Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2020 – 04:33 PM EST

PDB ID	:	5RVZ
Title	:	PanDDA analysis group deposition – Crystal Structure of DHTKD1 in complex with Z1929757385
Authors	:	Bezerra, G.A.; Foster, W.R.; Bailey, H.J.; Shrestha, L.; Krojer, T.; Brandao-Neto, J.; Douangamath, A.; Burgess-Brown, N.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Yue, W.W.
Deposited on	:	2020-10-27
Resolution	:	1.98 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

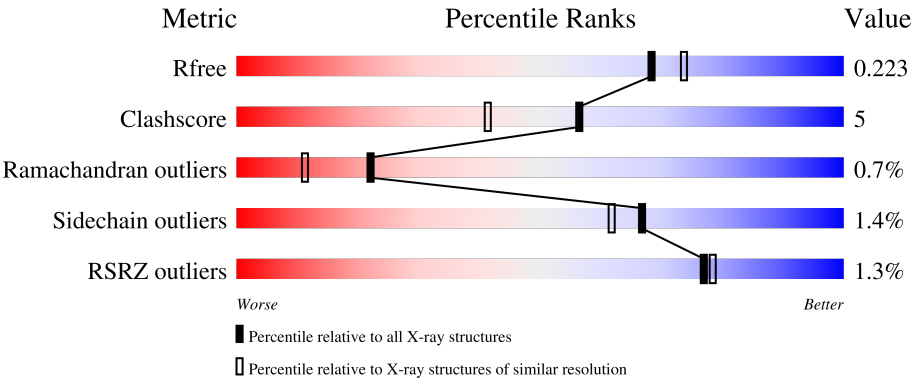
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

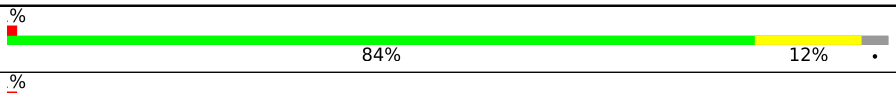
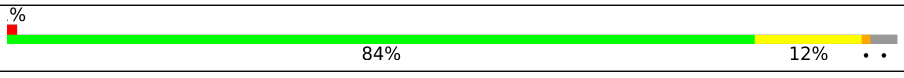
The reported resolution of this entry is 1.98 Å.

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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 >=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 <=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	898	
1	B	898	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15394 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 Probable 2-oxoglutarate dehydrogenase E1 component DHKTD1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	867	Total	C	N	O	S	0	5	0
			6775	4317	1169	1249	40			
1	B	867	Total	C	N	O	S	0	2	0
			6740	4296	1163	1243	38			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP Q96HY7
A	23	HIS	-	expression tag	UNP Q96HY7
A	24	HIS	-	expression tag	UNP Q96HY7
A	25	HIS	-	expression tag	UNP Q96HY7
A	26	HIS	-	expression tag	UNP Q96HY7
A	27	HIS	-	expression tag	UNP Q96HY7
A	28	HIS	-	expression tag	UNP Q96HY7
A	29	SER	-	expression tag	UNP Q96HY7
A	30	SER	-	expression tag	UNP Q96HY7
A	31	GLY	-	expression tag	UNP Q96HY7
A	32	VAL	-	expression tag	UNP Q96HY7
A	33	ASP	-	expression tag	UNP Q96HY7
A	34	LEU	-	expression tag	UNP Q96HY7
A	35	GLY	-	expression tag	UNP Q96HY7
A	36	THR	-	expression tag	UNP Q96HY7
A	37	GLU	-	expression tag	UNP Q96HY7
A	38	ASN	-	expression tag	UNP Q96HY7
A	39	LEU	-	expression tag	UNP Q96HY7
A	40	TYR	-	expression tag	UNP Q96HY7
A	41	PHE	-	expression tag	UNP Q96HY7
A	42	GLN	-	expression tag	UNP Q96HY7
A	43	SER	-	expression tag	UNP Q96HY7
A	44	MET	-	expression tag	UNP Q96HY7
B	22	MET	-	initiating methionine	UNP Q96HY7

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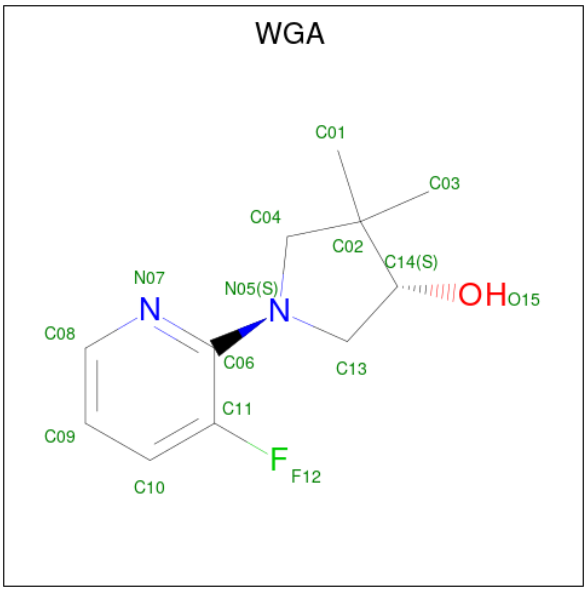
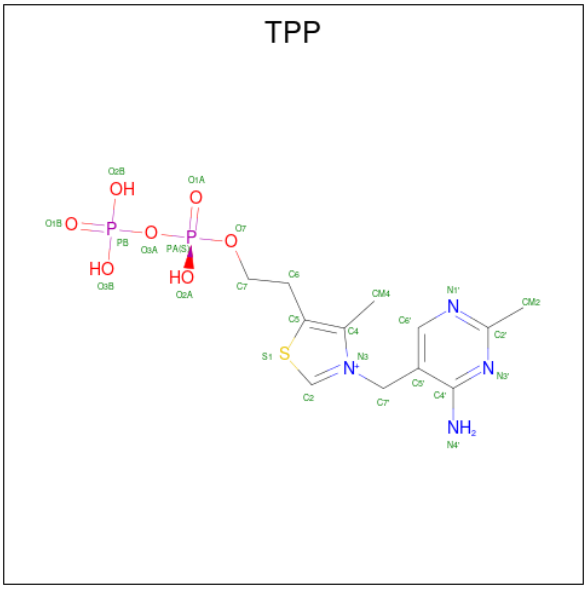
Chain	Residue	Modelled	Actual	Comment	Reference
B	23	HIS	-	expression tag	UNP Q96HY7
B	24	HIS	-	expression tag	UNP Q96HY7
B	25	HIS	-	expression tag	UNP Q96HY7
B	26	HIS	-	expression tag	UNP Q96HY7
B	27	HIS	-	expression tag	UNP Q96HY7
B	28	HIS	-	expression tag	UNP Q96HY7
B	29	SER	-	expression tag	UNP Q96HY7
B	30	SER	-	expression tag	UNP Q96HY7
B	31	GLY	-	expression tag	UNP Q96HY7
B	32	VAL	-	expression tag	UNP Q96HY7
B	33	ASP	-	expression tag	UNP Q96HY7
B	34	LEU	-	expression tag	UNP Q96HY7
B	35	GLY	-	expression tag	UNP Q96HY7
B	36	THR	-	expression tag	UNP Q96HY7
B	37	GLU	-	expression tag	UNP Q96HY7
B	38	ASN	-	expression tag	UNP Q96HY7
B	39	LEU	-	expression tag	UNP Q96HY7
B	40	TYR	-	expression tag	UNP Q96HY7
B	41	PHE	-	expression tag	UNP Q96HY7
B	42	GLN	-	expression tag	UNP Q96HY7
B	43	SER	-	expression tag	UNP Q96HY7
B	44	MET	-	expression tag	UNP Q96HY7

- Molecule 2 is (3S)-1-(3-fluoropyridin-2-yl)-4,4-dimethylpyrrolidin-3-ol (three-letter code: WGA) (formula: $C_{11}H_{15}FN_2O$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	1
			15	11	1	2	1		

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

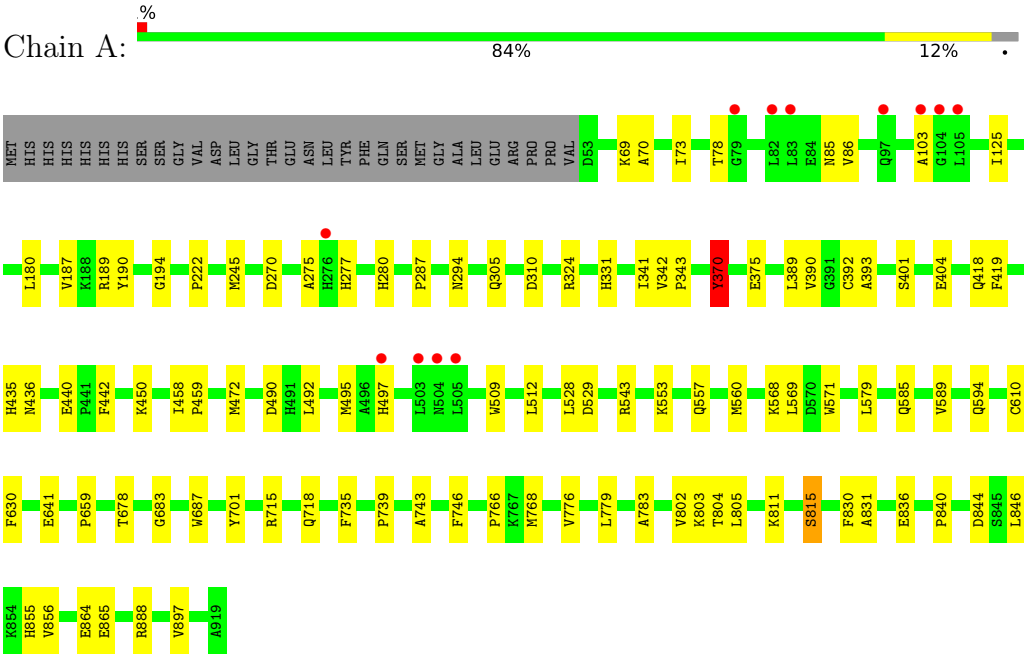
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1009	Total	O	0	4
			1009	1009		
5	B	800	Total	O	0	0
			800	800		

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.

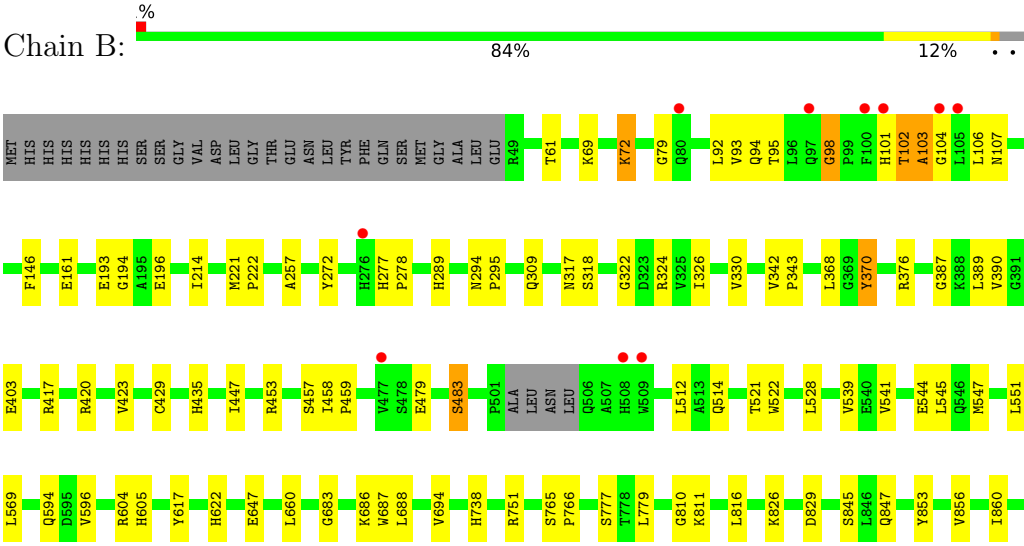
• Molecule 1: Probable 2-oxoglutarate dehydrogenase E1 component DHKTD1, mitochondrial

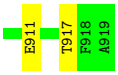
Chain A:



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

Chain B:




E911
T917
F918
A919

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.15Å 146.91Å 87.33Å 90.00° 102.90° 90.00°	Depositor
Resolution (Å)	85.12 – 1.98 85.12 – 1.98	Depositor EDS
% Data completeness (in resolution range)	58.3 (85.12-1.98) 58.4 (85.12-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.166 , 0.225 0.172 , 0.223	Depositor DCC
R_{free} test set	3950 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15394	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, WGA, 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	0.70	0/6959	0.84	0/9439
1	B	0.70	0/6914	0.83	1/9385 (0.0%)
All	All	0.70	0/13873	0.83	1/18824 (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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	751	ARG	NE-CZ-NH2	-6.56	117.02	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	98	GLY	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	6775	0	6624	73	0
1	B	6740	0	6571	61	0
2	A	15	0	0	1	0
3	A	26	0	16	3	0
3	B	26	0	16	1	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	1009	0	0	22	2
5	B	800	0	0	15	2
All	All	15394	0	13227	135	2

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 (135) 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:107:ASN:O	5:B:1101:HOH:O	1.96	0.84
1:A:543:ARG:HA	5:A:1693:HOH:O	1.86	0.76
1:A:389:LEU:HD12	1:A:390:VAL:HG13	1.68	0.76
1:A:815:SER:HB3	5:A:1389:HOH:O	1.89	0.72
1:A:324:ARG:NH2	5:A:1107:HOH:O	2.22	0.71
1:B:376:ARG:NH1	5:B:1103:HOH:O	2.11	0.71
1:A:528:LEU:HD21	1:A:783:ALA:HB2	1.73	0.69
1:A:275:ALA:O	5:A:1102:HOH:O	2.11	0.68
1:B:61:THR:OG1	5:B:1102:HOH:O	2.11	0.67
1:A:853:TYR:HA	1:A:855:HIS:CE1	2.30	0.67
1:A:324:ARG:CZ	5:A:1107:HOH:O	2.43	0.66
1:B:103:ALA:HA	5:B:1699:HOH:O	1.95	0.66
1:B:92:LEU:O	1:B:95:THR:HB	1.95	0.66
1:A:375:GLU:OE2	5:A:1103:HOH:O	2.14	0.64
1:B:911:GLU:HB3	5:B:1638:HOH:O	1.96	0.64
1:A:375:GLU:OE1	5:A:1104:HOH:O	2.15	0.64
1:A:129:GLN:HB2	1:A:404:GLU:HG3	1.80	0.63
1:A:768:MET:HE1	5:A:1389:HOH:O	1.98	0.62
1:B:660:LEU:HD23	1:B:694:VAL:HB	1.84	0.60
1:B:569:LEU:HB2	1:B:777:SER:O	2.02	0.59
1:B:847:GLN:HG2	5:B:1835:HOH:O	2.02	0.59
1:A:557:GLN:HA	1:A:560:MET:HE2	1.85	0.58
1:B:194:GLY:O	1:B:429:CYS:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:GLU:OE2	5:A:1105:HOH:O	2.17	0.58
1:A:78:THR:HG22	5:A:1261:HOH:O	2.03	0.57
1:A:490:ASP:HB3	5:A:1942:HOH:O	2.05	0.56
1:A:492:LEU:HD12	1:A:495:MET:CE	2.36	0.56
1:A:571:TRP:CE2	1:A:766:PRO:HG3	2.41	0.55
1:B:272:TYR:CE2	1:B:278:PRO:HB3	2.41	0.55
1:A:180:LEU:HD22	1:A:245:MET:HE1	1.89	0.55
1:B:479:GLU:O	1:B:483:SER:OG	2.21	0.55
1:B:853:TYR:HB3	1:B:856:VAL:HG23	1.88	0.54
1:A:579:LEU:HD22	1:A:589:VAL:HG11	1.88	0.54
1:A:70:ALA:HB2	1:A:86:VAL:HG23	1.90	0.54
1:A:418:GLN:HG2	1:A:419:PHE:CE2	2.43	0.54
1:A:529:ASP:HA	5:A:1864:HOH:O	2.07	0.53
1:A:610:CYS:SG	1:A:613:THR:OG1	2.59	0.53
3:A:1002:TPP:HN42	3:A:1002:TPP:C2	2.23	0.52
1:B:541:VAL:HG11	1:B:547:MET:HE3	1.92	0.52
1:B:528:LEU:HD13	1:B:779:LEU:HB3	1.92	0.51
1:B:124:GLN:HG2	5:B:1148:HOH:O	2.10	0.51
1:A:735:PHE:CD2	1:A:840:PRO:HD2	2.46	0.51
1:A:630:PHE:CG	2:A:1001[A]:WGA:C13	2.94	0.50
1:A:392[B]:CYS:SG	1:A:422:ASP:HB2	2.51	0.50
1:B:453:ARG:HD2	5:B:1806:HOH:O	2.12	0.50
1:A:844:ASP:HB2	5:A:1771:HOH:O	2.11	0.50
1:B:106:LEU:HG	1:B:121:TYR:CE2	2.47	0.50
1:A:569:LEU:HD11	1:A:779:LEU:HD13	1.94	0.49
1:A:802:VAL:HG21	1:A:831:ALA:HB2	1.94	0.49
1:B:370:TYR:HA	1:B:435:HIS:HB2	1.94	0.49
1:A:389:LEU:CD1	1:A:390:VAL:HG13	2.39	0.49
1:A:418:GLN:NE2	5:A:1135:HOH:O	2.42	0.49
1:B:342:VAL:HB	1:B:343:PRO:CD	2.42	0.49
1:B:860:ILE:HD11	1:B:888:ARG:NH2	2.28	0.49
1:A:194:GLY:O	1:A:429:CYS:HB2	2.13	0.48
1:A:190:TYR:CE1	1:A:436:ASN:HB3	2.48	0.48
1:B:853:TYR:HB3	1:B:856:VAL:CG2	2.42	0.48
1:B:102:THR:O	1:B:104:GLY:N	2.46	0.48
1:A:125:ILE:O	1:A:154:GLN:NE2	2.46	0.48
1:B:93:VAL:C	1:B:95:THR:H	2.17	0.48
1:A:129:GLN:OE1	1:A:401:SER:OG	2.30	0.48
1:A:440:GLU:OE1	1:A:442:PHE:HB2	2.14	0.48
1:A:277:HIS:CB	5:A:1102:HOH:O	2.62	0.48
1:A:393:ALA:HB3	1:A:423:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:GLN:NE2	5:B:1142:HOH:O	2.45	0.48
1:B:69:LYS:HE3	5:B:1118:HOH:O	2.14	0.48
1:B:403:GLU:HB2	5:B:1731:HOH:O	2.14	0.47
1:B:447:ILE:HG23	5:B:1211:HOH:O	2.14	0.47
1:B:544:GLU:HG2	1:B:545:LEU:N	2.29	0.46
1:A:509:TRP:CE3	1:A:512:LEU:HD12	2.49	0.46
1:B:221:MET:HB2	1:B:330:VAL:HB	1.97	0.46
3:A:1002:TPP:H6'	1:B:594:GLN:OE1	2.16	0.46
1:B:738:HIS:CE1	1:B:810:GLY:HA3	2.51	0.45
1:B:294:ASN:HB2	1:B:295:PRO:HD3	1.99	0.45
1:A:442:PHE:HE1	1:A:450:LYS:HG3	1.82	0.45
1:A:270:ASP:OD1	1:A:280[B]:HIS:ND1	2.49	0.45
1:A:492:LEU:HD12	1:A:495:MET:HE2	1.98	0.45
1:A:70:ALA:HB2	1:A:86:VAL:CG2	2.47	0.45
1:A:897:VAL:HG11	1:B:686:LYS:HG3	1.97	0.45
1:A:803:LYS:O	1:A:856:VAL:HG13	2.16	0.45
1:B:389:LEU:HD12	1:B:390:VAL:HG13	1.97	0.45
1:B:193:GLU:HA	1:B:196:GLU:OE2	2.16	0.45
1:B:551:LEU:HD21	1:B:605:HIS:CE1	2.52	0.45
1:A:585:GLN:CD	5:A:1109:HOH:O	2.55	0.45
1:B:326:ILE:HA	5:B:1302:HOH:O	2.17	0.44
1:A:743:ALA:O	1:A:746:PHE:HB3	2.18	0.44
1:B:101:HIS:O	1:B:102:THR:CB	2.65	0.44
1:B:393:ALA:HB3	1:B:423:VAL:HG23	1.97	0.44
1:A:458:ILE:HB	1:A:459:PRO:HD3	1.99	0.44
1:A:811:LYS:HE3	1:A:864:GLU:OE1	2.17	0.44
1:B:420:ARG:HA	1:B:420:ARG:HD3	1.84	0.44
1:A:450:LYS:NZ	5:A:1182:HOH:O	2.50	0.44
1:A:715:ARG:O	1:A:718:GLN:HB3	2.17	0.44
1:A:370:TYR:HA	1:A:435:HIS:HB2	1.99	0.43
1:B:539:VAL:HG13	1:B:559:ARG:HD2	2.00	0.43
3:A:1002:TPP:HN42	3:A:1002:TPP:H2	1.82	0.43
1:A:85:ASN:CB	5:A:1936:HOH:O	2.66	0.43
1:B:521:THR:C	1:B:522:TRP:CD1	2.92	0.43
1:B:101:HIS:O	1:B:102:THR:HB	2.19	0.43
1:B:765:SER:HB2	1:B:766:PRO:HD2	1.99	0.43
1:B:863:GLN:O	1:B:891:GLY:HA2	2.18	0.43
1:B:131:SER:OG	1:B:396:HIS:HB2	2.19	0.43
1:A:294:ASN:ND2	1:A:331:HIS:HE1	2.17	0.43
1:A:341:ILE:HD12	1:A:641:GLU:HG2	2.01	0.43
1:A:805:LEU:HD23	1:A:831:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ILE:N	1:B:459:PRO:CD	2.82	0.42
1:A:701:TYR:CE1	1:A:865:GLU:HG3	2.53	0.42
1:A:594:GLN:OE1	3:B:1001:TPP:H6'	2.19	0.42
1:B:683:GLY:HA2	1:B:687:TRP:CE3	2.54	0.42
1:B:816:LEU:HD22	1:B:917:THR:HG21	2.01	0.42
1:B:826:LYS:CG	5:B:1768:HOH:O	2.68	0.42
1:A:187:VAL:HG11	1:A:245:MET:HG2	2.01	0.42
1:A:450:LYS:HG2	5:A:2069:HOH:O	2.20	0.42
1:A:804:THR:HB	1:A:830:PHE:CD1	2.54	0.42
1:A:683:GLY:HA2	1:A:687:TRP:CE3	2.54	0.42
1:B:596:VAL:O	1:B:604:ARG:HD2	2.20	0.42
1:B:647:GLU:HA	1:B:647:GLU:OE1	2.19	0.42
1:A:180:LEU:HD12	1:A:189:ARG:HD2	2.02	0.41
1:A:69:LYS:NZ	5:A:1195:HOH:O	2.52	0.41
1:B:322:GLY:O	1:B:417:ARG:NH2	2.34	0.41
1:A:73:ILE:HD13	5:A:1457:HOH:O	2.19	0.41
1:B:387:GLY:O	1:B:392:CYS:HB2	2.19	0.41
1:A:846:LEU:O	1:A:850:MET:HG3	2.20	0.41
1:B:617:TYR:CZ	1:B:622:HIS:CD2	3.08	0.41
1:B:214:ILE:HG23	1:B:324:ARG:O	2.21	0.41
1:A:305:GLN:HA	1:A:310:ASP:HB3	2.03	0.41
1:A:342:VAL:HB	1:A:343:PRO:CD	2.51	0.41
1:B:257:ALA:HB2	1:B:688:LEU:HD21	2.02	0.41
1:A:568:LYS:HA	1:A:776:VAL:HB	2.03	0.41
1:A:855:HIS:C	5:A:1222:HOH:O	2.59	0.41
1:B:553:LYS:CG	5:B:1796:HOH:O	2.68	0.41
1:B:368:LEU:HD13	1:B:370:TYR:O	2.21	0.40
1:B:72:LYS:HG2	1:B:79:GLY:O	2.21	0.40
1:A:739:PRO:HA	1:A:836:GLU:OE1	2.20	0.40
1:A:287:PRO:HB3	1:A:678:THR:HB	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1464:HOH:O	5:B:1593:HOH:O[1_655]	2.09	0.11
5:A:1975:HOH:O	5:B:1755:HOH:O[1_554]	2.18	0.02

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	870/898 (97%)	829 (95%)	37 (4%)	4 (0%)	29 16
1	B	865/898 (96%)	806 (93%)	51 (6%)	8 (1%)	17 8
All	All	1735/1796 (97%)	1635 (94%)	88 (5%)	12 (1%)	22 11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	THR
1	B	103	ALA
1	A	222	PRO
1	B	222	PRO
1	B	277	HIS
1	B	289	HIS
1	B	457	SER
1	A	103	ALA
1	B	94	GLN
1	A	370	TYR
1	B	98	GLY
1	A	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	729/776 (94%)	720 (99%)	9 (1%)	71 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	723/776 (93%)	711 (98%)	12 (2%)	60 53
All	All	1452/1552 (94%)	1431 (99%)	21 (1%)	67 62

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	PHE
1	A	370	TYR
1	A	472	MET
1	A	497[A]	HIS
1	A	497[B]	HIS
1	A	553	LYS
1	A	628	LYS
1	A	815	SER
1	A	888	ARG
1	B	72	LYS
1	B	146	PHE
1	B	161	GLU
1	B	309	GLN
1	B	317	ASN
1	B	318	SER
1	B	370	TYR
1	B	483	SER
1	B	512	LEU
1	B	811	LYS
1	B	829	ASP
1	B	845	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	317	ASN
1	A	418	GLN
1	A	546	GLN
1	A	626	ASN
1	B	124	GLN
1	B	317	ASN
1	B	518	GLN
1	B	557	GLN
1	B	626	ASN

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Mol	Chain	Res	Type
1	B	848	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	WGA	A	1001[A]	-	15,16,16	5.87	8 (53%)	20,24,24	2.95	10 (50%)
3	TPP	B	1001	4	22,27,27	0.76	1 (4%)	29,40,40	1.01	2 (6%)
3	TPP	A	1002	4	22,27,27	0.67	0	29,40,40	0.81	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	WGA	A	1001[A]	-	-	4/4/19/19	0/2/2/2
3	TPP	B	1001	4	-	1/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	A	1002	4	-	3/16/17/17	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001[A]	WGA	C04-N05	11.95	1.67	1.46
2	A	1001[A]	WGA	C13-N05	-11.93	1.30	1.46
2	A	1001[A]	WGA	C04-C02	-10.73	1.40	1.54
2	A	1001[A]	WGA	O15-C14	-8.17	1.30	1.43
2	A	1001[A]	WGA	C06-C11	-3.70	1.37	1.42
2	A	1001[A]	WGA	C06-N05	3.42	1.46	1.37
2	A	1001[A]	WGA	F12-C11	2.98	1.43	1.35
2	A	1001[A]	WGA	C03-C02	2.96	1.60	1.53
3	B	1001	TPP	C4-N3	2.13	1.41	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001[A]	WGA	C13-N05-C04	-7.07	102.46	112.27
2	A	1001[A]	WGA	C11-C06-N05	-4.87	117.07	123.82
2	A	1001[A]	WGA	C01-C02-C04	4.47	116.56	110.63
2	A	1001[A]	WGA	C10-C11-C06	-4.22	119.03	121.73
2	A	1001[A]	WGA	C13-C14-C02	-3.23	99.63	103.40
2	A	1001[A]	WGA	C04-N05-C06	3.07	132.51	123.61
2	A	1001[A]	WGA	C01-C02-C14	-2.99	107.53	111.39
3	B	1001	TPP	C7'-N3-C2	-2.95	120.03	125.35
2	A	1001[A]	WGA	C03-C02-C14	2.91	115.15	111.39
2	A	1001[A]	WGA	C08-N07-C06	2.76	121.54	115.14
3	B	1001	TPP	C6-C5-C4	2.23	129.22	127.43
2	A	1001[A]	WGA	N07-C06-N05	2.20	122.04	116.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001[A]	WGA	N07-C06-N05-C13
2	A	1001[A]	WGA	C11-C06-N05-C13
2	A	1001[A]	WGA	N07-C06-N05-C04
2	A	1001[A]	WGA	C11-C06-N05-C04
3	A	1002	TPP	C4-C5-C6-C7
3	A	1002	TPP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	A	1002	TPP	PA-O3A-PB-O3B
3	B	1001	TPP	PA-O3A-PB-O3B

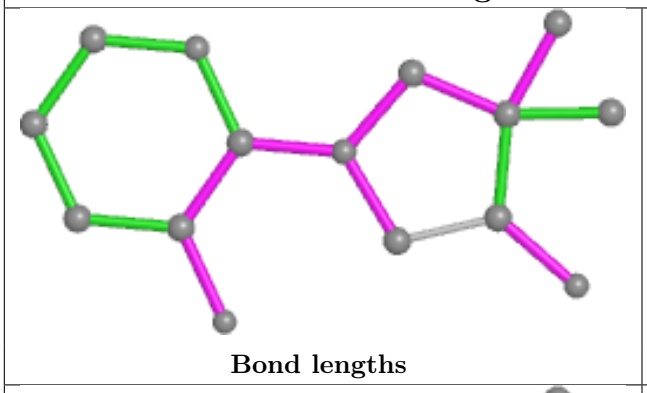
There are no ring outliers.

3 monomers are involved in 5 short contacts:

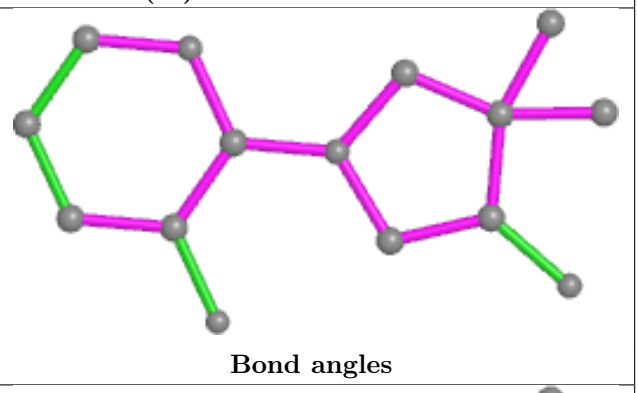
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001[A]	WGA	1	0
3	B	1001	TPP	1	0
3	A	1002	TPP	3	0

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 then 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.

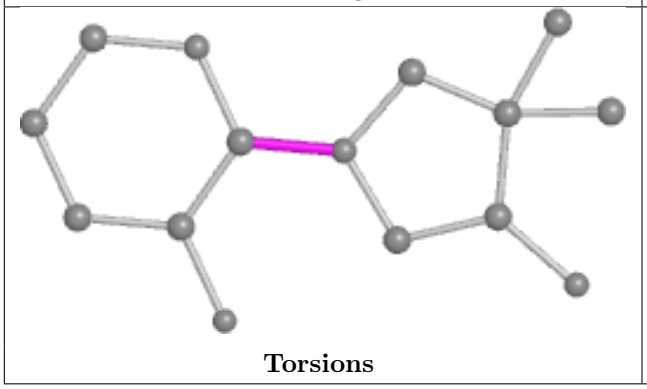
Ligand WGA A 1001 (A)



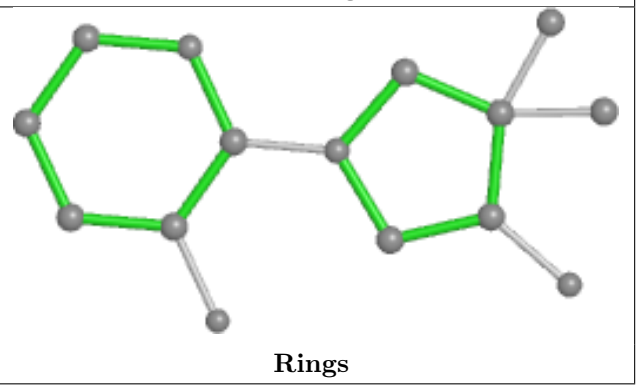
Bond lengths



Bond angles

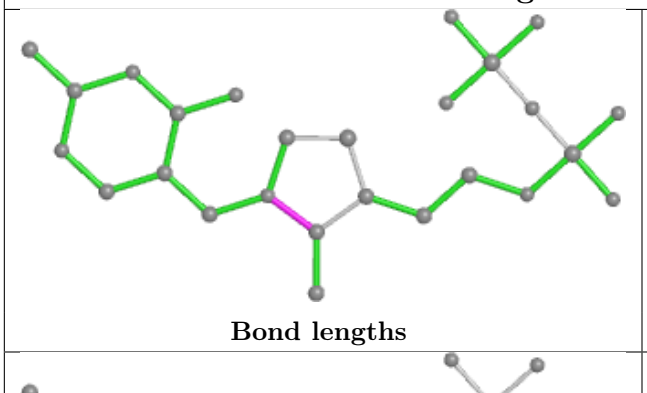


Torsions

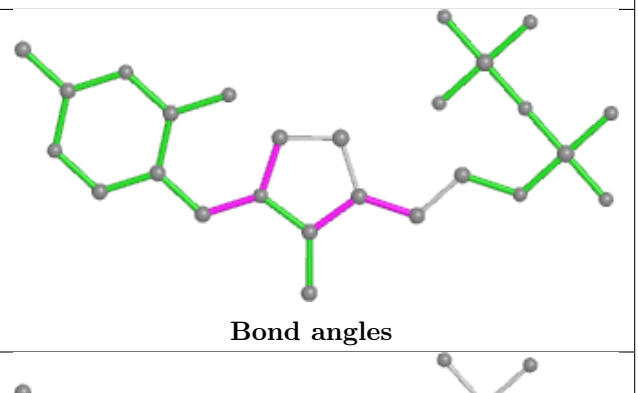


Rings

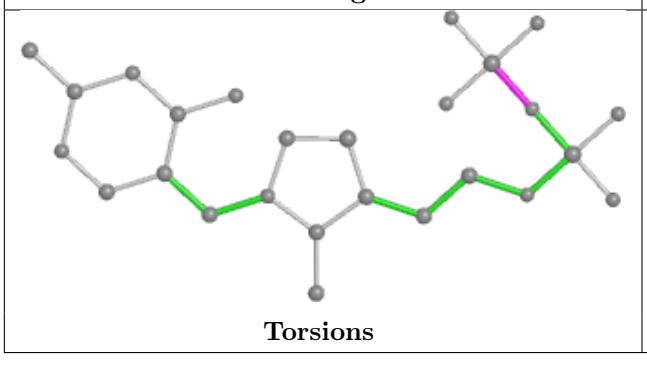
Ligand TPP B 1001



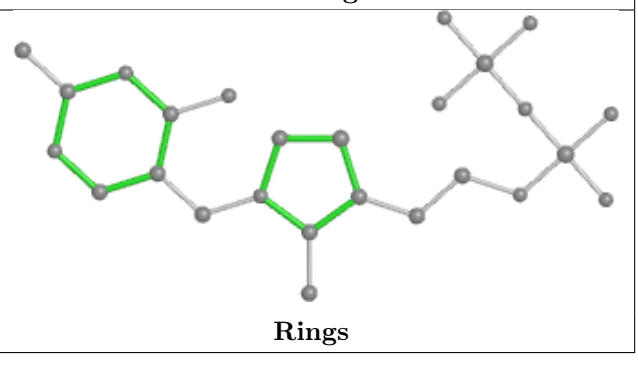
Bond lengths



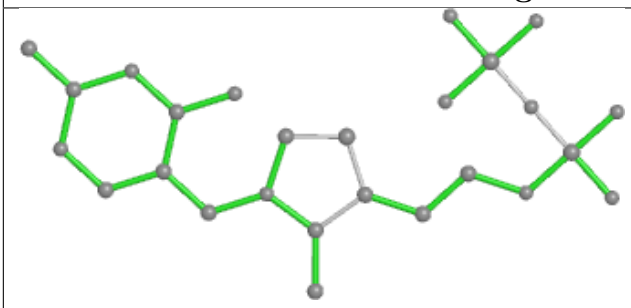
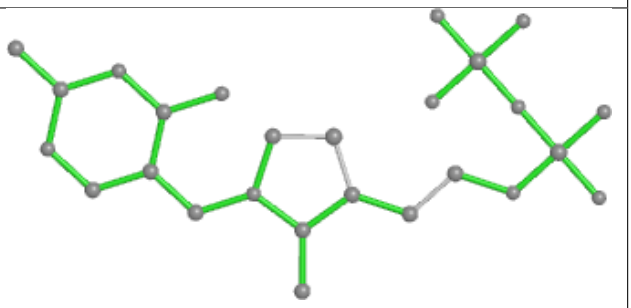
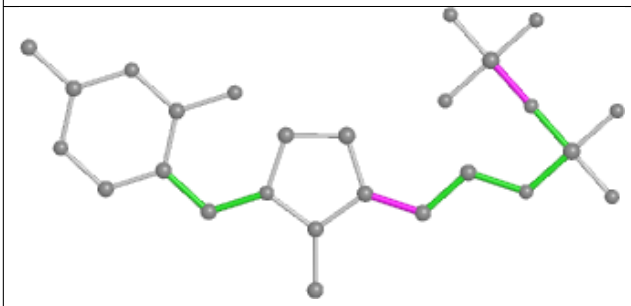
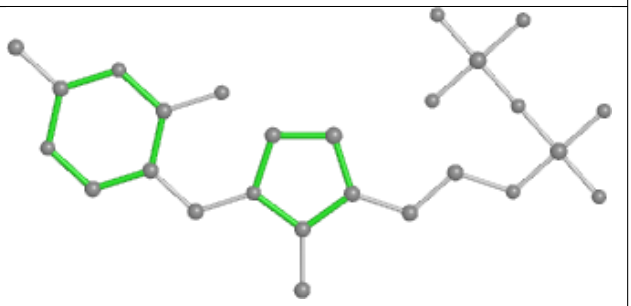
Bond angles



Torsions



Rings

Ligand TPP A 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

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^{th} 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^2)	Q<0.9
1	A	867/898 (96%)	-0.42	12 (1%)	75	77	8, 21, 51, 94	0
1	B	867/898 (96%)	-0.34	10 (1%)	79	80	10, 25, 63, 92	0
All	All	1734/1796 (96%)	-0.38	22 (1%)	77	78	8, 23, 57, 94	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	GLY	7.1
1	A	505	LEU	6.6
1	A	503	LEU	5.7
1	A	103	ALA	4.8
1	A	82	LEU	4.6
1	B	104	GLY	4.0
1	A	276	HIS	3.1
1	A	504	ASN	2.9
1	A	83	LEU	2.9
1	B	101	HIS	2.8
1	B	105	LEU	2.7
1	A	497[A]	HIS	2.6
1	A	105	LEU	2.5
1	B	477	VAL	2.4
1	B	508	HIS	2.2
1	B	276	HIS	2.2
1	B	80	GLN	2.2
1	B	100	PHE	2.1
1	A	79	GLY	2.1
1	B	97	GLN	2.1
1	B	509	TRP	2.0
1	A	97	GLN	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)

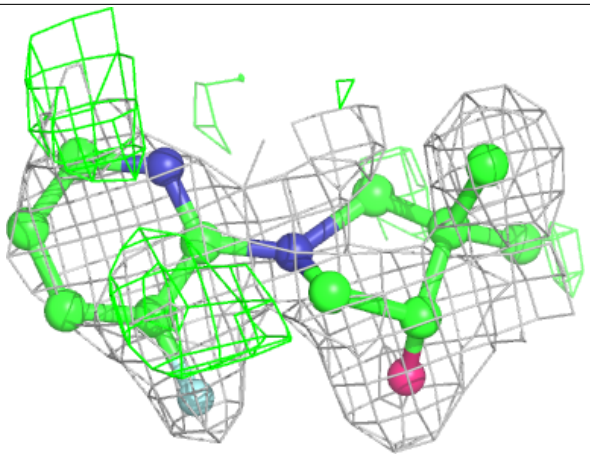
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

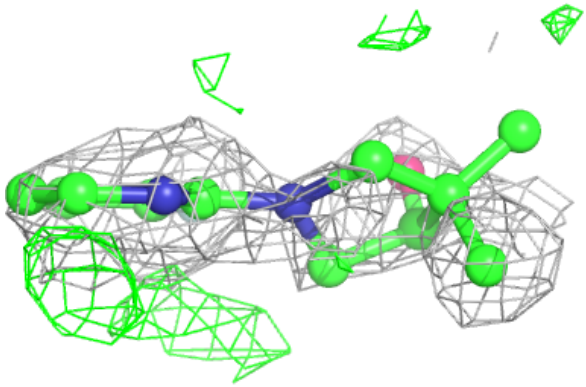
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	WGA	A	1001[A]	15/15	0.84	0.23	27,33,34,35	15
3	TPP	B	1001	26/26	0.98	0.07	13,15,18,18	0
4	MG	B	1003	1/1	0.99	0.03	11,11,11,11	0
4	MG	A	1003	1/1	0.99	0.03	15,15,15,15	0
3	TPP	A	1002	26/26	0.99	0.07	11,14,15,15	0
4	MG	B	1002	1/1	1.00	0.04	12,12,12,12	0

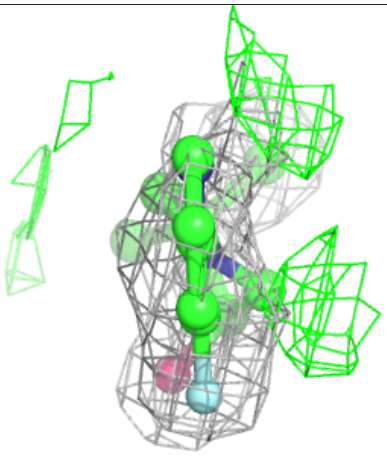
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WGA A 1001 (A):

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

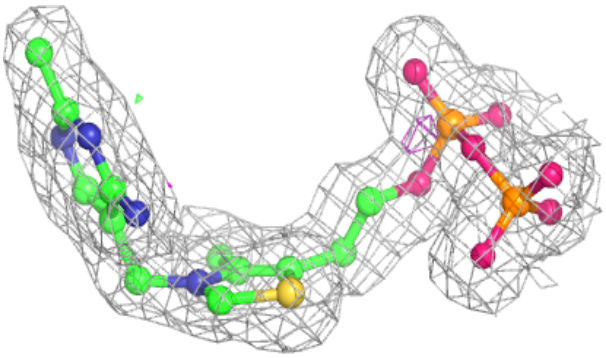


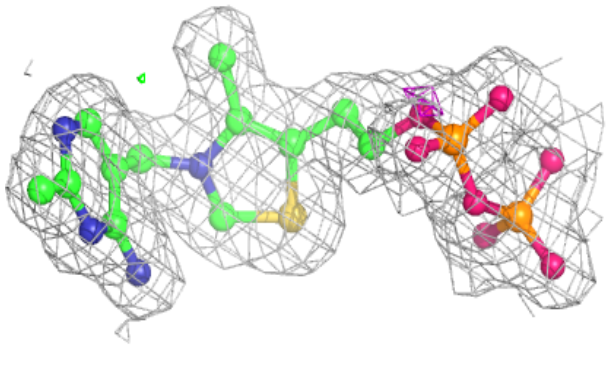


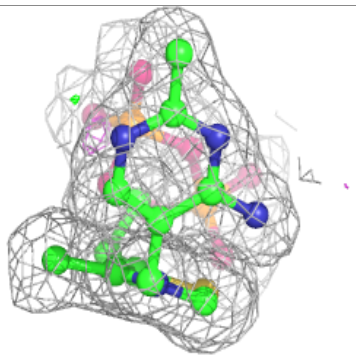


Electron density around TPP B 1001:

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

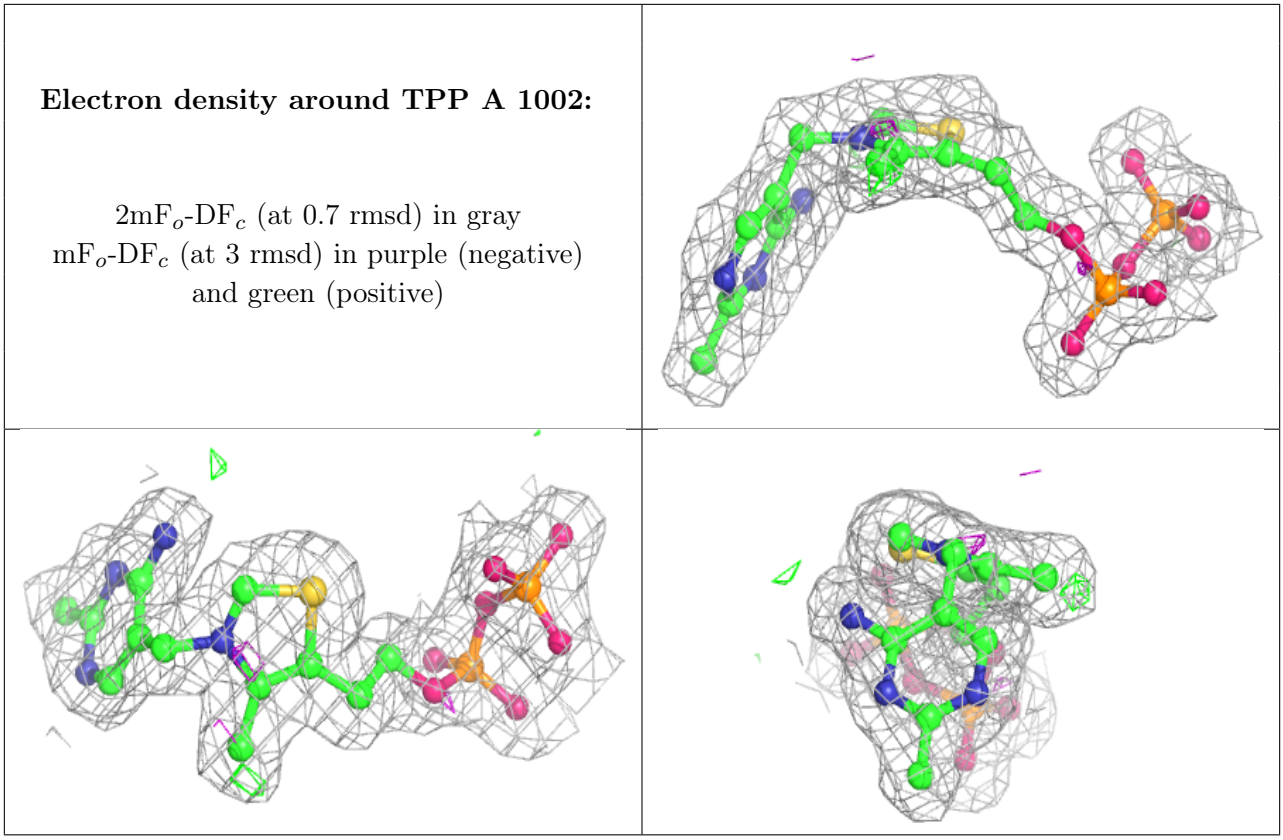






Electron density around TPP A 1002:

$2mF_o$-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.