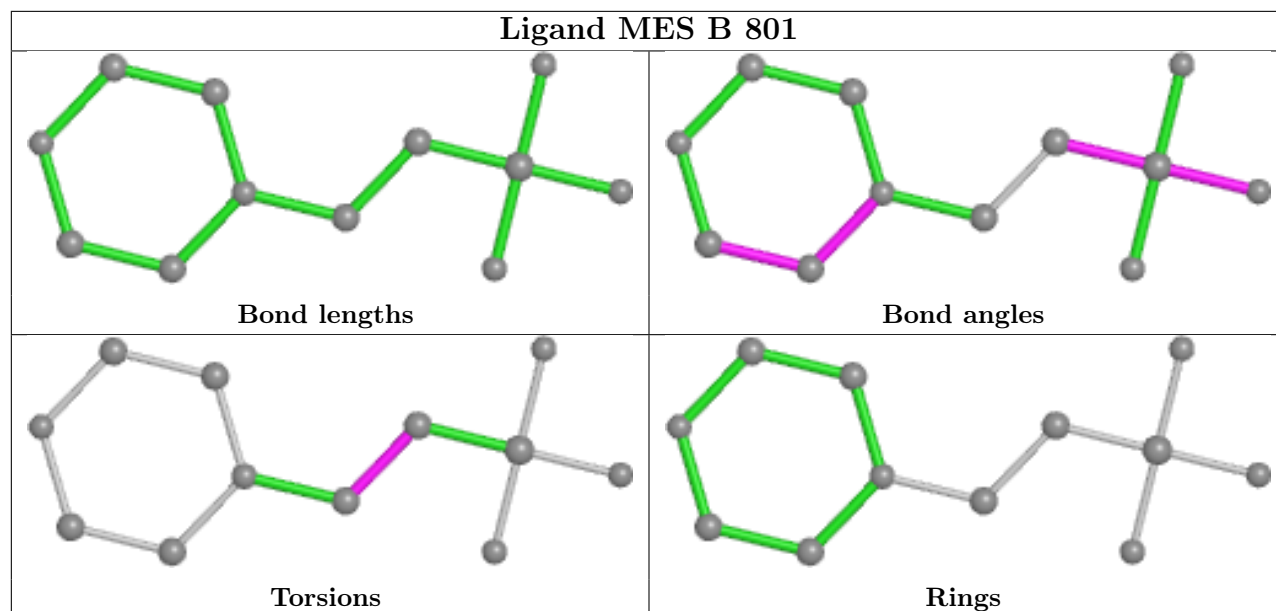
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 C 701

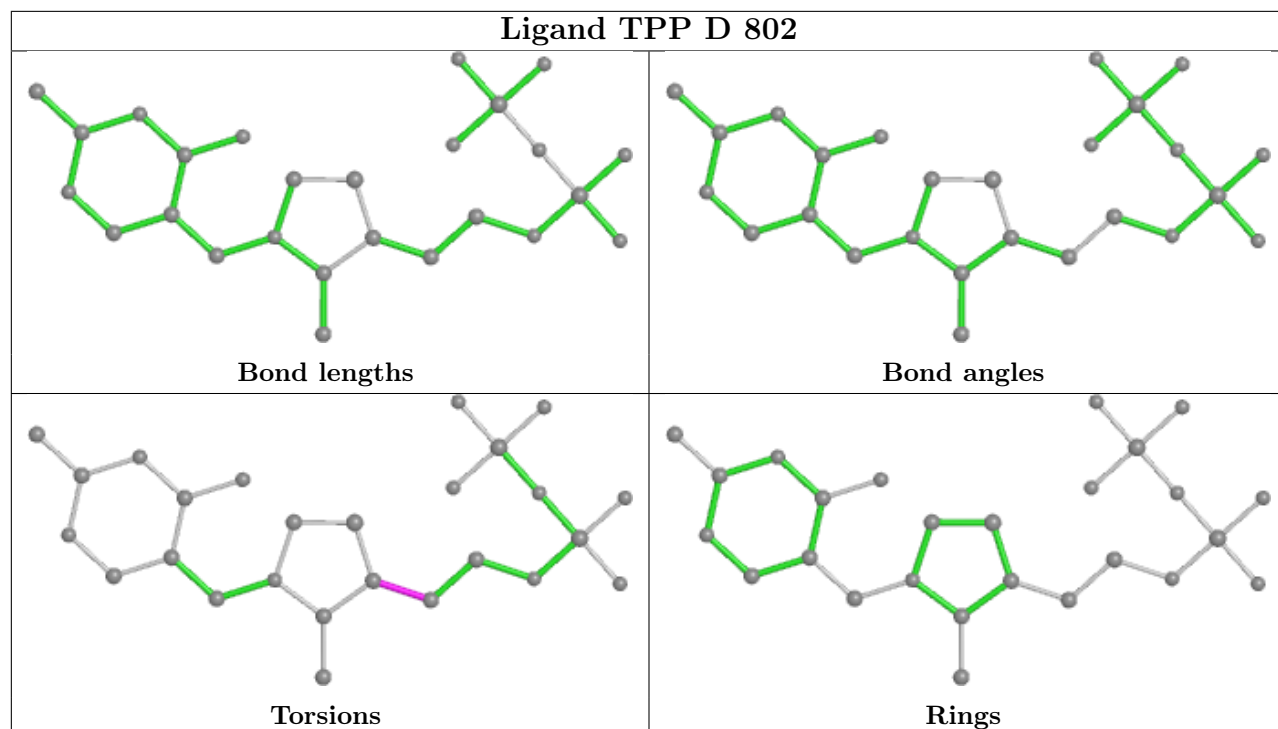


## Ligand TPP B 802

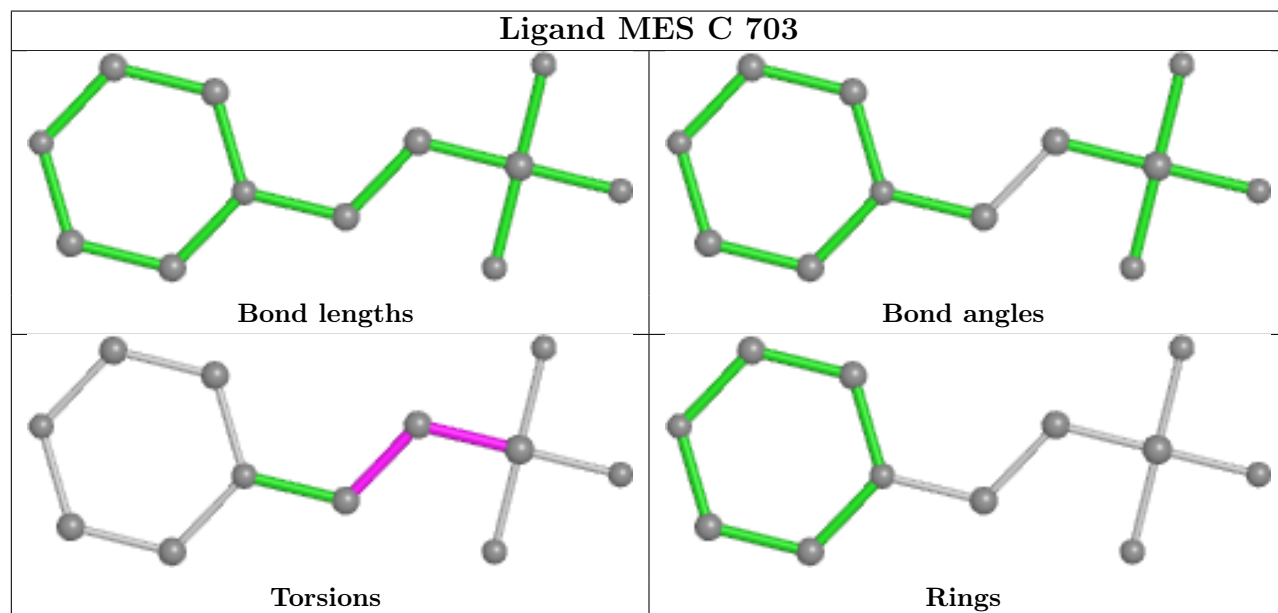


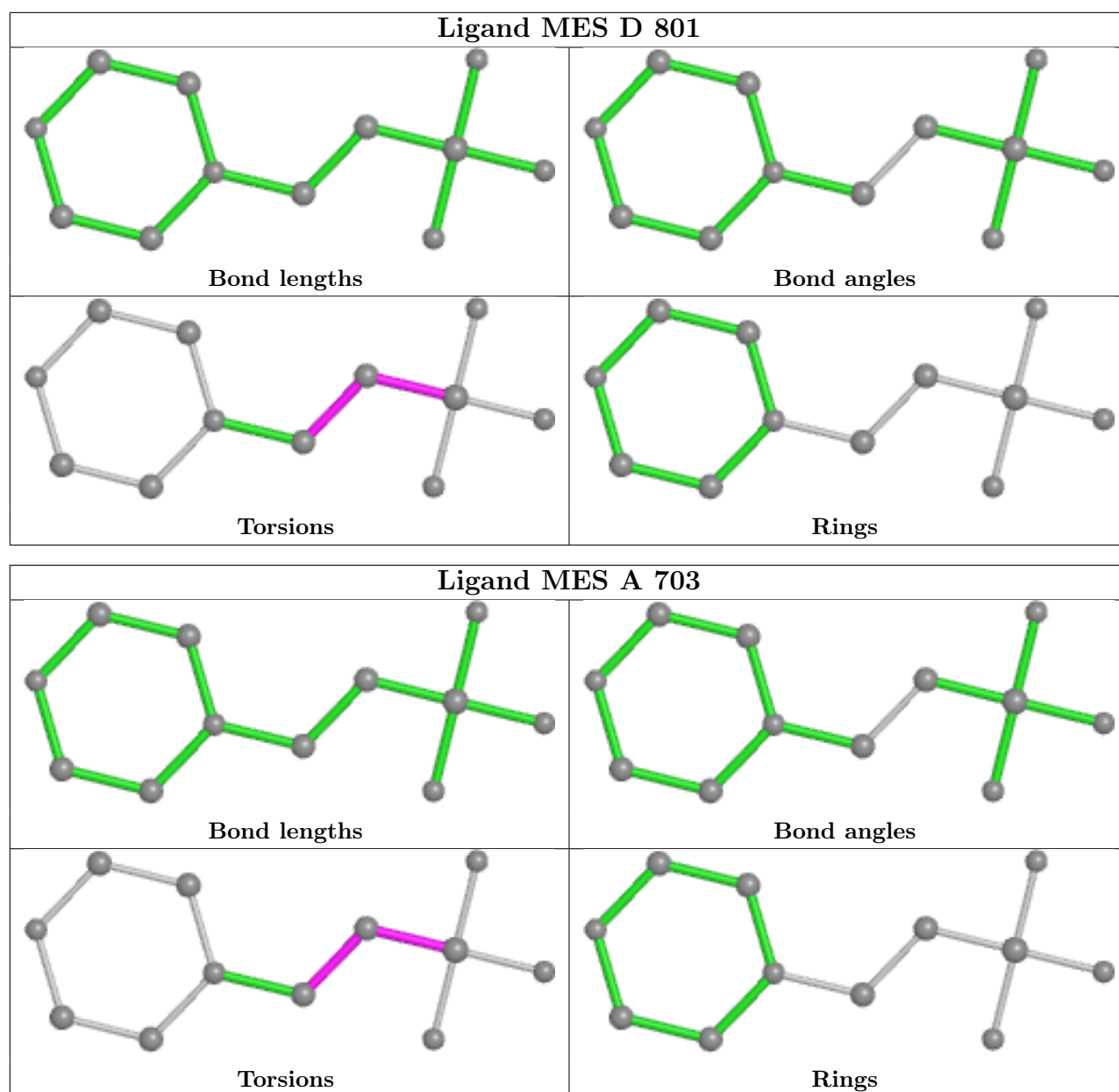


## Ligand TPP D 802



## Ligand MES C 703





## 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	650/672 (96%)	-0.18	8 (1%) 79 78	21, 32, 51, 105	0
1	B	650/672 (96%)	-0.19	10 (1%) 73 72	23, 35, 54, 105	0
1	C	650/672 (96%)	0.08	21 (3%) 47 46	35, 47, 69, 105	0
1	D	650/672 (96%)	0.80	107 (16%) 1 1	38, 59, 83, 136	0
All	All	2600/2688 (96%)	0.13	146 (5%) 24 23	21, 43, 73, 136	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	THR	6.8
1	D	4	THR	5.6
1	A	2	LYS	5.1
1	D	144	PRO	5.0
1	B	4	THR	4.9
1	D	3	GLU	4.8
1	D	320	TYR	4.5
1	C	2	LYS	4.5
1	D	148	VAL	4.3
1	C	322	ASP	4.3
1	D	2	LYS	4.1
1	D	5	ARG	4.1
1	D	312	ALA	4.1
1	D	597	LEU	4.0
1	D	280	GLY	4.0
1	D	316	TYR	3.9
1	B	651	VAL	3.9
1	D	166	VAL	3.9
1	B	3	GLU	3.8
1	D	313	LEU	3.7
1	D	323	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	564	ARG	3.7
1	D	438	PRO	3.6
1	D	318	ARG	3.6
1	D	338	LEU	3.5
1	D	436	MET	3.5
1	C	5	ARG	3.5
1	D	237	LEU	3.5
1	D	651	VAL	3.4
1	B	2	LYS	3.3
1	D	432	PHE	3.2
1	D	340	GLU	3.2
1	D	152	TYR	3.2
1	D	230	LYS	3.1
1	D	568	VAL	3.1
1	C	562	LEU	3.1
1	D	54	LEU	3.1
1	D	288	VAL	3.1
1	D	227	ALA	3.1
1	D	561	ALA	3.1
1	C	337	PRO	3.1
1	A	3	GLU	3.1
1	D	145	GLY	3.0
1	D	308	ALA	3.0
1	D	411	ALA	3.0
1	D	309	TRP	3.0
1	C	3	GLU	3.0
1	D	563	LEU	2.9
1	D	269	PRO	2.9
1	D	570	VAL	2.8
1	D	566	LYS	2.8
1	C	120	LEU	2.8
1	D	48	VAL	2.8
1	D	644	ALA	2.8
1	B	5	ARG	2.8
1	D	541	GLU	2.7
1	D	234	LEU	2.7
1	D	542	PRO	2.7
1	D	559	ALA	2.7
1	D	141	PHE	2.7
1	D	433	SER	2.7
1	D	404	VAL	2.7
1	D	324	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	536	LEU	2.7
1	D	294	ARG	2.7
1	C	148	VAL	2.6
1	D	435	TYR	2.6
1	D	303	ARG	2.6
1	C	651	VAL	2.6
1	D	319	ALA	2.6
1	D	311	LYS	2.6
1	C	166	VAL	2.6
1	B	440	ILE	2.6
1	A	166	VAL	2.6
1	D	437	ARG	2.6
1	C	218	ARG	2.5
1	C	438	PRO	2.5
1	D	544	GLY	2.5
1	D	539	VAL	2.5
1	D	121	GLY	2.5
1	D	314	GLU	2.5
1	D	431	VAL	2.4
1	D	283	TYR	2.4
1	D	643	VAL	2.4
1	B	435	TYR	2.4
1	D	315	ALA	2.4
1	D	365	ARG	2.4
1	D	496	TYR	2.3
1	A	432	PHE	2.3
1	D	439	ALA	2.3
1	C	435	TYR	2.3
1	D	112	GLY	2.3
1	C	439	ALA	2.3
1	D	327	LEU	2.3
1	D	527	ARG	2.3
1	B	439	ALA	2.2
1	D	120	LEU	2.2
1	D	221	ASP	2.2
1	D	272	VAL	2.2
1	D	407	HIS	2.2
1	D	650	LEU	2.2
1	D	42	TYR	2.2
1	D	495	PHE	2.2
1	D	567	GLY	2.2
1	D	239	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	431	VAL	2.2
1	D	147	VAL	2.2
1	D	255	PRO	2.2
1	D	543	GLN	2.2
1	D	260	ALA	2.2
1	D	646	ALA	2.2
1	D	10	LEU	2.2
1	D	413	LEU	2.2
1	D	295	HIS	2.2
1	D	540	GLU	2.2
1	C	124	ILE	2.2
1	B	438	PRO	2.2
1	D	252	PHE	2.2
1	C	160	GLY	2.2
1	D	428	THR	2.2
1	A	438	PRO	2.2
1	D	282	PRO	2.2
1	D	284	PRO	2.2
1	A	120	LEU	2.1
1	D	278	ASN	2.1
1	D	257	GLN	2.1
1	D	557	LEU	2.1
1	D	277	ARG	2.1
1	C	121	GLY	2.1
1	A	444	ALA	2.1
1	D	341	GLU	2.1
1	D	339	PRO	2.1
1	D	374	ALA	2.1
1	B	436	MET	2.1
1	D	429	PHE	2.1
1	D	337	PRO	2.1
1	C	408	ALA	2.1
1	D	146	HIS	2.1
1	D	524	GLU	2.0
1	D	124	ILE	2.0
1	D	441	ARG	2.0
1	A	435	TYR	2.0
1	C	364	PRO	2.0
1	D	442	LEU	2.0
1	D	335	LEU	2.0
1	D	430	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

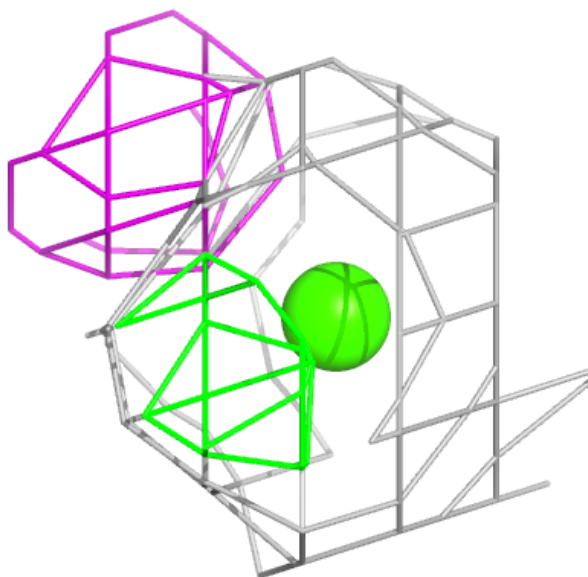
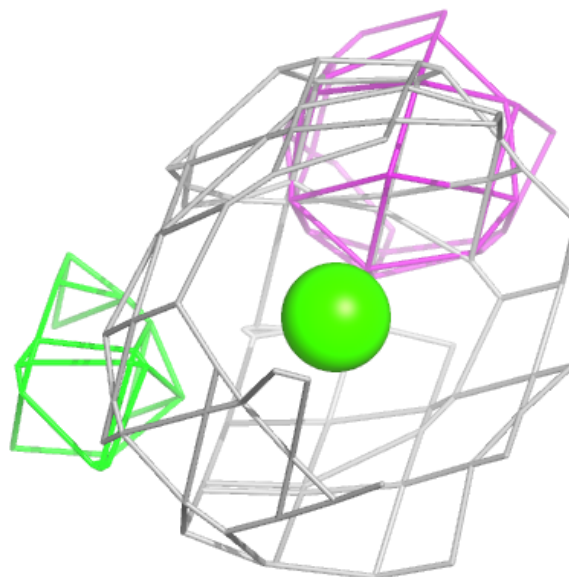
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	D	803	1/1	0.79	0.10	72,72,72,72	0
2	TPP	D	802	26/26	0.85	0.20	55,69,95,101	0
4	MES	C	703	12/12	0.90	0.20	58,93,105,108	0
2	TPP	C	701	26/26	0.91	0.16	47,61,75,81	0
2	TPP	A	701	26/26	0.93	0.12	27,41,50,51	0
3	CA	B	803	1/1	0.93	0.04	43,43,43,43	0
3	CA	C	702	1/1	0.94	0.05	52,52,52,52	0
4	MES	A	703	12/12	0.95	0.14	44,71,83,83	0
2	TPP	B	802	26/26	0.95	0.12	34,42,54,59	0
4	MES	D	801	12/12	0.95	0.17	74,95,103,104	0
4	MES	B	801	12/12	0.96	0.15	38,76,92,94	0
3	CA	A	702	1/1	0.99	0.05	38,38,38,38	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.

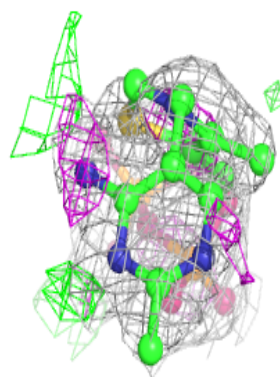
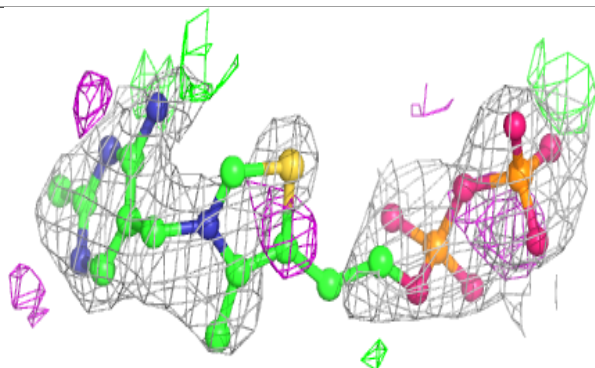
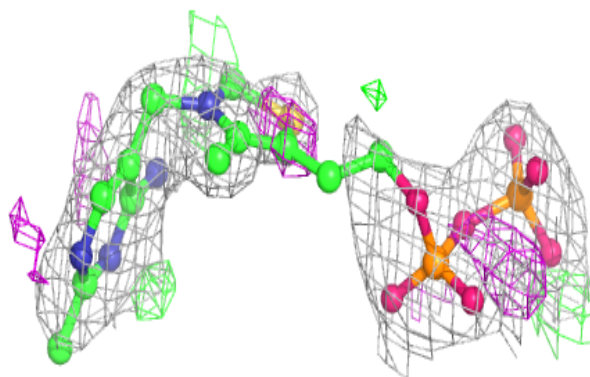
**Electron density around CA D 803:**

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

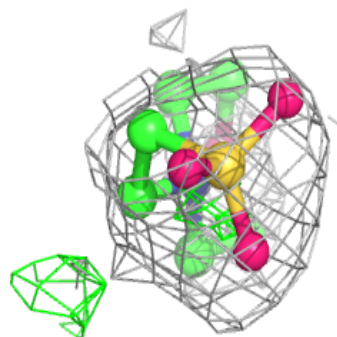
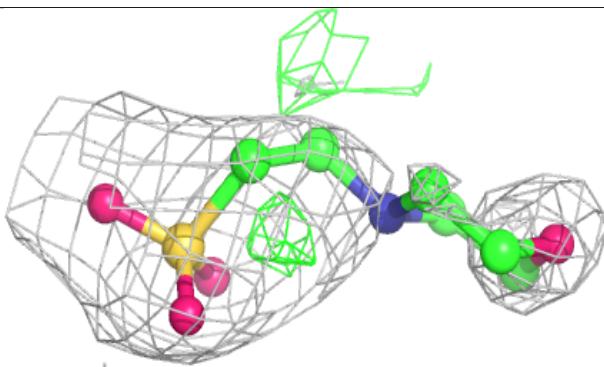
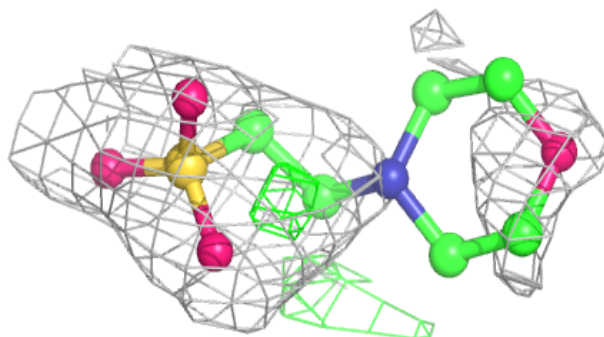


**Electron density around TPP D 802:**

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

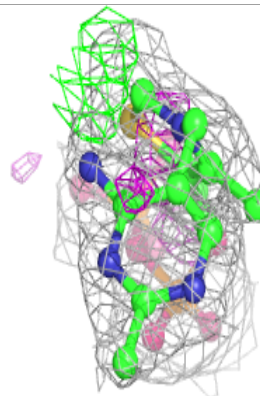
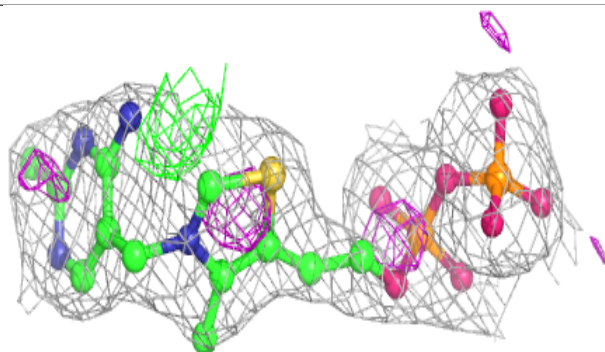
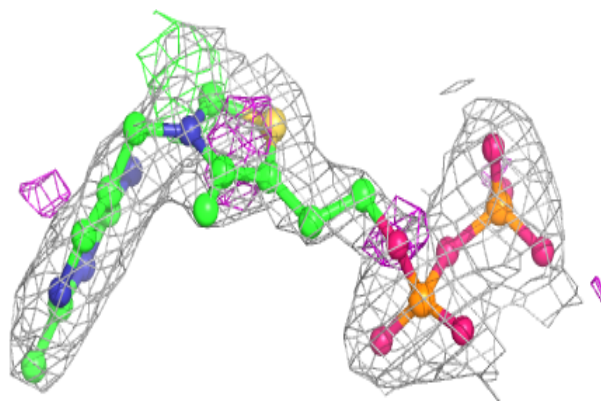
**Electron density around MES C 703:**

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

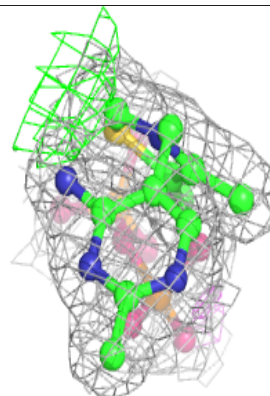
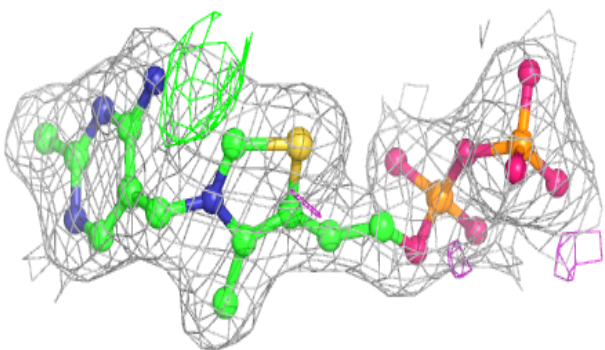
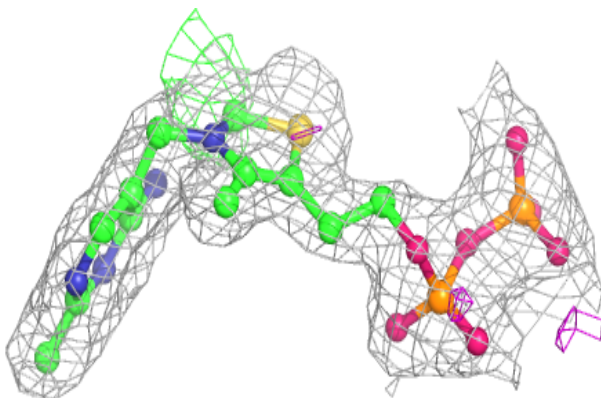


**Electron density around TPP C 701:**

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

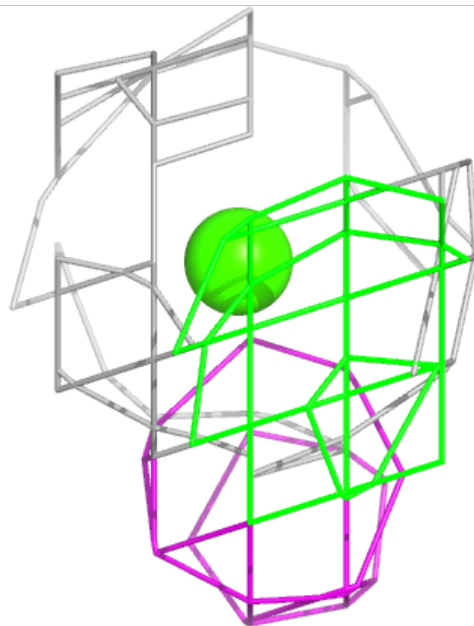
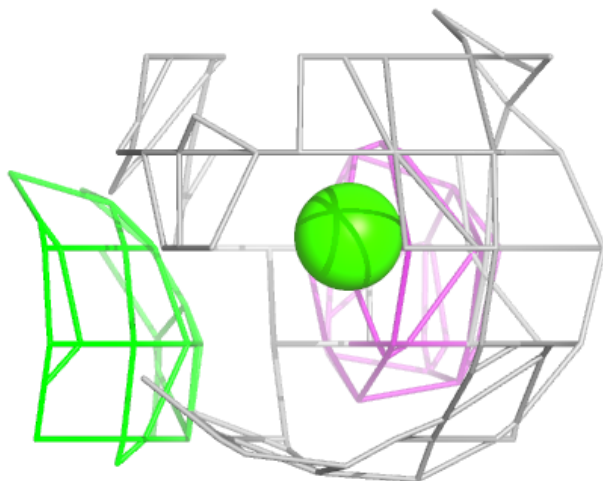
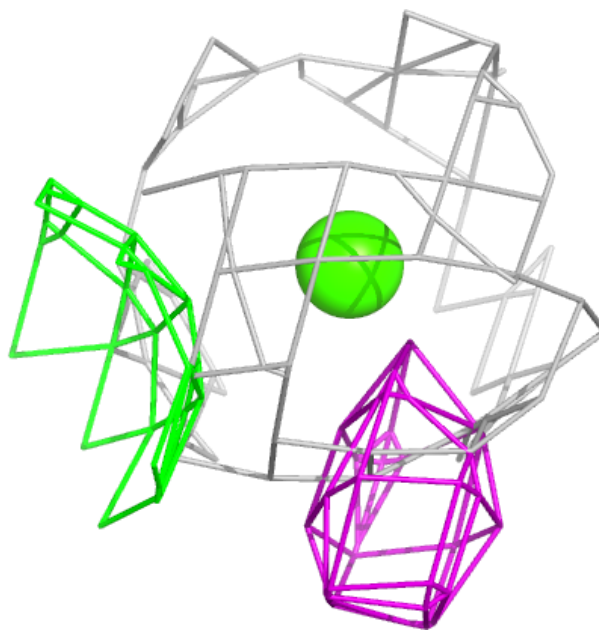
**Electron density around TPP A 701:**

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



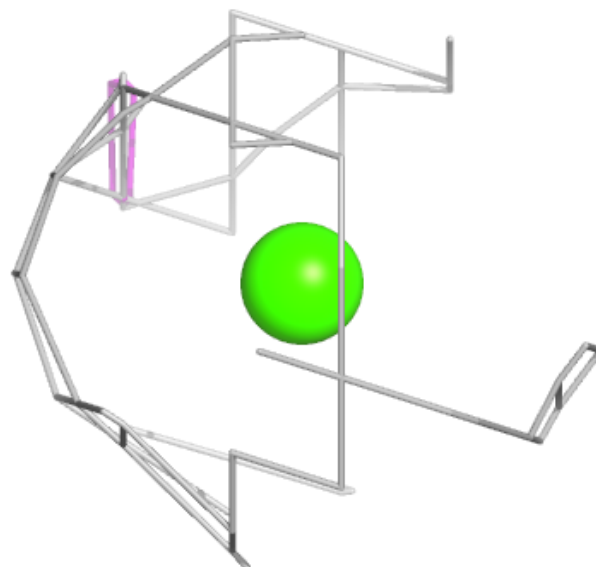
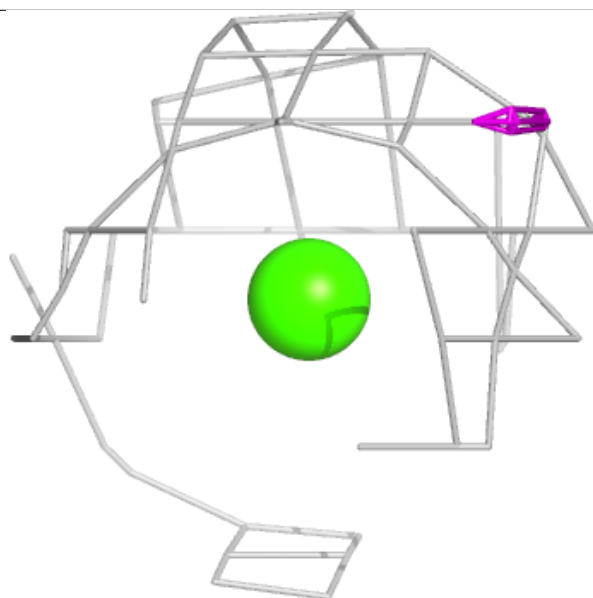
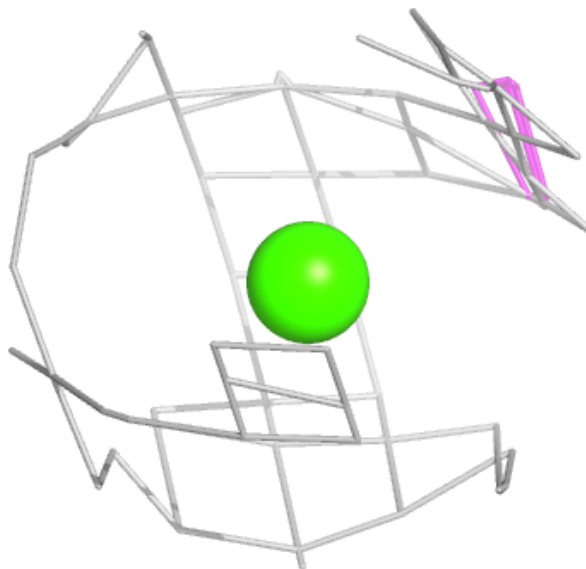
**Electron density around CA B 803:**

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and green (positive)



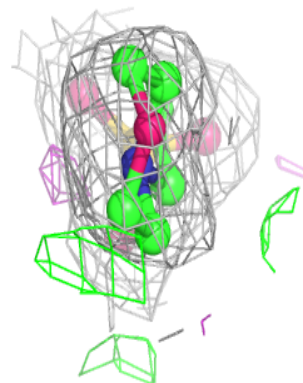
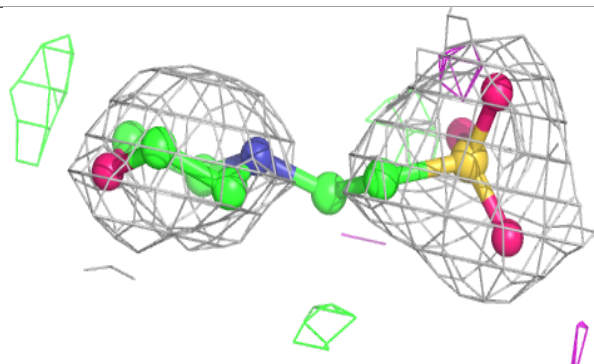
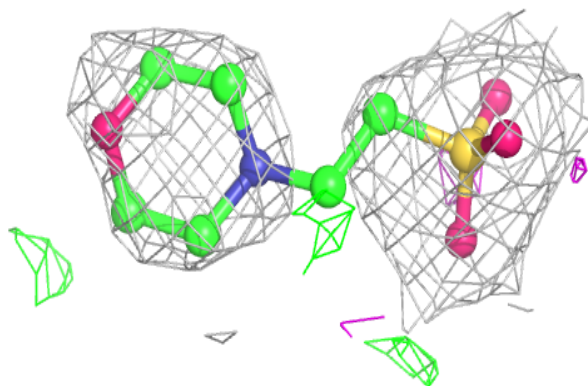
**Electron density around CA C 702:**

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and green (positive)

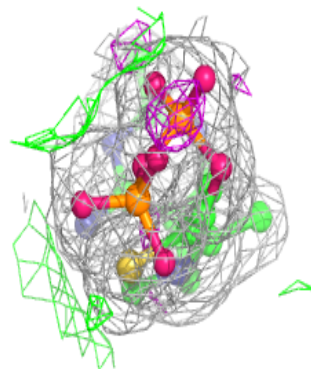
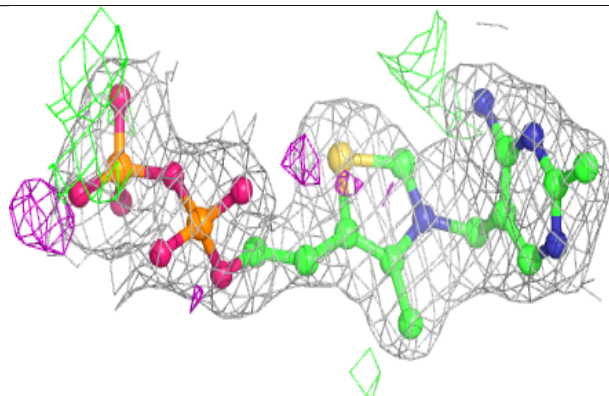
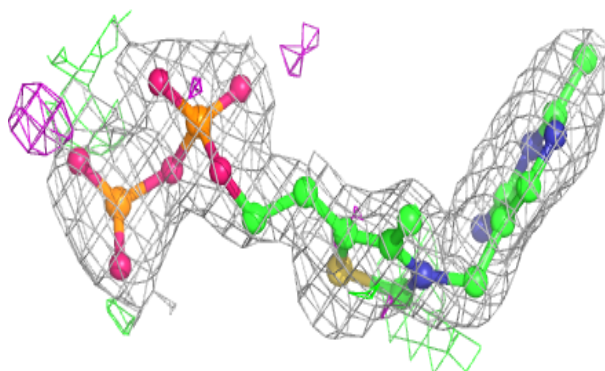


**Electron density around MES A 703:**

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

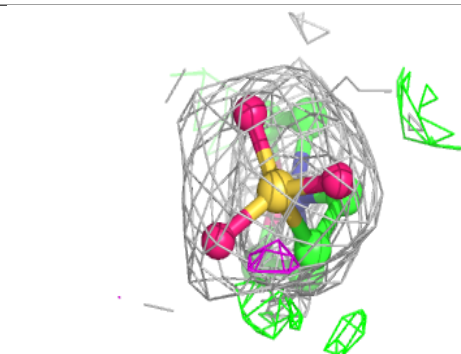
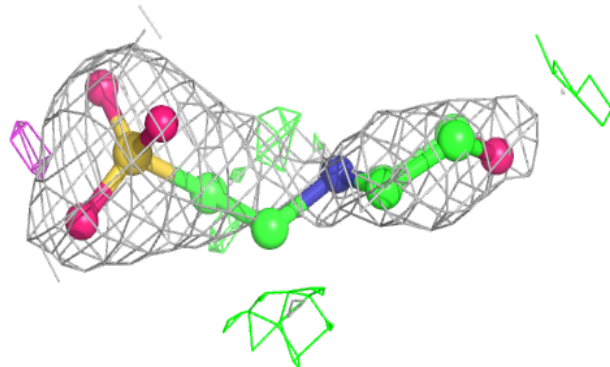
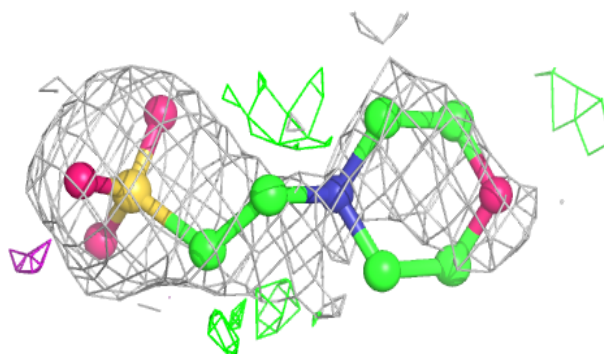
**Electron density around TPP B 802:**

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

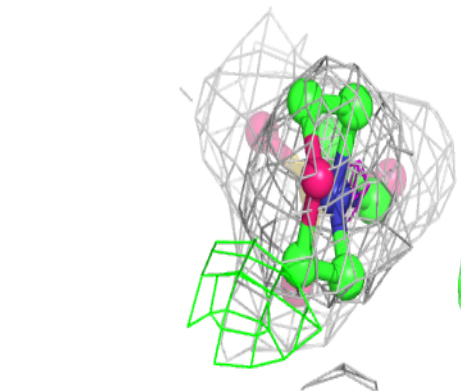
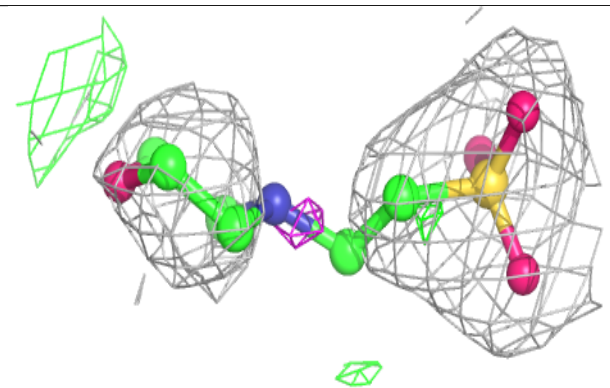
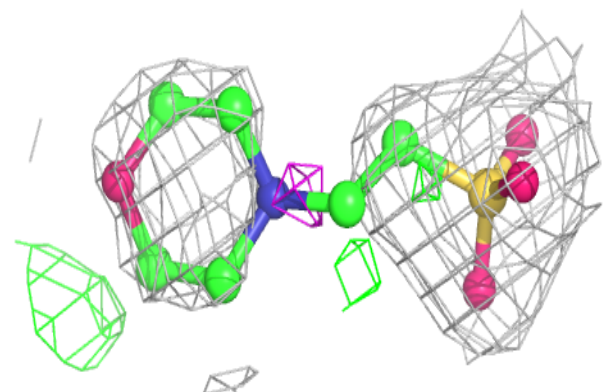


**Electron density around MES D 801:**

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

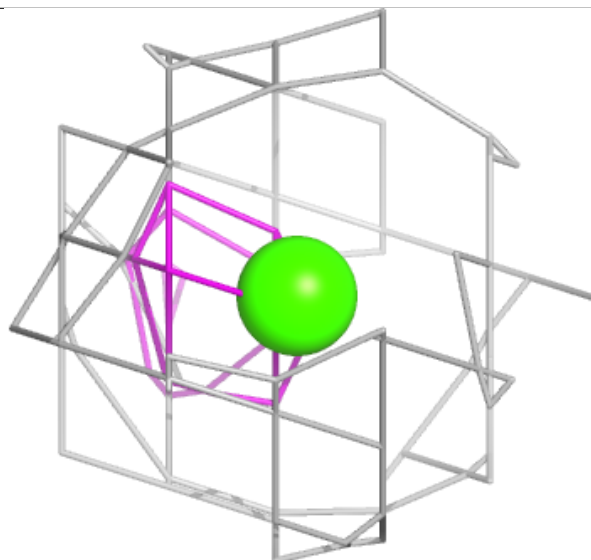
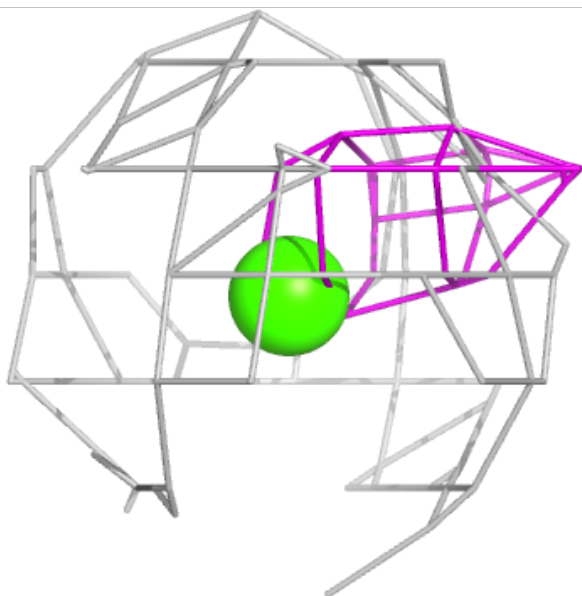
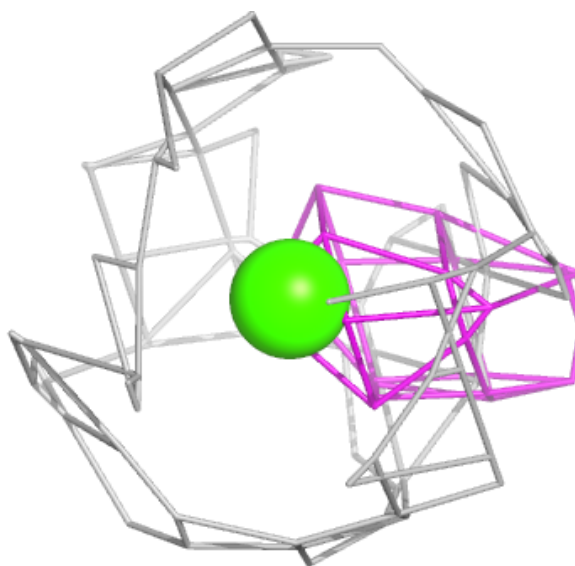
**Electron density around MES B 801:**

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



**Electron density around CA A 702:**

$2mF_o-DF_c$  (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.