



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:25 AM BST

PDB ID : 6U3J  
Title : Structure of the 2-oxoadipate dehydrogenase DHTKD1  
Authors : Khamrui, S.; Lazarus, M.B.  
Deposited on : 2019-08-21  
Resolution : 2.25 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 : 2.14.6  
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) : 2.14.6

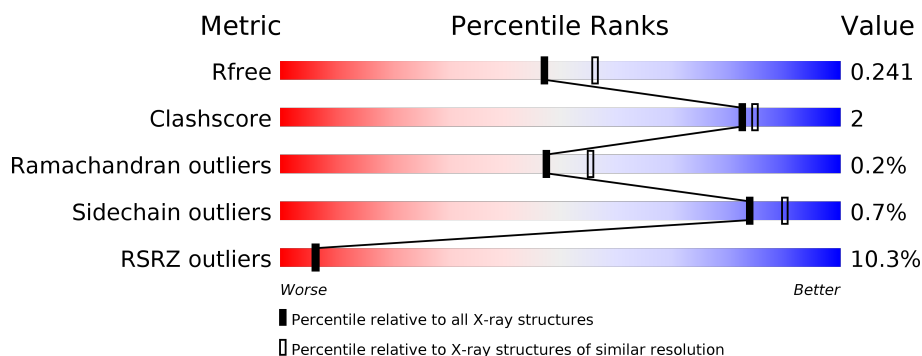
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	904	<div> <div>10%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div> </div>
1	B	904	<div> <div>10%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div></div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14773 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

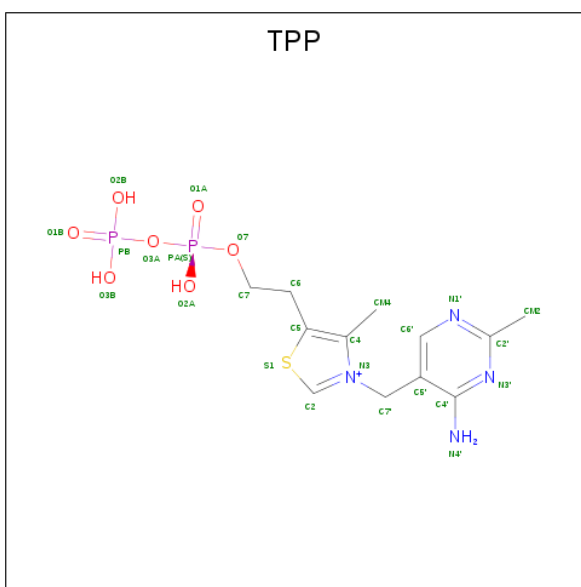
- Molecule 1 is a protein called 2-oxoglutarate dehydrogenase E1 component DHKTD1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	876	Total	C	N	O	S	0	1	0
			6878	4381	1196	1261	40			
1	B	876	Total	C	N	O	S	0	1	0
			6878	4381	1196	1261	40			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP Q96HY7
A	24	GLY	-	expression tag	UNP Q96HY7
A	920	HIS	-	expression tag	UNP Q96HY7
A	921	HIS	-	expression tag	UNP Q96HY7
A	922	HIS	-	expression tag	UNP Q96HY7
A	923	HIS	-	expression tag	UNP Q96HY7
A	924	HIS	-	expression tag	UNP Q96HY7
A	925	HIS	-	expression tag	UNP Q96HY7
A	926	HIS	-	expression tag	UNP Q96HY7
B	23	MET	-	initiating methionine	UNP Q96HY7
B	24	GLY	-	expression tag	UNP Q96HY7
B	920	HIS	-	expression tag	UNP Q96HY7
B	921	HIS	-	expression tag	UNP Q96HY7
B	922	HIS	-	expression tag	UNP Q96HY7
B	923	HIS	-	expression tag	UNP Q96HY7
B	924	HIS	-	expression tag	UNP Q96HY7
B	925	HIS	-	expression tag	UNP Q96HY7
B	926	HIS	-	expression tag	UNP Q96HY7

- 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) (labeled as "Ligand of Interest" by author).



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

- 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	2	Total	Mg	0	0
			2	2		

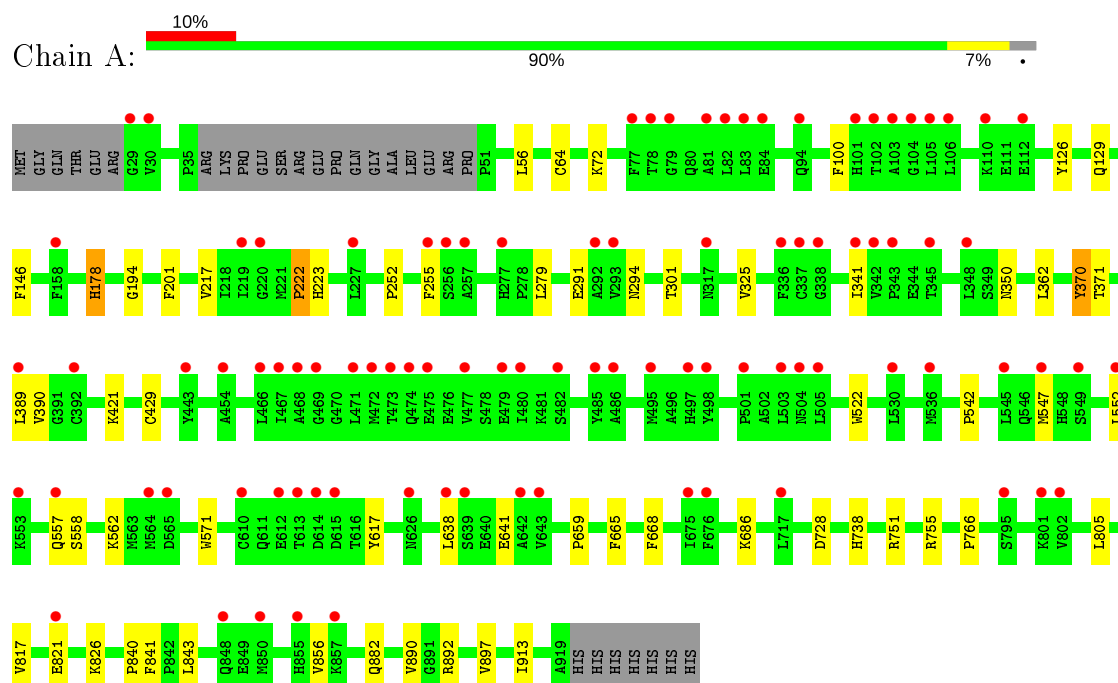
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	472	Total	O	0	0
			472	472		
4	B	490	Total	O	0	0
			490	490		

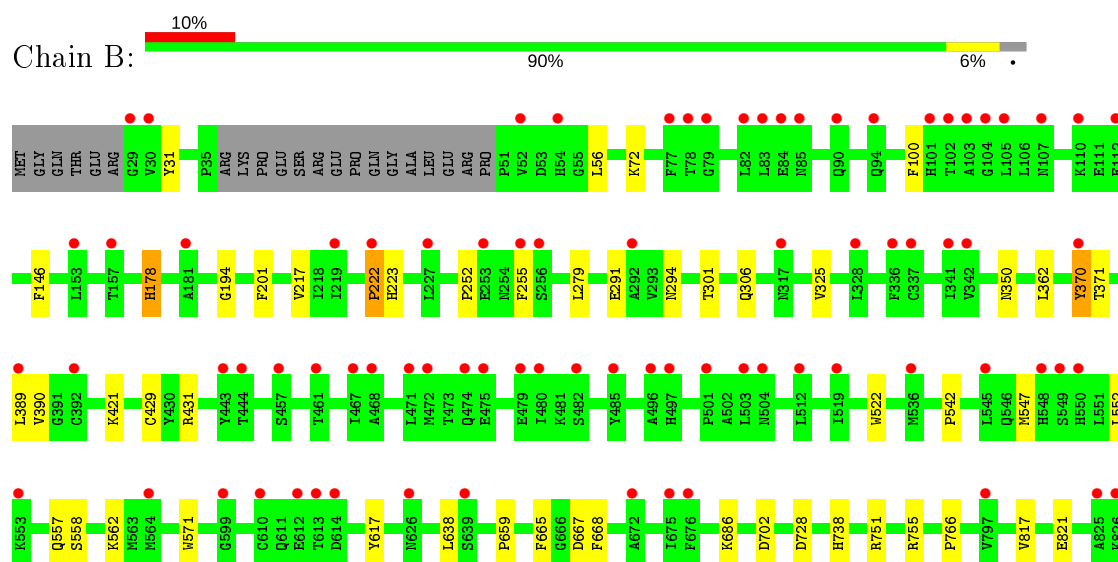
### 3 Residue-property plots

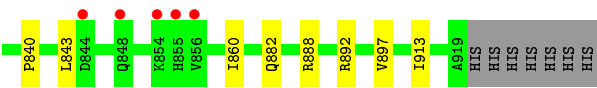
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 2-oxoglutarate dehydrogenase E1 component DHKTD1, mitochondrial



- Molecule 1: 2-oxoglutarate dehydrogenase E1 component DHKTD1, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	332.31Å 72.61Å 79.67Å 90.00° 91.87° 90.00°	Depositor
Resolution (Å)	49.01 – 2.25 49.01 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.01-2.25) 100.0 (49.01-2.25)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.209 , 0.241 0.209 , 0.241	Depositor DCC
$R_{free}$ test set	4591 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, 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	0.24	0/7029	0.41	0/9525
1	B	0.24	0/7029	0.41	0/9525
All	All	0.24	0/14058	0.41	0/19050

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

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	6878	0	6756	33	0
1	B	6878	0	6756	32	0
2	A	26	0	16	2	0
2	B	26	0	16	2	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	472	0	0	2	0
4	B	490	0	0	2	0
All	All	14773	0	13544	67	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 (67) 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:291:GLU:OE1	1:B:294:ASN:ND2	2.22	0.72
1:A:291:GLU:OE1	1:A:294:ASN:ND2	2.22	0.71
1:A:389:LEU:HD12	1:A:390:VAL:HG13	1.75	0.68
1:B:389:LEU:HD12	1:B:390:VAL:HG13	1.75	0.66
1:A:129:GLN:NE2	4:A:1111:HOH:O	2.37	0.57
1:A:350:ASN:HD21	1:A:421:LYS:HE3	1.72	0.54
1:B:350:ASN:HD21	1:B:421:LYS:HE3	1.72	0.54
1:B:178:HIS:C	1:B:178:HIS:HD1	2.12	0.53
1:B:431:ARG:NH1	4:B:1117:HOH:O	2.39	0.51
1:B:552:LEU:O	1:B:557:GLN:HG2	2.11	0.51
1:A:552:LEU:O	1:A:557:GLN:HG2	2.11	0.50
1:A:558:SER:O	1:A:562:LYS:HG2	2.11	0.50
1:B:558:SER:O	1:B:562:LYS:HG2	2.11	0.50
1:B:547:MET:HG2	1:B:552:LEU:HG	1.94	0.49
1:A:817:VAL:O	1:A:821:GLU:HG2	2.12	0.49
1:B:571:TRP:CE2	1:B:766:PRO:HG3	2.48	0.49
1:A:547:MET:HG2	1:A:552:LEU:HG	1.94	0.49
1:B:817:VAL:O	1:B:821:GLU:HG2	2.12	0.49
1:A:571:TRP:CE2	1:A:766:PRO:HG3	2.48	0.49
1:B:702:ASP:OD2	4:B:1101:HOH:O	2.19	0.48
1:A:686:LYS:HG3	1:B:897:VAL:HG11	1.97	0.46
1:A:751:ARG:O	1:A:755:ARG:HG3	2.16	0.46
1:B:751:ARG:O	1:B:755:ARG:HG3	2.16	0.46
1:B:892:ARG:HG3	1:B:913:ILE:HD11	1.98	0.45
1:B:843:LEU:HD13	1:B:882:GLN:HB3	1.98	0.45
2:A:1001:TPP:HN42	2:A:1001:TPP:H2	1.81	0.45
1:A:194:GLY:O	1:A:429:CYS:HB2	2.17	0.45
1:A:665:PHE:HB2	1:A:668:PHE:CE2	2.52	0.45
1:B:665:PHE:HB2	1:B:668:PHE:CE2	2.52	0.45
1:A:843:LEU:HD13	1:A:882:GLN:HB3	1.98	0.44
1:B:194:GLY:O	1:B:429:CYS:HB2	2.17	0.44
1:A:897:VAL:HG11	1:B:686:LYS:HG3	1.98	0.44
2:B:1001:TPP:H2	2:B:1001:TPP:HN42	1.81	0.44
2:B:1001:TPP:HN42	2:B:1001:TPP:C2	2.31	0.44
1:A:892:ARG:HG3	1:A:913:ILE:HD11	1.99	0.44
2:A:1001:TPP:C2	2:A:1001:TPP:HN42	2.31	0.44
1:A:728:ASP:HB3	1:A:840:PRO:HB3	2.00	0.43
1:A:64[B]:CYS:HG	1:A:126:TYR:HH	1.65	0.43
1:A:522:TRP:CE2	1:A:755:ARG:HG2	2.54	0.43
1:B:522:TRP:CE2	1:B:755:ARG:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:TYR:HB3	1:B:371:THR:H	1.68	0.43
1:B:728:ASP:HB3	1:B:840:PRO:HB3	2.00	0.43
1:B:178:HIS:C	1:B:178:HIS:ND1	2.71	0.42
1:B:56:LEU:HD22	1:B:100:PHE:HB3	2.01	0.42
1:B:217:VAL:HG23	1:B:279:LEU:HD11	2.02	0.42
1:A:542:PRO:HD3	1:A:617:TYR:CE2	2.54	0.42
1:B:542:PRO:HD3	1:B:617:TYR:CE2	2.55	0.42
1:B:252:PRO:HD2	1:B:255:PHE:CD2	2.56	0.41
1:B:201:PHE:CD2	1:B:362:LEU:HD22	2.55	0.41
1:A:217:VAL:HG23	1:A:279:LEU:HD11	2.02	0.41
1:A:341:ILE:HD12	1:A:641:GLU:HG2	2.02	0.41
1:A:841:PHE:O	4:A:1101:HOH:O	2.21	0.41
1:B:222:PRO:HB2	1:B:223:HIS:H	1.69	0.41
1:A:201:PHE:CD2	1:A:362:LEU:HD22	2.55	0.41
1:A:890:VAL:HG12	1:A:913:ILE:HG23	2.03	0.41
1:A:826:LYS:HE2	1:A:826:LYS:HB3	1.87	0.41
1:B:301:THR:HG23	1:B:325:VAL:HG12	2.03	0.41
1:A:222:PRO:HB2	1:A:223:HIS:H	1.69	0.40
1:A:301:THR:HG23	1:A:325:VAL:HG12	2.03	0.40
1:A:252:PRO:HD2	1:A:255:PHE:CD2	2.56	0.40
1:A:370:TYR:HB3	1:A:371:THR:H	1.69	0.40
1:A:56:LEU:HD22	1:A:100:PHE:HB3	2.01	0.40
1:A:805:LEU:HG	1:A:856:VAL:HG11	2.02	0.40
1:B:522:TRP:CD1	1:B:755:ARG:HG2	2.57	0.40
1:A:178:HIS:C	1:A:178:HIS:HD1	2.25	0.40
1:B:31:TYR:OH	1:B:306:GLN:NE2	2.49	0.40
1:B:860:ILE:HD11	1:B:888:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	871/904 (96%)	847 (97%)	22 (2%)	2 (0%)	47	55
1	B	871/904 (96%)	845 (97%)	24 (3%)	2 (0%)	47	55
All	All	1742/1808 (96%)	1692 (97%)	46 (3%)	4 (0%)	47	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	PRO
1	B	222	PRO
1	A	659	PRO
1	B	659	PRO

### 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	742/779 (95%)	737 (99%)	5 (1%)	84	90
1	B	742/779 (95%)	736 (99%)	6 (1%)	81	88
All	All	1484/1558 (95%)	1473 (99%)	11 (1%)	84	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	PHE
1	A	178	HIS
1	A	370	TYR
1	A	638	LEU
1	A	738	HIS
1	B	146	PHE
1	B	178	HIS
1	B	370	TYR
1	B	638	LEU
1	B	667	ASP
1	B	738	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	605	HIS
1	B	228	ASN
1	B	605	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	MLZ	B	72	1	8,9,10	1.02	1 (12%)	4,9,11	0.47	0
1	MLZ	A	537	1	8,9,10	0.89	0	4,9,11	0.37	0
1	MLZ	B	537	1	8,9,10	0.88	0	4,9,11	0.36	0
1	MLZ	A	72	1	8,9,10	1.01	1 (12%)	4,9,11	0.46	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
1	MLZ	B	72	1	-	2/7/8/10	-
1	MLZ	A	537	1	-	0/7/8/10	-
1	MLZ	B	537	1	-	0/7/8/10	-
1	MLZ	A	72	1	-	2/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	MLZ	CB-CA	2.24	1.56	1.53
1	A	72	MLZ	CB-CA	2.19	1.56	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	72	MLZ	CG-CD-CE-NZ
1	A	72	MLZ	CG-CD-CE-NZ
1	B	72	MLZ	CD-CE-NZ-CM
1	A	72	MLZ	CD-CE-NZ-CM

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	1001	3	22,27,27	1.59	5 (22%)	29,40,40	1.95	9 (31%)
2	TPP	B	1001	3	22,27,27	1.59	5 (22%)	29,40,40	1.94	9 (31%)

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	1001	3	-	3/16/17/17	0/2/2/2
2	TPP	B	1001	3	-	4/16/17/17	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	TPP	C4-N3	-4.47	1.35	1.39
2	A	1001	TPP	C4-N3	-4.47	1.35	1.39
2	A	1001	TPP	C2'-N1'	2.56	1.38	1.34
2	B	1001	TPP	C2'-N1'	2.56	1.38	1.34
2	A	1001	TPP	C2'-N3'	2.38	1.38	1.34
2	B	1001	TPP	C2'-N3'	2.38	1.38	1.34
2	A	1001	TPP	C4'-N3'	2.35	1.38	1.35
2	B	1001	TPP	C4'-N3'	2.31	1.38	1.35
2	A	1001	TPP	C7'-N3	-2.17	1.44	1.48
2	B	1001	TPP	C7'-N3	-2.14	1.44	1.48

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	TPP	C6-C5-C4	5.82	132.11	127.43
2	B	1001	TPP	C6-C5-C4	5.76	132.06	127.43
2	B	1001	TPP	N1'-C2'-N3'	-3.19	120.06	125.54
2	B	1001	TPP	PA-O3A-PB	-3.14	122.05	132.83
2	A	1001	TPP	N1'-C2'-N3'	-3.12	120.17	125.54
2	A	1001	TPP	PA-O3A-PB	-3.12	122.13	132.83
2	B	1001	TPP	CM2-C2'-N1'	2.86	120.29	117.14
2	A	1001	TPP	CM2-C2'-N1'	2.77	120.19	117.14
2	A	1001	TPP	C6'-C5'-C4'	2.73	119.44	115.72
2	B	1001	TPP	C6'-C5'-C4'	2.70	119.39	115.72
2	A	1001	TPP	CM4-C4-N3	2.65	125.90	122.53
2	B	1001	TPP	CM4-C4-N3	2.60	125.84	122.53
2	B	1001	TPP	C5'-C7'-N3	-2.43	109.23	113.28
2	A	1001	TPP	C5'-C7'-N3	-2.42	109.24	113.28
2	B	1001	TPP	C6'-N1'-C2'	2.42	120.08	115.96
2	A	1001	TPP	C6'-N1'-C2'	2.36	119.98	115.96
2	B	1001	TPP	C5'-C6'-N1'	-2.18	120.18	123.82
2	A	1001	TPP	C5'-C6'-N1'	-2.17	120.20	123.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

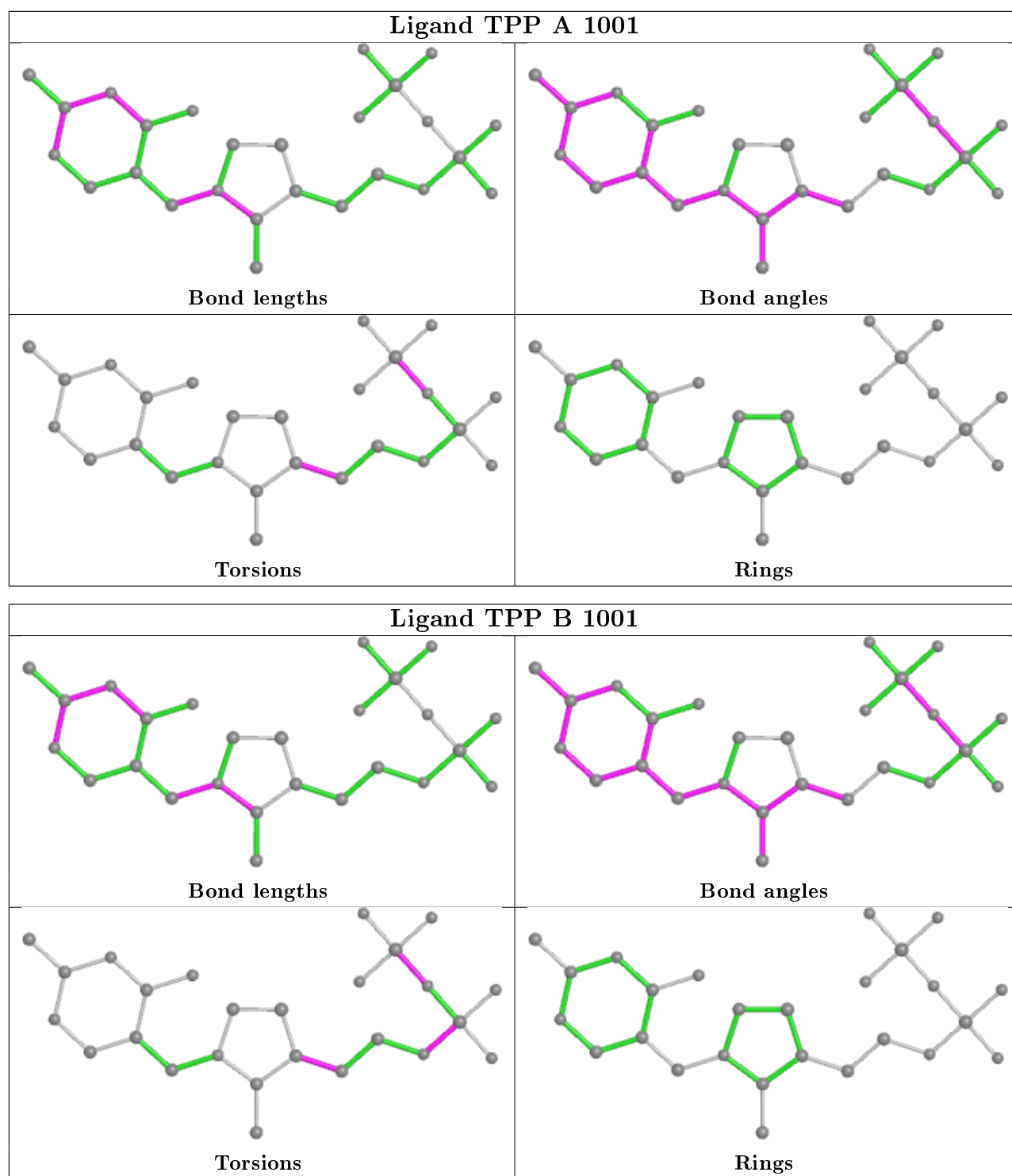
Mol	Chain	Res	Type	Atoms
2	A	1001	TPP	PA-O3A-PB-O2B
2	A	1001	TPP	PA-O3A-PB-O3B
2	B	1001	TPP	PA-O3A-PB-O3B
2	A	1001	TPP	C4-C5-C6-C7
2	B	1001	TPP	C4-C5-C6-C7
2	B	1001	TPP	PA-O3A-PB-O1B
2	B	1001	TPP	C7-O7-PA-O1A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	TPP	2	0
2	B	1001	TPP	2	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 ⓘ

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	874/904 (96%)	0.68	94 (10%) 5 5	17, 37, 77, 151	0
1	B	874/904 (96%)	0.67	86 (9%) 7 8	17, 37, 77, 137	0
All	All	1748/1808 (96%)	0.68	180 (10%) 6 6	17, 37, 77, 151	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	ALA	10.3
1	B	110	LYS	5.8
1	B	77	PHE	5.3
1	B	82	LEU	5.3
1	A	110	LYS	5.2
1	B	504	ASN	5.1
1	B	854	LYS	5.0
1	B	78	THR	4.8
1	A	84	GLU	4.8
1	A	83	LEU	4.8
1	A	103	ALA	4.7
1	A	104	GLY	4.7
1	B	468	ALA	4.5
1	B	613	THR	4.5
1	B	256	SER	4.5
1	A	443	TYR	4.4
1	A	504	ASN	4.4
1	A	82	LEU	4.3
1	A	468	ALA	4.3
1	A	564	MET	4.1
1	B	474	GLN	4.1
1	B	467	ILE	4.1
1	B	553	LYS	4.1
1	B	614	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	473	THR	4.0
1	B	104	GLY	4.0
1	A	855	HIS	4.0
1	A	341	ILE	3.9
1	A	78	THR	3.9
1	A	77	PHE	3.8
1	A	255	PHE	3.8
1	B	29	GLY	3.7
1	A	552	LEU	3.6
1	B	84	GLU	3.6
1	A	475	GLU	3.6
1	A	105	LEU	3.6
1	B	443	TYR	3.6
1	B	519	ILE	3.5
1	B	292	ALA	3.5
1	B	855	HIS	3.5
1	A	29	GLY	3.5
1	B	564	MET	3.4
1	A	675	ILE	3.4
1	A	549	SER	3.4
1	B	480	ILE	3.4
1	A	474	GLN	3.4
1	A	482	SER	3.4
1	A	857	LYS	3.4
1	B	253	GLU	3.3
1	A	638	LEU	3.3
1	A	613	THR	3.3
1	A	536	MET	3.3
1	A	547	MET	3.2
1	B	83	LEU	3.2
1	B	485	TYR	3.2
1	A	466	LEU	3.2
1	A	503	LEU	3.2
1	A	102	THR	3.2
1	B	610	CYS	3.1
1	A	471	LEU	3.1
1	B	341	ILE	3.1
1	A	30	VAL	3.1
1	B	255	PHE	3.1
1	A	342	VAL	3.0
1	B	79	GLY	3.0
1	A	610	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	102	THR	3.0
1	B	317	ASN	3.0
1	A	480	ILE	2.9
1	B	471	LEU	2.9
1	B	461	THR	2.9
1	B	90	GLN	2.9
1	A	565	ASP	2.9
1	A	802	VAL	2.9
1	A	389	LEU	2.9
1	B	475	GLU	2.8
1	B	389	LEU	2.8
1	A	472	MET	2.8
1	A	257	ALA	2.8
1	B	797	VAL	2.8
1	B	536	MET	2.7
1	A	256	SER	2.7
1	B	336	PHE	2.7
1	A	821	GLU	2.7
1	A	467	ILE	2.7
1	A	612	GLU	2.7
1	A	642	ALA	2.7
1	A	101	HIS	2.7
1	A	345	THR	2.7
1	A	486	ALA	2.7
1	B	496	ALA	2.7
1	A	477	VAL	2.7
1	A	79	GLY	2.7
1	B	370	TYR	2.6
1	B	503	LEU	2.6
1	B	848	GLN	2.6
1	A	501	PRO	2.6
1	B	105	LEU	2.6
1	A	292	ALA	2.6
1	A	337	CYS	2.5
1	A	293	VAL	2.5
1	B	337	CYS	2.5
1	B	548	HIS	2.5
1	A	219	ILE	2.5
1	A	220	GLY	2.5
1	B	497	HIS	2.5
1	B	612	GLU	2.5
1	B	825	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	501	PRO	2.5
1	A	795	SER	2.4
1	B	639	SER	2.4
1	B	675	ILE	2.4
1	B	626	ASN	2.4
1	B	112	GLU	2.4
1	A	626	ASN	2.4
1	A	158	PHE	2.4
1	A	106	LEU	2.4
1	A	227	LEU	2.4
1	A	343	PRO	2.4
1	A	336	PHE	2.4
1	A	553	LYS	2.4
1	A	498	TYR	2.3
1	A	505	LEU	2.3
1	A	717	LEU	2.3
1	B	549	SER	2.3
1	A	348	LEU	2.3
1	B	550	HIS	2.3
1	A	639	SER	2.3
1	B	457	SER	2.3
1	A	615	ASP	2.3
1	B	219	ILE	2.3
1	B	482	SER	2.3
1	A	485	TYR	2.3
1	B	599	GLY	2.3
1	A	479	GLU	2.3
1	A	643	VAL	2.2
1	B	52	VAL	2.2
1	A	469	GLY	2.2
1	B	444	THR	2.2
1	A	317	ASN	2.2
1	A	801	LYS	2.2
1	A	338	GLY	2.2
1	A	454	ALA	2.2
1	A	614	ASP	2.2
1	B	222	PRO	2.2
1	B	545	LEU	2.2
1	B	826	LYS	2.2
1	B	85	ASN	2.2
1	B	672	ALA	2.2
1	A	392	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	545	LEU	2.2
1	B	328	LEU	2.2
1	B	107	ASN	2.1
1	B	153	LEU	2.1
1	A	277	HIS	2.1
1	B	101	HIS	2.1
1	B	30	VAL	2.1
1	B	512	LEU	2.1
1	B	392	CYS	2.1
1	A	557	GLN	2.1
1	A	112	GLU	2.1
1	A	850	MET	2.1
1	B	676	PHE	2.1
1	B	54	HIS	2.1
1	B	479	GLU	2.1
1	A	497	HIS	2.1
1	A	530	LEU	2.1
1	A	848	GLN	2.1
1	B	227	LEU	2.1
1	B	157	THR	2.1
1	B	181	ALA	2.1
1	A	81	ALA	2.0
1	B	342	VAL	2.0
1	B	844	ASP	2.0
1	B	472	MET	2.0
1	A	94	GLN	2.0
1	B	856	VAL	2.0
1	A	676	PHE	2.0
1	A	495	MET	2.0
1	B	94	GLN	2.0

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

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
1	MLZ	A	537	10/11	0.81	0.17	33,39,47,48	0
1	MLZ	B	537	10/11	0.85	0.15	32,38,46,47	0
1	MLZ	B	72	10/11	0.87	0.17	24,42,57,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLZ	A	72	10/11	0.93	0.13	22,43,56,65	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

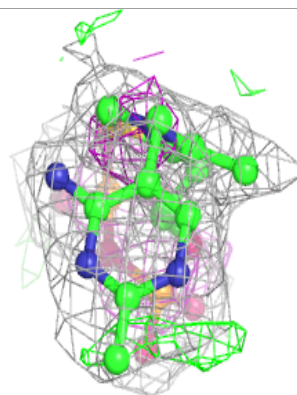
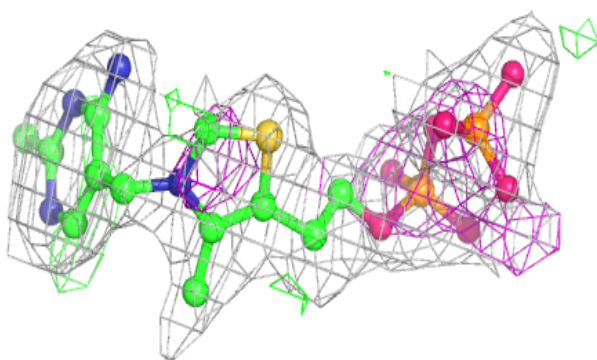
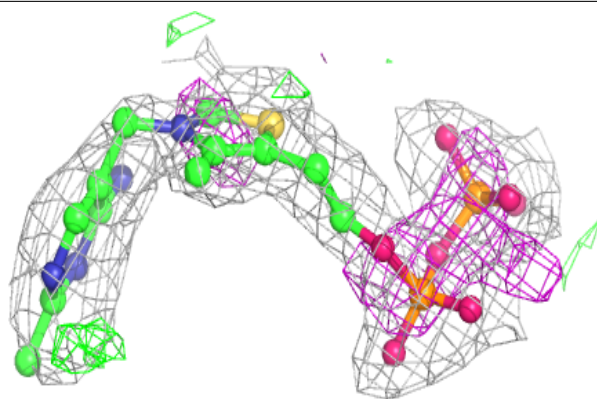
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	MG	B	1002	1/1	0.81	0.08	27,27,27,27	0
3	MG	A	1002	1/1	0.83	0.27	36,36,36,36	0
3	MG	A	1003	1/1	0.88	0.07	28,28,28,28	0
2	TPP	B	1001	26/26	0.89	0.19	18,36,50,60	0
2	TPP	A	1001	26/26	0.91	0.16	18,35,51,59	0

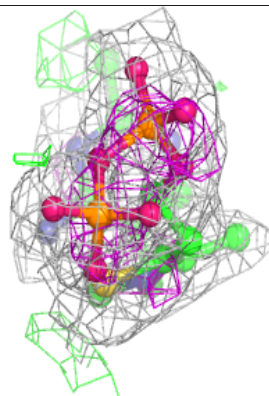
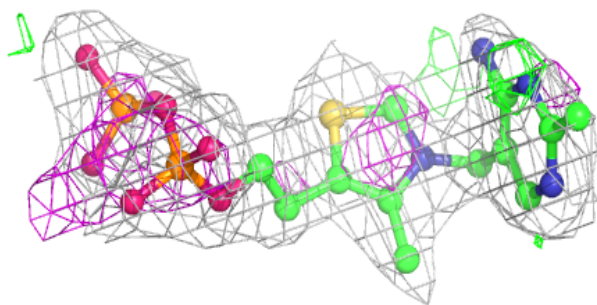
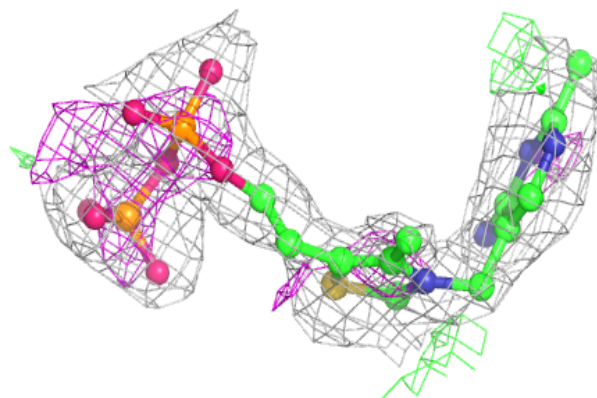
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPP B 1001:**

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

**Electron density around TPP A 1001:**

$2mF_o-DF_c$  (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.