



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:56 am BST

PDB ID : 3ZHR  
Title : Crystal structure of the H747A mutant of the SucA domain of Mycobacterium smegmatis KGD showing the active site lid closed  
Authors : Wagner, T.; Barilone, N.; Bellinzoni, M.; Alzari, P.M.  
Deposited on : 2012-12-24  
Resolution : 2.10 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.

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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	:	2.11
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)	:	2.11

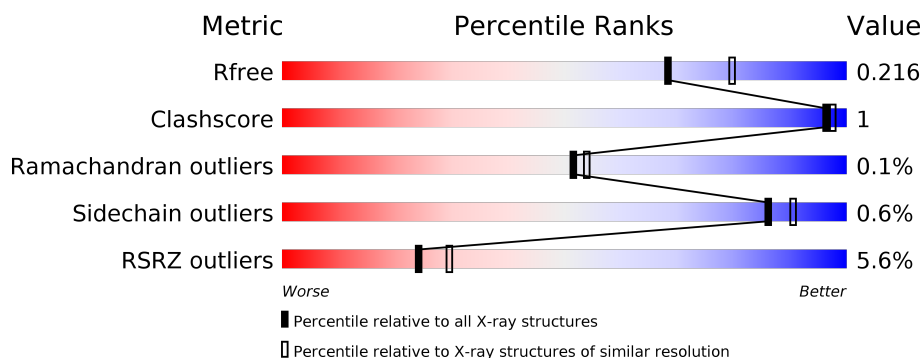
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	868	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	B	868	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
1	C	868	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>6%</div> </div> </div>
1	D	868	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26675 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.

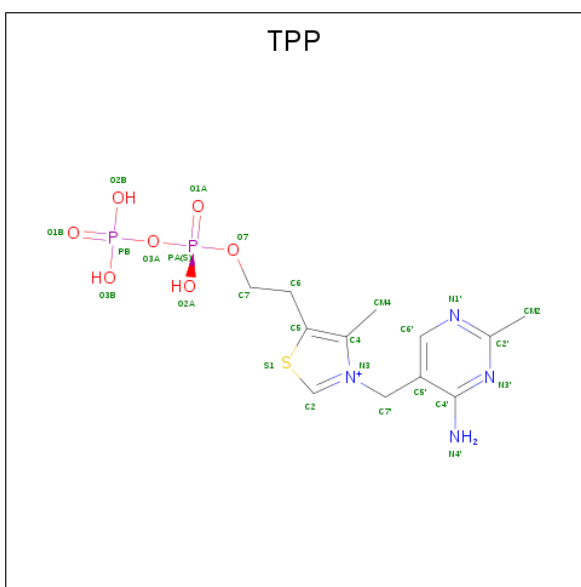
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	2	0
			6376	4017	1124	1210	25			
1	B	823	Total	C	N	O	S	0	2	0
			6371	4010	1130	1205	26			
1	C	813	Total	C	N	O	S	0	1	0
			6307	3973	1116	1193	25			
1	D	823	Total	C	N	O	S	0	1	0
			6302	3971	1109	1197	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	expression tag	UNP A0R2B1
A	747	ALA	HIS	engineered mutation	UNP A0R2B1
B	360	GLY	-	expression tag	UNP A0R2B1
B	747	ALA	HIS	engineered mutation	UNP A0R2B1
C	360	GLY	-	expression tag	UNP A0R2B1
C	747	ALA	HIS	engineered mutation	UNP A0R2B1
D	360	GLY	-	expression tag	UNP A0R2B1
D	747	ALA	HIS	engineered mutation	UNP A0R2B1

- Molecule 2 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
2	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

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

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

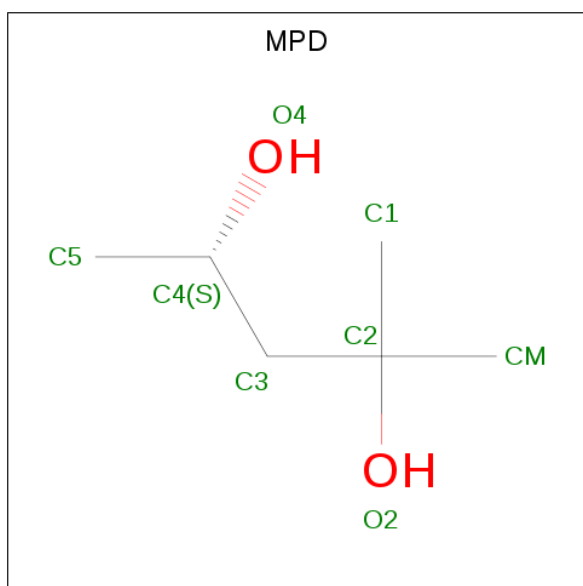
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	C	1	Total	C	O	0	0
			8	6	2		
5	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	339	Total	O	0	0
			339	339		
6	B	259	Total	O	0	0
			259	259		

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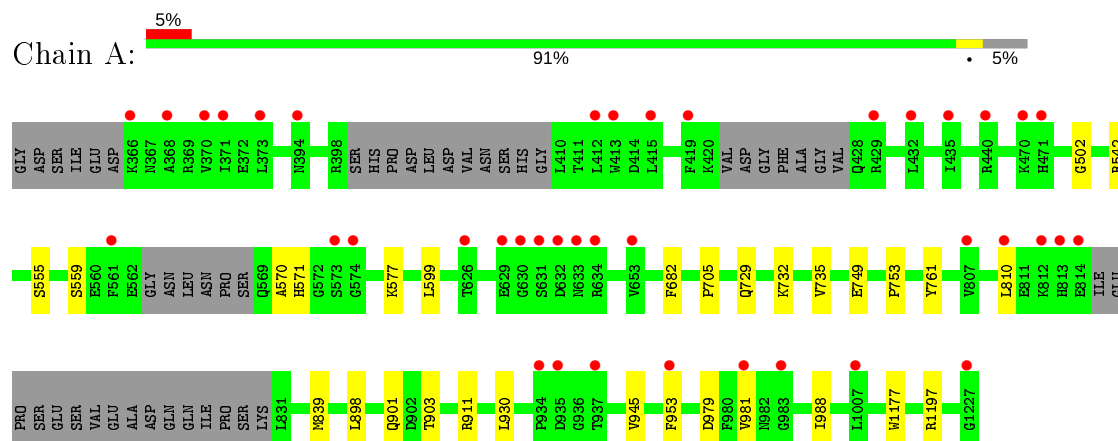
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	326	Total 326	O 326	0	0
6	D	251	Total 251	O 251	0	0

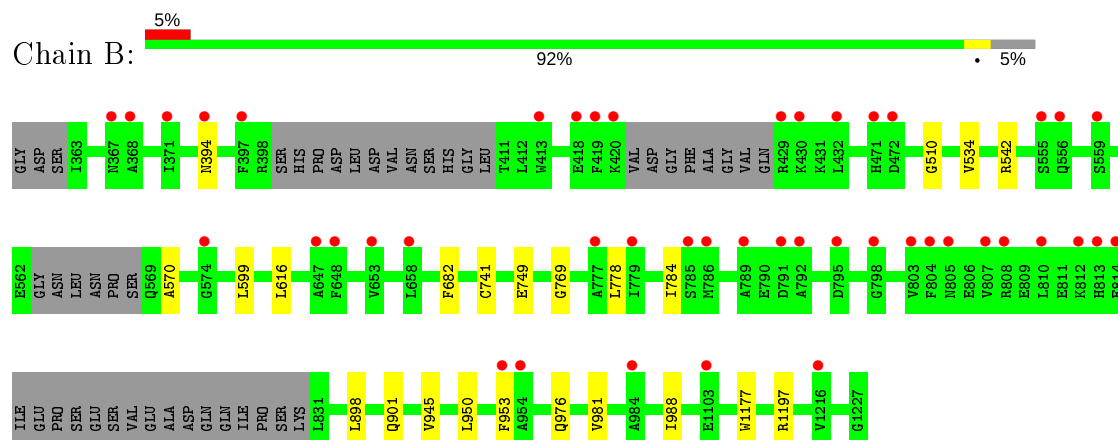
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

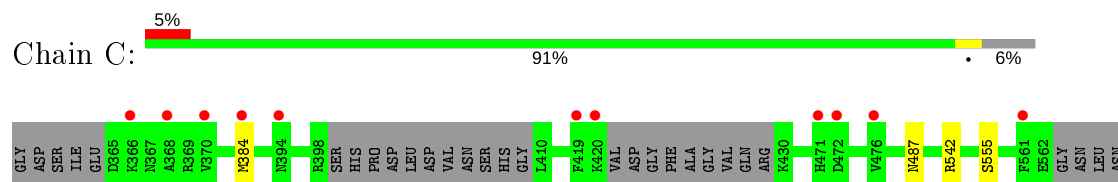
#### • Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

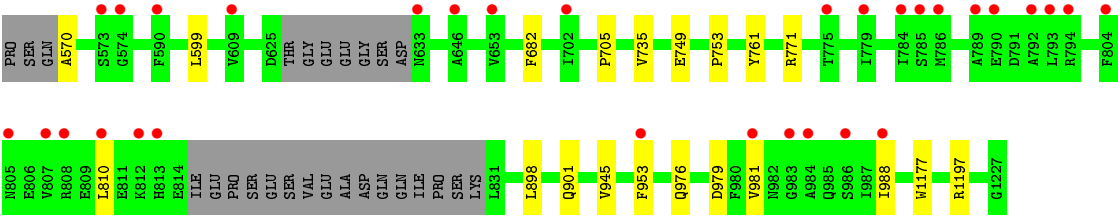


#### • Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

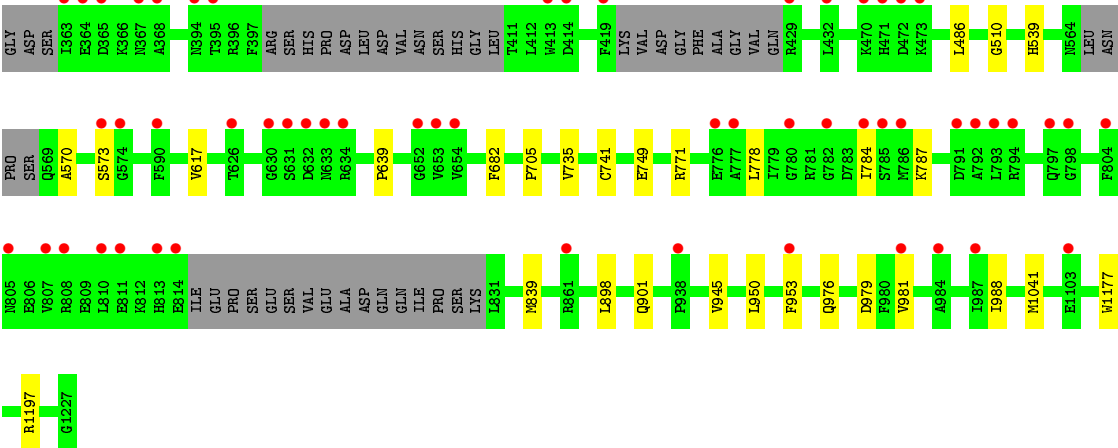
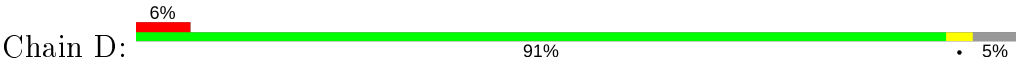


#### • Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME





• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.97Å 83.45Å 159.67Å 99.64° 98.82° 100.98°	Depositor
Resolution (Å)	30.75 – 2.10 48.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.75-2.10) 96.6 (48.75-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.180 , 0.202 0.193 , 0.216	Depositor DCC
$R_{free}$ test set	11124 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26675	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.34% 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: MPD, CA, MG, 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	0.51	0/6511	0.61	0/8828
1	B	0.49	0/6501	0.60	0/8812
1	C	0.50	0/6436	0.60	0/8724
1	D	0.50	0/6431	0.60	0/8725
All	All	0.50	0/25879	0.60	0/35089

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	6376	0	6164	15	0
1	B	6371	0	6158	10	0
1	C	6307	0	6102	10	0
1	D	6302	0	6048	13	0
2	A	26	0	16	2	0
2	B	26	0	16	1	0
2	C	26	0	16	1	0
2	D	26	0	16	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	8	0	14	0	0
5	B	8	0	14	0	0
5	C	8	0	14	0	0
5	D	8	0	14	0	0
6	A	339	0	0	1	0
6	B	259	0	0	1	0
6	C	326	0	0	0	0
6	D	251	0	0	1	0
All	All	26675	0	24592	49	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 1.

All (49) 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:A:570:ALA:HA	1:A:749:GLU:HB2	1.81	0.62
1:B:542:ARG:NE	1:B:599:LEU:HD21	2.17	0.59
1:C:570:ALA:HA	1:C:749:GLU:HB2	1.87	0.56
1:D:570:ALA:HA	1:D:749:GLU:HB2	1.88	0.56
1:A:705:PRO:HG2	1:A:735:VAL:HG13	1.93	0.51
1:B:534:VAL:HG11	1:B:616:LEU:HD22	1.94	0.50
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.93	0.50
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.95	0.49
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.94	0.49
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.95	0.48
1:A:559:SER:O	1:A:577:LYS:NZ	2.45	0.48
1:A:901:GLN:OE1	2:B:2001:TPP:H6'	2.15	0.47
1:A:571:HIS:HE1	6:A:3056:HOH:O	1.98	0.47
1:A:898:LEU:O	1:A:945:VAL:HA	2.15	0.46
1:B:570:ALA:HA	1:B:749:GLU:HB2	1.98	0.46
1:A:542:ARG:NE	1:A:599:LEU:HD21	2.30	0.46
1:D:617:VAL:HG11	1:D:639:PRO:HG3	1.98	0.45
1:C:898:LEU:O	1:C:945:VAL:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:510:GLY:O	1:D:741:CYS:HB2	2.15	0.45
2:A:2001:TPP:H6'	1:B:901:GLN:OE1	2.16	0.45
1:C:901:GLN:OE1	2:D:2001:TPP:H6'	2.16	0.45
1:D:539:HIS:HE1	1:D:573:SER:HB2	1.81	0.45
1:B:898:LEU:O	1:B:945:VAL:HA	2.18	0.44
2:C:2001:TPP:H6'	1:D:901:GLN:OE1	2.17	0.44
1:D:898:LEU:O	1:D:945:VAL:HA	2.18	0.44
1:C:542:ARG:NE	1:C:599:LEU:HD21	2.33	0.44
1:A:839:MET:HE3	1:A:839:MET:O	2.18	0.43
1:B:510:GLY:O	1:B:741:CYS:HB2	2.18	0.43
1:B:778:LEU:HB3	1:B:784:ILE:HG12	2.00	0.43
1:D:705:PRO:HG2	1:D:735:VAL:HG13	2.00	0.43
1:A:555:SER:HA	1:A:810:LEU:HD22	2.01	0.43
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.55	0.42
2:A:2001:TPP:H61	2:A:2001:TPP:HM41	1.94	0.42
1:C:555:SER:HA	1:C:810:LEU:HD22	2.01	0.42
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.55	0.42
1:D:778:LEU:HB3	1:D:784:ILE:HG12	2.01	0.42
1:A:729:GLN:O	1:A:732:LYS:HE3	2.19	0.42
1:C:487:ASN:OD1	1:C:771:ARG:HD2	2.20	0.42
1:D:1041[A]:MET:HE1	6:D:3235:HOH:O	2.20	0.42
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.55	0.42
1:B:769:GLY:HA3	6:B:3024:HOH:O	2.20	0.41
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.55	0.41
1:C:753:PRO:HB2	1:C:761:TYR:CE1	2.56	0.41
1:D:486:LEU:HD13	1:D:771:ARG:HA	2.02	0.41
1:A:502:GLY:HA2	1:A:749:GLU:HG3	2.03	0.41
1:A:753:PRO:HB2	1:A:761:TYR:CE1	2.57	0.40
1:A:903:THR:O	1:A:911:ARG:HD2	2.22	0.40
1:C:705:PRO:HG2	1:C:735:VAL:HG13	2.02	0.40
1:D:839:MET:O	1:D:839:MET:HE2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	814/868 (94%)	797 (98%)	16 (2%)	1 (0%)	51	54
1	B	815/868 (94%)	798 (98%)	16 (2%)	1 (0%)	51	54
1	C	802/868 (92%)	789 (98%)	12 (2%)	1 (0%)	51	54
1	D	814/868 (94%)	793 (97%)	20 (2%)	1 (0%)	51	54
All	All	3245/3472 (94%)	3177 (98%)	64 (2%)	4 (0%)	51	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	682	PHE
1	B	682	PHE
1	C	682	PHE
1	D	682	PHE

### 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	657/725 (91%)	654 (100%)	3 (0%)	88	92
1	B	653/725 (90%)	649 (99%)	4 (1%)	86	90
1	C	649/725 (90%)	645 (99%)	4 (1%)	86	90
1	D	639/725 (88%)	634 (99%)	5 (1%)	81	86
All	All	2598/2900 (90%)	2582 (99%)	16 (1%)	86	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	930	LEU
1	A	953	PHE
1	A	979	ASP
1	B	394	ASN

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Mol	Chain	Res	Type
1	B	950	LEU
1	B	953	PHE
1	B	976	GLN
1	C	384	MET
1	C	953	PHE
1	C	976	GLN
1	C	979	ASP
1	D	787	LYS
1	D	950	LEU
1	D	953	PHE
1	D	976	GLN
1	D	979	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1020	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 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	A	2001	3	22,27,27	1.93	4 (18%)	29,40,40	1.86	8 (27%)
2	TPP	C	2001	3	22,27,27	2.12	4 (18%)	29,40,40	1.96	8 (27%)
5	MPD	C	2228	-	7,7,7	0.70	0	9,10,10	0.35	0
2	TPP	D	2001	3	22,27,27	2.10	5 (22%)	29,40,40	1.90	11 (37%)
5	MPD	B	2228	-	7,7,7	0.69	0	9,10,10	0.45	0
5	MPD	A	2228	-	7,7,7	0.73	0	9,10,10	0.45	0
5	MPD	D	2228	-	7,7,7	0.66	0	9,10,10	0.47	0
2	TPP	B	2001	3	22,27,27	2.00	4 (18%)	29,40,40	1.90	10 (34%)

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	A	2001	3	-	1/16/17/17	0/2/2/2
2	TPP	C	2001	3	-	2/16/17/17	0/2/2/2
5	MPD	C	2228	-	-	0/5/5/5	-
2	TPP	D	2001	3	-	2/16/17/17	0/2/2/2
5	MPD	B	2228	-	-	0/5/5/5	-
5	MPD	A	2228	-	-	0/5/5/5	-
5	MPD	D	2228	-	-	0/5/5/5	-
2	TPP	B	2001	3	-	0/16/17/17	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	TPP	C4-N3	-7.57	1.33	1.39
2	B	2001	TPP	C4-N3	-6.91	1.33	1.39
2	C	2001	TPP	C4-N3	-6.34	1.34	1.39
2	A	2001	TPP	C4-N3	-6.07	1.34	1.39
2	C	2001	TPP	C6-C5	5.26	1.53	1.50
2	A	2001	TPP	C6-C5	4.03	1.52	1.50
2	B	2001	TPP	PB-O1B	3.17	1.60	1.50
2	C	2001	TPP	C2-N3	-3.07	1.29	1.36
2	B	2001	TPP	C6-C5	3.00	1.52	1.50
2	A	2001	TPP	C2-N3	-2.80	1.30	1.36
2	A	2001	TPP	PB-O1B	2.79	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	TPP	C6-C5	2.76	1.52	1.50
2	D	2001	TPP	C2-N3	-2.73	1.30	1.36
2	D	2001	TPP	PB-O1B	2.63	1.59	1.50
2	C	2001	TPP	PB-O1B	2.61	1.59	1.50
2	B	2001	TPP	C2-N3	-2.34	1.31	1.36
2	D	2001	TPP	C4'-N4'	2.14	1.39	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	TPP	CM4-C4-C5	-4.70	117.33	127.60
2	A	2001	TPP	CM4-C4-C5	-4.40	117.97	127.60
2	C	2001	TPP	C5-C4-N3	4.14	115.85	107.57
2	B	2001	TPP	CM4-C4-C5	-4.07	118.71	127.60
2	B	2001	TPP	C5-C4-N3	4.03	115.64	107.57
2	A	2001	TPP	C5-C4-N3	3.96	115.49	107.57
2	D	2001	TPP	C5-C4-N3	3.88	115.33	107.57
2	D	2001	TPP	CM4-C4-C5	-3.86	119.16	127.60
2	D	2001	TPP	C6'-N1'-C2'	3.81	122.45	115.96
2	C	2001	TPP	C7'-N3-C2	-3.62	118.81	125.35
2	B	2001	TPP	C6-C5-C4	3.55	130.28	127.43
2	C	2001	TPP	C6-C5-C4	3.29	130.07	127.43
2	B	2001	TPP	C6'-N1'-C2'	3.28	121.55	115.96
2	C	2001	TPP	C6'-N1'-C2'	3.22	121.45	115.96
2	C	2001	TPP	CM4-C4-N3	3.20	126.61	122.53
2	A	2001	TPP	C6'-N1'-C2'	3.16	121.34	115.96
2	D	2001	TPP	N1'-C2'-N3'	-3.15	120.11	125.54
2	B	2001	TPP	C7'-N3-C2	-3.04	119.85	125.35
2	A	2001	TPP	C7'-N3-C2	-3.01	119.91	125.35
2	A	2001	TPP	CM4-C4-N3	3.01	126.37	122.53
2	B	2001	TPP	N1'-C2'-N3'	-2.91	120.54	125.54
2	A	2001	TPP	N1'-C2'-N3'	-2.89	120.56	125.54
2	D	2001	TPP	C7'-N3-C2	-2.85	120.20	125.35
2	A	2001	TPP	C6-C5-C4	2.79	129.68	127.43
2	C	2001	TPP	N1'-C2'-N3'	-2.73	120.84	125.54
2	D	2001	TPP	C5'-C6'-N1'	-2.69	119.34	123.82
2	D	2001	TPP	C6-C5-C4	2.63	129.54	127.43
2	B	2001	TPP	C5'-C6'-N1'	-2.43	119.78	123.82
2	B	2001	TPP	C2'-N3'-C4'	2.29	121.66	118.08
2	D	2001	TPP	C2'-N3'-C4'	2.27	121.62	118.08
2	A	2001	TPP	CM2-C2'-N1'	2.27	119.63	117.14
2	B	2001	TPP	CM4-C4-N3	2.22	125.36	122.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	TPP	CM2-C2'-N1'	2.19	119.55	117.14
2	D	2001	TPP	CM4-C4-N3	2.18	125.31	122.53
2	D	2001	TPP	CM2-C2'-N1'	2.13	119.47	117.14
2	D	2001	TPP	CM2-C2'-N3'	2.06	120.37	117.15
2	C	2001	TPP	C5'-C6'-N1'	-2.05	120.41	123.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2001	TPP	PA-O3A-PB-O3B
2	D	2001	TPP	PA-O3A-PB-O3B
2	A	2001	TPP	C7-O7-PA-O1A
2	C	2001	TPP	C7-O7-PA-O1A
2	D	2001	TPP	C7-O7-PA-O1A

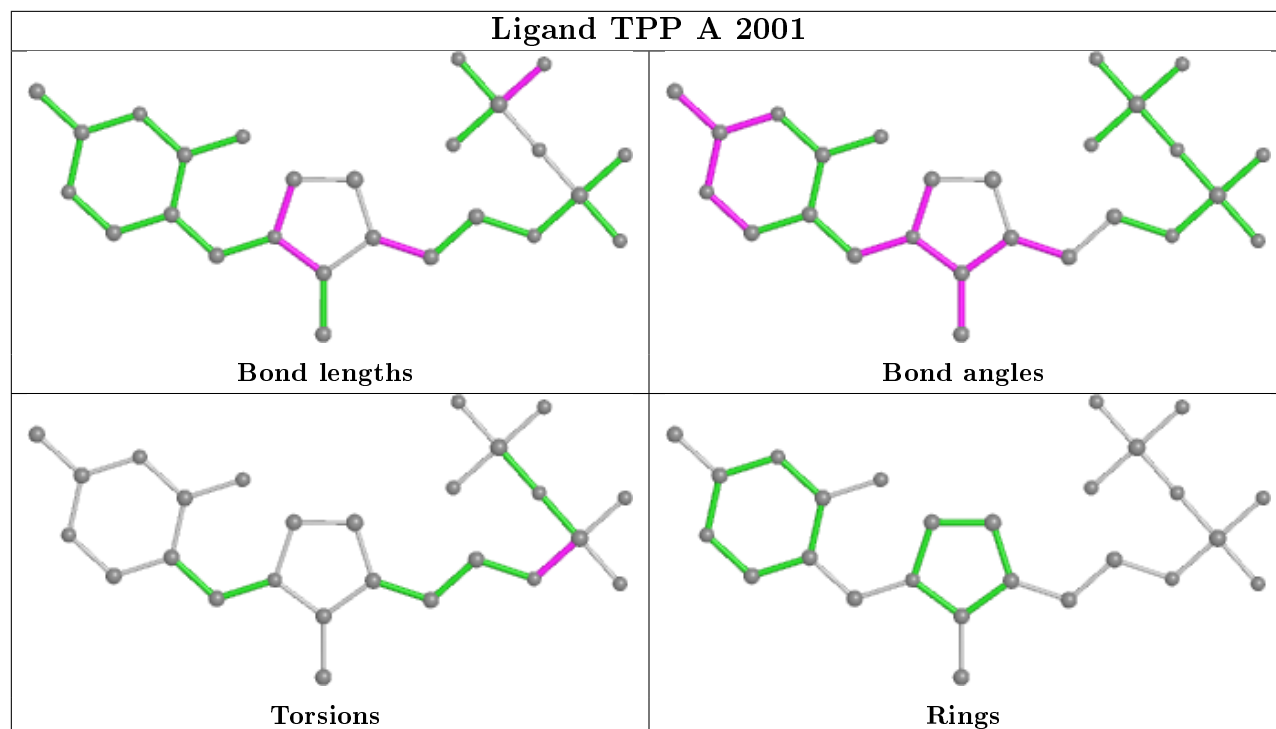
There are no ring outliers.

4 monomers are involved in 5 short contacts:

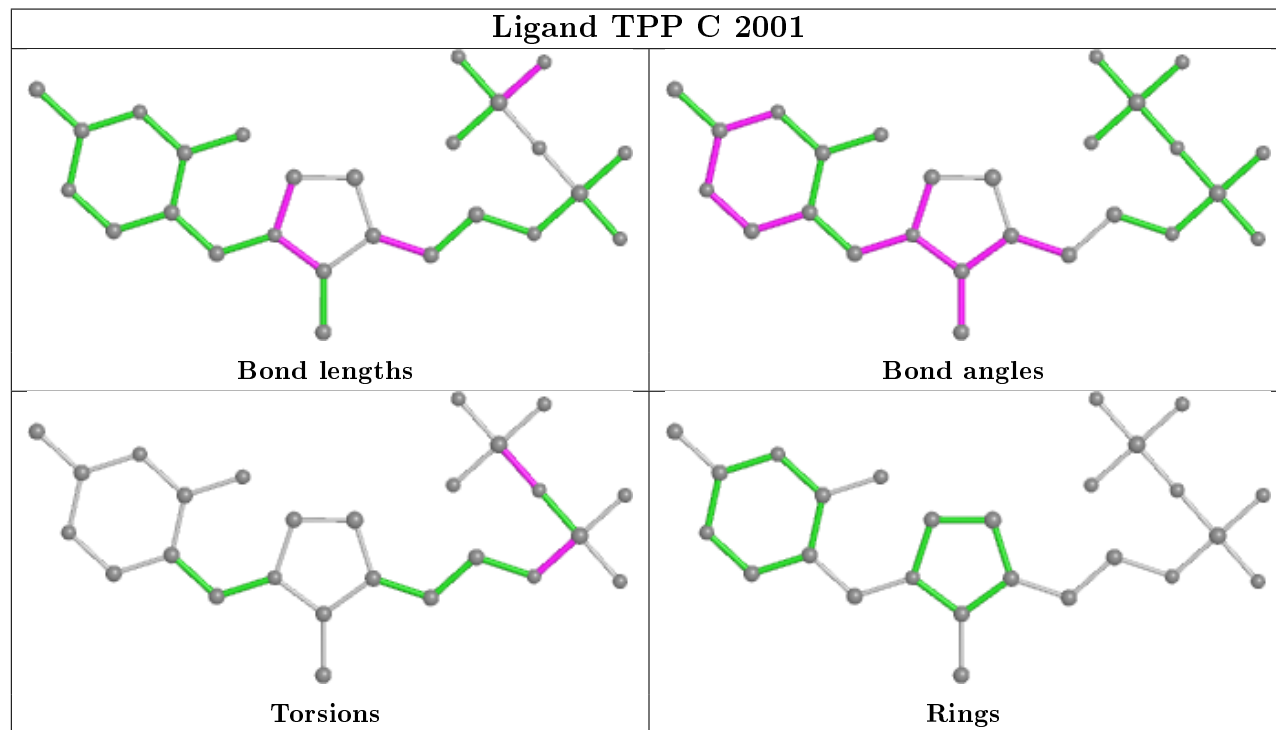
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	TPP	2	0
2	C	2001	TPP	1	0
2	D	2001	TPP	1	0
2	B	2001	TPP	1	0

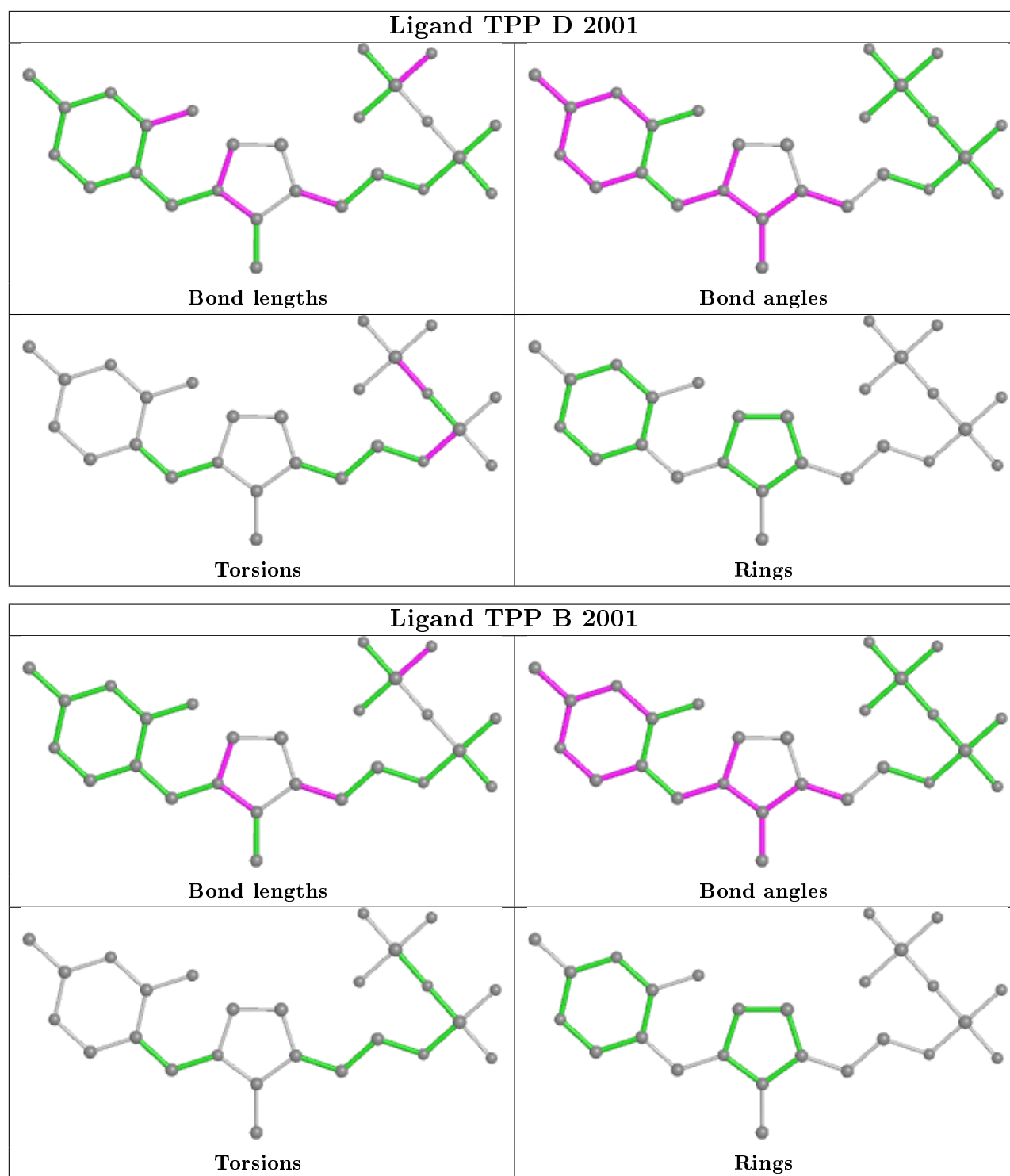
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand TPP A 2001



## Ligand TPP C 2001





## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	822/868 (94%)	0.11	40 (4%)	29	35	20, 35, 68, 99	0
1	B	823/868 (94%)	0.17	45 (5%)	25	31	20, 35, 73, 121	0
1	C	813/868 (93%)	0.10	42 (5%)	27	32	20, 33, 68, 108	0
1	D	823/868 (94%)	0.18	56 (6%)	17	21	20, 35, 74, 104	0
All	All	3281/3472 (94%)	0.14	183 (5%)	24	29	20, 35, 71, 121	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	574	GLY	15.9
1	D	413	TRP	7.8
1	B	419	PHE	7.1
1	D	807	VAL	6.2
1	D	472	ASP	5.7
1	C	785	SER	5.6
1	D	810	LEU	5.6
1	A	415	LEU	5.5
1	C	779	ILE	5.2
1	B	813	HIS	5.2
1	D	471	HIS	5.1
1	B	413	TRP	5.1
1	D	419	PHE	5.1
1	A	413	TRP	5.0
1	C	573	SER	5.0
1	A	810	LEU	4.9
1	B	420	LYS	4.9
1	A	633	ASN	4.8
1	B	574	GLY	4.8
1	B	807	VAL	4.4
1	C	420	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	630	GLY	4.3
1	B	368	ALA	4.2
1	A	368	ALA	4.1
1	D	368	ALA	4.1
1	D	634	ARG	4.1
1	D	473	LYS	4.1
1	D	626	THR	4.1
1	B	367	ASN	4.0
1	D	632	ASP	3.9
1	A	561	PHE	3.9
1	B	791	ASP	3.8
1	D	394	ASN	3.8
1	C	786	MET	3.8
1	C	471	HIS	3.8
1	D	429	ARG	3.8
1	A	631	SER	3.8
1	C	810	LEU	3.7
1	C	590	PHE	3.7
1	B	785	SER	3.6
1	B	397	PHE	3.6
1	D	414	ASP	3.5
1	A	371	ILE	3.5
1	B	429	ARG	3.4
1	B	779	ILE	3.4
1	B	808	ARG	3.4
1	C	574	GLY	3.4
1	B	430	LYS	3.4
1	B	810	LEU	3.4
1	B	786	MET	3.4
1	D	1103	GLU	3.4
1	B	371	ILE	3.3
1	D	631	SER	3.3
1	D	590	PHE	3.3
1	B	805	ASN	3.2
1	C	784	ILE	3.2
1	C	653	VAL	3.2
1	D	953	PHE	3.2
1	D	364	GLU	3.1
1	A	812	LYS	3.1
1	C	561	PHE	3.1
1	A	394	ASN	3.1
1	B	792	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	804	PHE	3.1
1	C	476	VAL	3.1
1	A	412	LEU	3.1
1	A	807	VAL	3.1
1	D	785	SER	3.1
1	C	419	PHE	3.1
1	C	953	PHE	3.1
1	A	471	HIS	3.0
1	A	440	ARG	3.0
1	A	419	PHE	3.0
1	B	804	PHE	3.0
1	C	807	VAL	3.0
1	B	472	ASP	2.9
1	A	953	PHE	2.9
1	A	429	ARG	2.9
1	B	418	GLU	2.9
1	A	435	ILE	2.9
1	D	805	ASN	2.9
1	D	981	VAL	2.9
1	D	808	ARG	2.8
1	D	798	GLY	2.8
1	B	394	ASN	2.8
1	A	626	THR	2.8
1	C	986	SER	2.8
1	C	394	ASN	2.8
1	C	805	ASN	2.8
1	D	811	GLU	2.7
1	A	632	ASP	2.7
1	A	981	VAL	2.7
1	B	812	LYS	2.7
1	D	987	ILE	2.7
1	B	798	GLY	2.7
1	C	984	ALA	2.7
1	A	366	LYS	2.7
1	D	793	LEU	2.7
1	D	786	MET	2.7
1	B	795	ASP	2.6
1	D	794	ARG	2.6
1	A	1007	LEU	2.6
1	A	934	PRO	2.6
1	D	633	ASN	2.6
1	B	1103	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	791	ASP	2.6
1	C	790	GLU	2.6
1	B	648	PHE	2.6
1	B	953	PHE	2.5
1	B	653	VAL	2.5
1	A	370	VAL	2.5
1	C	808	ARG	2.5
1	B	559	SER	2.5
1	B	954	ALA	2.5
1	C	792	ALA	2.5
1	C	804	PHE	2.5
1	D	938	PRO	2.4
1	A	573	SER	2.4
1	B	789	ALA	2.4
1	D	654	VAL	2.4
1	C	789	ALA	2.4
1	B	647	ALA	2.4
1	C	633	ASN	2.4
1	D	984	ALA	2.4
1	A	937	THR	2.4
1	D	780	GLY	2.4
1	D	574	GLY	2.4
1	D	814	GLU	2.3
1	C	609	VAL	2.3
1	B	555	SER	2.3
1	A	935	ASP	2.3
1	D	367	ASN	2.3
1	A	373	LEU	2.3
1	D	652	GLY	2.3
1	A	813	HIS	2.3
1	A	630	GLY	2.3
1	B	1216	VAL	2.3
1	D	395	THR	2.3
1	D	363	ILE	2.3
1	B	432	LEU	2.3
1	B	803	VAL	2.3
1	B	814	GLU	2.3
1	C	702	ILE	2.3
1	C	988	ILE	2.3
1	A	432	LEU	2.2
1	A	814	GLU	2.2
1	B	556	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	366	LYS	2.2
1	D	470	LYS	2.2
1	D	432	LEU	2.2
1	D	777	ALA	2.2
1	D	797	GLN	2.2
1	C	368	ALA	2.2
1	C	813	HIS	2.2
1	D	782	GLY	2.2
1	A	634	ARG	2.2
1	C	775	THR	2.2
1	A	470	LYS	2.2
1	A	653	VAL	2.1
1	D	813	HIS	2.1
1	C	812	LYS	2.1
1	D	365	ASP	2.1
1	D	784	ILE	2.1
1	D	653	VAL	2.1
1	B	984	ALA	2.1
1	C	794	ARG	2.1
1	D	861	ARG	2.1
1	A	1227	GLY	2.1
1	B	777	ALA	2.1
1	C	370	VAL	2.1
1	C	983	GLY	2.1
1	B	658	LEU	2.1
1	D	792	ALA	2.1
1	A	629	GLU	2.0
1	D	573	SER	2.0
1	C	472	ASP	2.0
1	A	983	GLY	2.0
1	D	776	GLU	2.0
1	B	471	HIS	2.0
1	C	646	ALA	2.0
1	C	981	VAL	2.0
1	C	384	MET	2.0
1	C	793	LEU	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

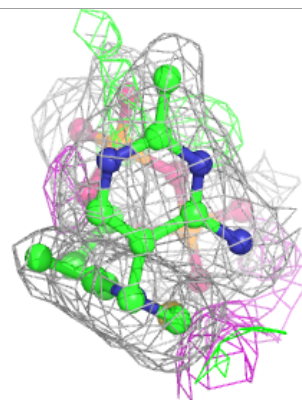
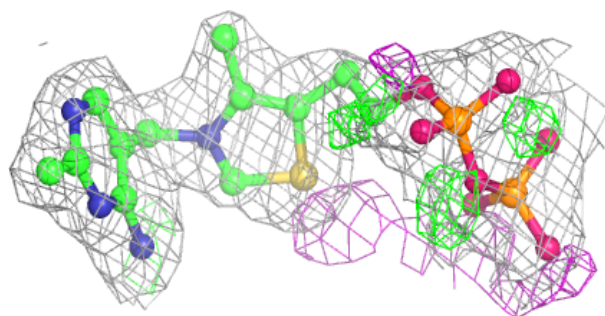
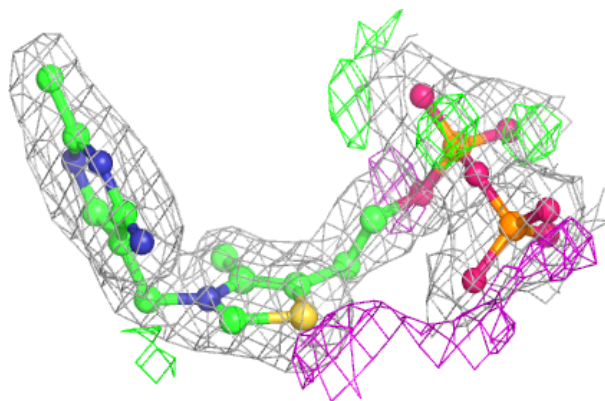
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MPD	B	2228	8/8	0.88	0.15	47,49,50,50	0
5	MPD	D	2228	8/8	0.91	0.18	48,51,52,53	0
5	MPD	C	2228	8/8	0.91	0.16	64,64,65,66	0
5	MPD	A	2228	8/8	0.91	0.17	68,69,71,71	0
2	TPP	B	2001	26/26	0.97	0.14	16,24,28,31	0
2	TPP	A	2001	26/26	0.98	0.11	19,22,26,27	0
2	TPP	D	2001	26/26	0.98	0.14	14,21,25,28	0
2	TPP	C	2001	26/26	0.98	0.13	17,23,25,26	0
3	MG	A	2002	1/1	0.98	0.14	12,12,12,12	0
3	MG	D	2002	1/1	0.99	0.16	16,16,16,16	0
4	CA	D	2003	1/1	0.99	0.05	30,30,30,30	0
3	MG	B	2002	1/1	0.99	0.14	16,16,16,16	0
4	CA	A	2003	1/1	0.99	0.04	29,29,29,29	0
4	CA	C	2003	1/1	0.99	0.04	29,29,29,29	0
4	CA	B	2003	1/1	0.99	0.05	32,32,32,32	0
3	MG	C	2002	1/1	0.99	0.16	11,11,11,11	0

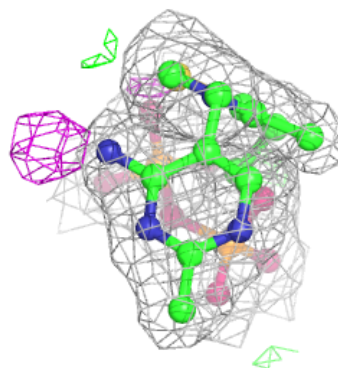
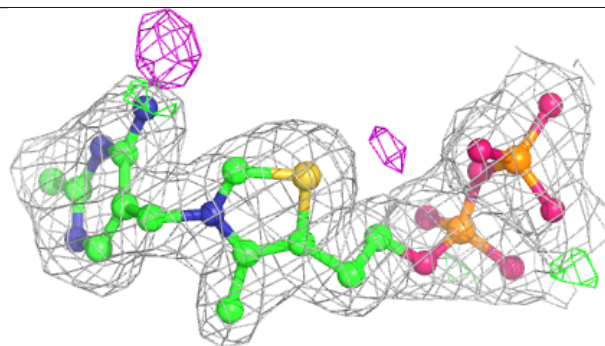
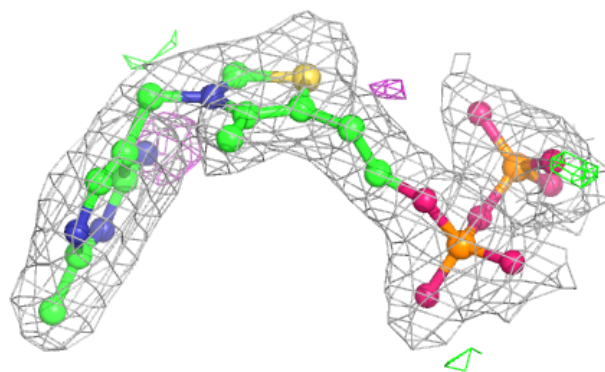
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPP B 2001:**

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

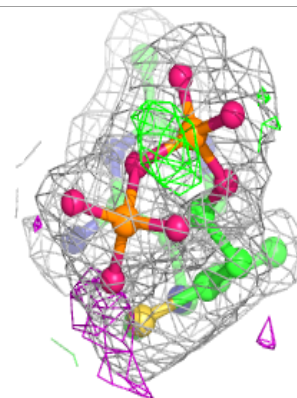
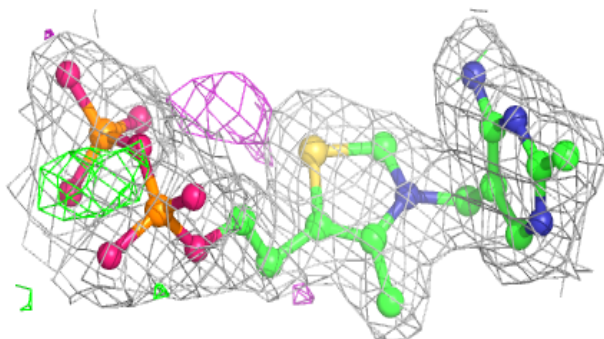
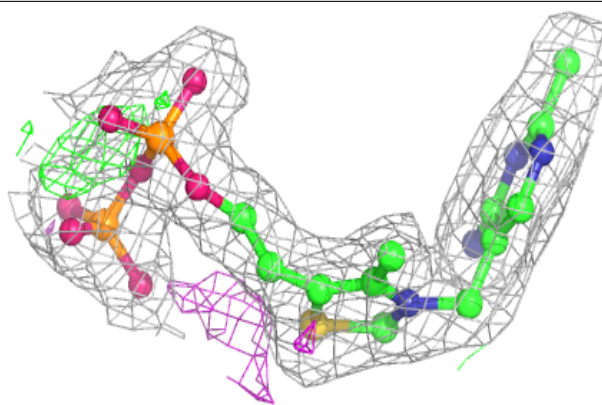
**Electron density around TPP A 2001:**

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

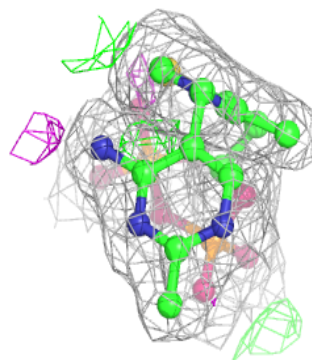
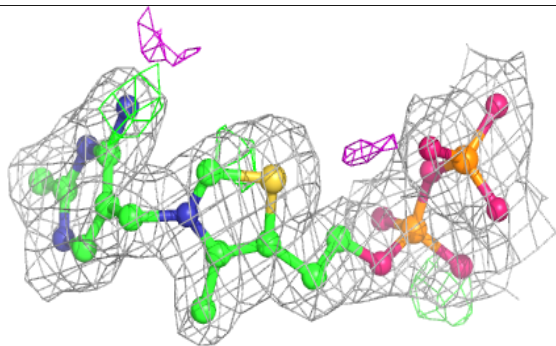
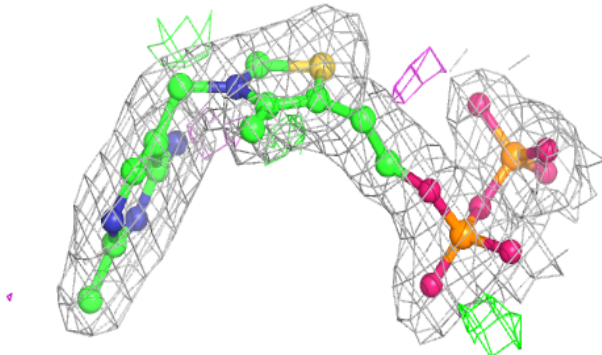


**Electron density around TPP D 2001:**

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

**Electron density around TPP C 2001:**

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



## 6.5 Other polymers

There are no such residues in this entry.