



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:24 am BST

PDB ID : 2YIC
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis alpha-ketoglutarate decarboxylase (triclinic form)
Authors : Wagner, T.; Bellinzoni, M.; Wehenkel, A.M.; O'Hare, H.M.; Alzari, P.M.
Deposited on : 2011-05-11
Resolution : 1.96 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 : 2.11
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

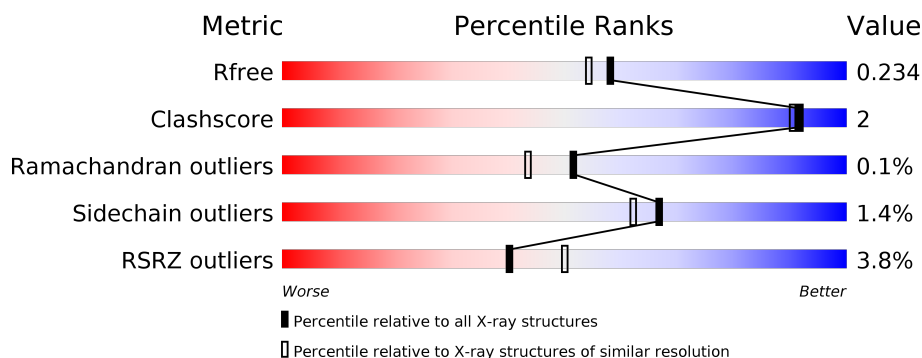
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 $\leq 5\%$. 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>3%</div> <div>89%</div> <div>6%</div> </div>
1	B	868	<div> <div>4%</div> <div>89%</div> <div>7%</div> </div>
1	C	868	<div> <div>3%</div> <div>89%</div> <div>7%</div> </div>
1	D	868	<div> <div>5%</div> <div>88%</div> <div>5%</div> <div>7%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26363 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.

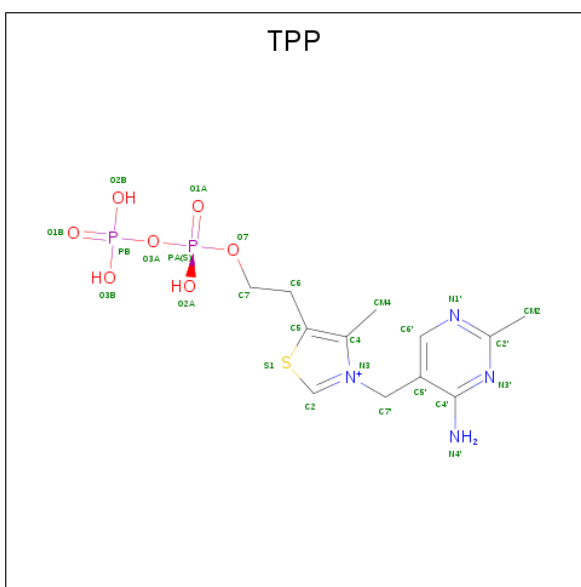
- Molecule 1 is a protein called 2-OXOGLUTARATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	814	Total	C	N	O	S	0	1	0
			6295	3965	1110	1196	24			
1	B	810	Total	C	N	O	S	0	1	0
			6241	3936	1106	1174	25			
1	C	806	Total	C	N	O	S	0	0	0
			6256	3939	1108	1187	22			
1	D	809	Total	C	N	O	S	0	1	0
			6238	3932	1096	1186	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	expression tag	UNP A0R2B1
B	360	GLY	-	expression tag	UNP A0R2B1
C	360	GLY	-	expression tag	UNP A0R2B1
D	360	GLY	-	expression tag	UNP A0R2B1

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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		
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	D	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	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 1	Ca 1	0	0
4	D	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0

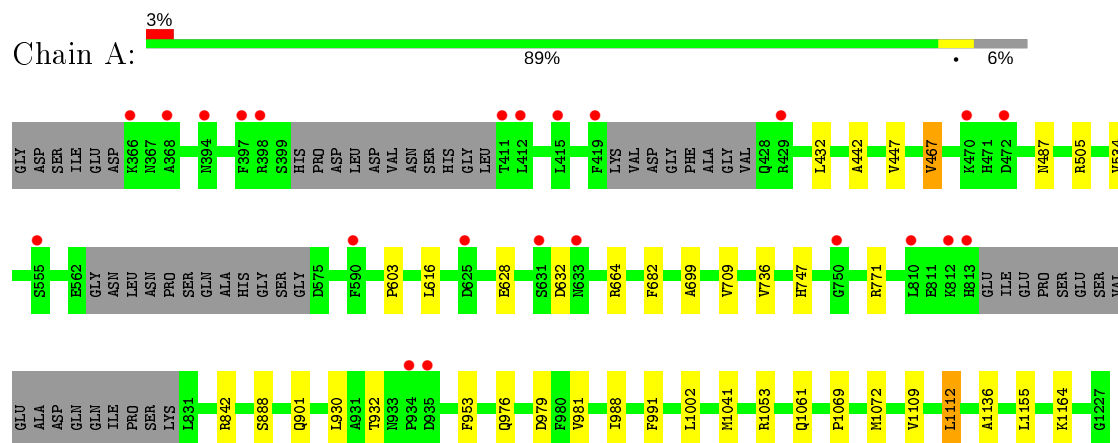
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	365	Total 365	O 365	0	0
5	B	275	Total 275	O 275	0	0
5	C	338	Total 338	O 338	0	0
5	D	243	Total 243	O 243	0	0

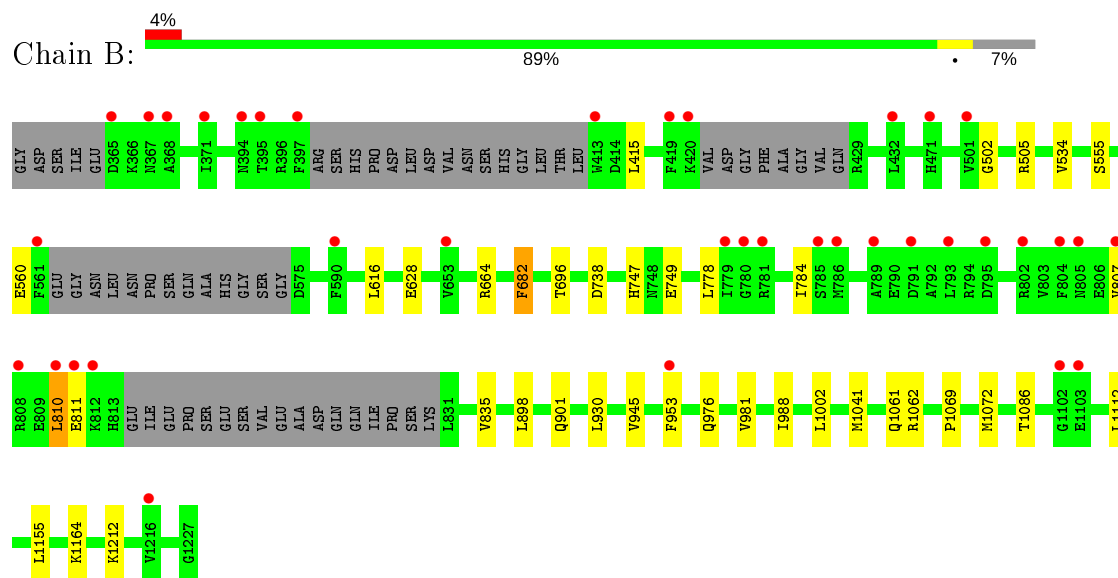
3 Residue-property plots [i](#)

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.

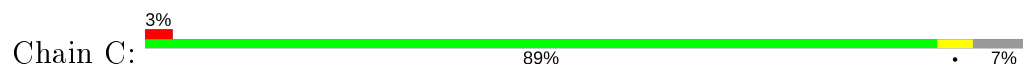
• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



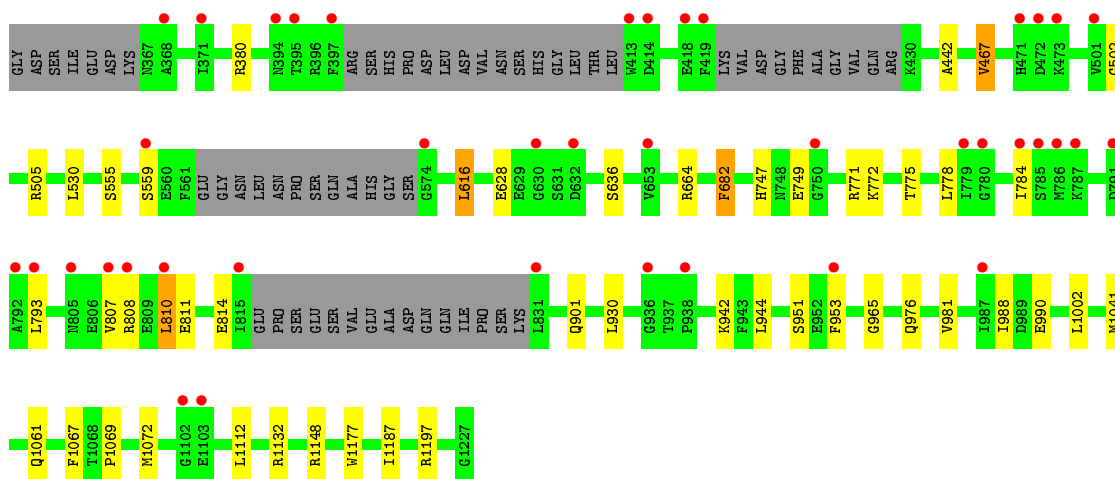
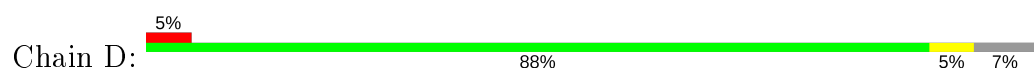
• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



- Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.54Å 83.24Å 158.61Å 99.48° 99.06° 101.25°	Depositor
Resolution (Å)	39.20 – 1.96 49.53 – 1.96	Depositor EDS
% Data completeness (in resolution range)	95.2 (39.20-1.96) 94.0 (49.53-1.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.97Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.188 , 0.211 0.207 , 0.234	Depositor DCC
R_{free} test set	13065 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.034 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26363	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0/6425	0.60	0/8715
1	B	0.50	0/6371	0.60	0/8645
1	C	0.51	0/6381	0.60	0/8650
1	D	0.50	0/6367	0.60	0/8640
All	All	0.50	0/25544	0.60	0/34650

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	6295	0	6066	18	0
1	B	6241	0	6017	19	0
1	C	6256	0	6055	16	0
1	D	6238	0	6009	26	0
2	A	26	0	16	1	0
2	B	26	0	16	2	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	365	0	0	1	0
5	B	275	0	0	3	0
5	C	338	0	0	0	0
5	D	243	0	0	0	0
All	All	26363	0	24211	78	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 (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1041[B]:MET:HG2	1:D:1067:PHE:HB2	1.49	0.94
1:D:1041[B]:MET:CG	1:D:1067:PHE:HB2	2.16	0.74
1:C:505:ARG:HA	1:C:747:HIS:O	2.03	0.58
1:D:505:ARG:HA	1:D:747:HIS:O	2.03	0.57
1:D:771:ARG:HH12	1:D:793:LEU:HD23	1.71	0.55
1:D:559:SER:HA	1:D:814:GLU:OE2	2.07	0.55
1:B:1041[B]:MET:HE2	5:B:3246:HOH:O	2.06	0.54
1:D:1069:PRO:HB2	1:D:1072:MET:HB3	1.90	0.54
1:B:1002:LEU:HB3	1:B:1061:GLN:HB2	1.93	0.52
1:D:1002:LEU:HB3	1:D:1061:GLN:HB2	1.92	0.51
1:B:778:LEU:HB3	1:B:784:ILE:HG12	1.92	0.51
1:C:901:GLN:OE1	2:D:2001:TPP:H6'	2.12	0.50
1:D:616:LEU:HD13	1:D:965:GLY:HA2	1.92	0.50
1:D:772:LYS:HA	1:D:775:THR:HG22	1.94	0.50
1:B:1069:PRO:HB2	1:B:1072:MET:HB3	1.94	0.49
1:B:534:VAL:HG11	1:B:616:LEU:HD22	1.94	0.49
1:A:534:VAL:HG11	1:A:616:LEU:HD22	1.95	0.49
1:A:1069:PRO:HB2	1:A:1072:MET:HB3	1.94	0.48
1:B:807:VAL:O	1:B:811:GLU:HG3	2.13	0.48
1:D:628:GLU:HG2	1:D:664:ARG:O	2.13	0.48
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.96	0.48
1:B:505:ARG:HA	1:B:747:HIS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:SER:HA	1:D:810:LEU:HG	1.95	0.47
1:A:901:GLN:OE1	2:B:2001:TPP:H6'	2.15	0.47
1:A:628:GLU:HG2	1:A:664:ARG:O	2.14	0.47
1:B:628:GLU:HG2	1:B:664:ARG:O	2.15	0.47
1:C:1155:LEU:HD11	1:C:1192:PHE:CZ	2.50	0.47
1:A:1002:LEU:HB3	1:A:1061:GLN:HB2	1.97	0.47
2:A:2001:TPP:H6'	1:B:901:GLN:OE1	2.15	0.46
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.97	0.45
1:A:447:VAL:HG22	1:A:709:VAL:HG23	1.99	0.45
1:D:442:ALA:HB1	1:D:467:VAL:HG13	2.00	0.45
1:A:442:ALA:HB1	1:A:467:VAL:HG13	1.98	0.44
1:C:555:SER:HA	1:C:810:LEU:HG	1.98	0.44
1:D:616:LEU:HD13	1:D:965:GLY:CA	2.47	0.44
2:C:2001:TPP:H6'	1:D:901:GLN:OE1	2.17	0.44
1:C:442:ALA:HB1	1:C:467:VAL:HG13	2.00	0.44
1:A:1109:VAL:HG21	1:A:1136:ALA:HB2	2.00	0.43
1:B:1155:LEU:HD13	1:B:1164:LYS:HE2	1.99	0.43
1:B:555:SER:HA	1:B:810:LEU:HG	2.00	0.43
1:A:487:ASN:OD1	1:A:771:ARG:HD2	2.18	0.43
1:B:502:GLY:HA2	1:B:749:GLU:CD	2.39	0.43
1:C:778:LEU:HB3	1:C:784:ILE:HG12	2.01	0.43
1:A:1155:LEU:HD13	1:A:1164:LYS:HE2	2.01	0.42
1:C:807:VAL:O	1:C:811:GLU:HG3	2.19	0.42
1:C:842:ARG:NH2	1:C:932:THR:O	2.53	0.42
1:D:1069:PRO:CB	1:D:1072:MET:HB3	2.48	0.42
1:B:1062:ARG:NH2	5:B:3194:HOH:O	2.51	0.42
2:B:2001:TPP:HM41	2:B:2001:TPP:H61	1.94	0.42
1:B:696:THR:HG21	1:B:738:ASP:HB2	2.01	0.42
1:D:807:VAL:O	1:D:811:GLU:HG3	2.18	0.42
1:D:502:GLY:HA2	1:D:749:GLU:CD	2.41	0.42
1:A:842:ARG:NH2	1:A:932:THR:O	2.53	0.42
1:B:898:LEU:O	1:B:945:VAL:HA	2.20	0.41
1:C:452:THR:O	1:D:380:ARG:NH2	2.53	0.41
1:C:603:PRO:HD3	1:C:991:PHE:CZ	2.55	0.41
1:D:530:LEU:HD22	1:D:636:SER:HA	2.01	0.41
1:C:1069:PRO:HB2	1:C:1072:MET:HB3	2.01	0.41
1:D:1148:ARG:NH1	1:D:1187:ILE:O	2.53	0.41
1:B:835:VAL:O	1:B:1086:THR:HA	2.20	0.41
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.55	0.41
1:A:603:PRO:HD3	1:A:991:PHE:CZ	2.56	0.41
1:B:1069:PRO:CB	1:B:1072:MET:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ARG:HA	1:A:747:HIS:O	2.21	0.41
1:C:1019:ASP:OD1	1:D:990:GLU:OE1	2.39	0.41
1:D:749:GLU:CD	1:D:749:GLU:H	2.24	0.41
1:B:981:VAL:HG22	1:B:988:ILE:HD11	2.03	0.41
1:D:778:LEU:HB3	1:D:784:ILE:HG12	2.02	0.41
1:A:1041[A]:MET:HE2	5:A:3328:HOH:O	2.20	0.41
1:A:699:ALA:CB	1:A:736:VAL:HG21	2.51	0.41
1:A:888:SER:OG	1:A:1053:ARG:HD2	2.20	0.41
1:C:1002:LEU:HB3	1:C:1061:GLN:HB2	2.03	0.41
1:D:942:LYS:HE2	1:D:944:LEU:HD21	2.03	0.41
1:C:696:THR:HG21	1:C:738:ASP:HB2	2.03	0.40
1:D:981:VAL:HG22	1:D:988:ILE:HD11	2.03	0.40
1:A:1112:LEU:HD22	1:A:1136:ALA:HB3	2.03	0.40
1:B:1041[B]:MET:HE1	5:B:3261:HOH:O	2.21	0.40
1:C:1174:GLN:OE1	1:C:1206:PRO:HA	2.22	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	805/868 (93%)	790 (98%)	15 (2%)	0	100	100
1	B	801/868 (92%)	785 (98%)	14 (2%)	2 (0%)	47	38
1	C	794/868 (92%)	778 (98%)	16 (2%)	0	100	100
1	D	800/868 (92%)	783 (98%)	16 (2%)	1 (0%)	51	43
All	All	3200/3472 (92%)	3136 (98%)	61 (2%)	3 (0%)	51	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	415	LEU
1	B	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	647/726 (89%)	638 (99%)	9 (1%)	67	62
1	B	637/726 (88%)	629 (99%)	8 (1%)	69	65
1	C	645/726 (89%)	636 (99%)	9 (1%)	67	62
1	D	640/726 (88%)	629 (98%)	11 (2%)	60	55
All	All	2569/2904 (88%)	2532 (99%)	37 (1%)	67	62

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	432	LEU
1	A	467	VAL
1	A	632	ASP
1	A	682	PHE
1	A	930	LEU
1	A	953	PHE
1	A	976	GLN
1	A	979	ASP
1	A	1112	LEU
1	B	560	GLU
1	B	682	PHE
1	B	810	LEU
1	B	930	LEU
1	B	953	PHE
1	B	976	GLN
1	B	1112	LEU
1	B	1212	LYS
1	C	418	GLU
1	C	467	VAL

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Mol	Chain	Res	Type
1	C	682	PHE
1	C	810	LEU
1	C	868	ARG
1	C	930	LEU
1	C	953	PHE
1	C	976	GLN
1	C	1112	LEU
1	D	467	VAL
1	D	616	LEU
1	D	682	PHE
1	D	808	ARG
1	D	810	LEU
1	D	930	LEU
1	D	951	SER
1	D	953	PHE
1	D	976	GLN
1	D	1112	LEU
1	D	1132	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	D	2001	3	22,27,27	1.88	4 (18%)	29,40,40	1.90	9 (31%)
2	TPP	C	2001	3	22,27,27	1.81	2 (9%)	29,40,40	1.88	7 (24%)
2	TPP	B	2001	3	22,27,27	1.86	2 (9%)	29,40,40	1.85	10 (34%)
2	TPP	A	2001	3	22,27,27	1.92	4 (18%)	29,40,40	1.94	7 (24%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	TPP	C4-N3	-7.11	1.33	1.39
2	D	2001	TPP	C4-N3	-6.86	1.33	1.39
2	C	2001	TPP	C4-N3	-6.51	1.34	1.39
2	A	2001	TPP	C4-N3	-6.33	1.34	1.39
2	A	2001	TPP	C6-C5	4.31	1.52	1.50
2	C	2001	TPP	C2-N3	-2.71	1.30	1.36
2	D	2001	TPP	C4'-N4'	2.68	1.40	1.34
2	B	2001	TPP	C2-N3	-2.54	1.30	1.36
2	D	2001	TPP	C2-N3	-2.45	1.30	1.36
2	A	2001	TPP	PB-O1B	2.28	1.57	1.50
2	A	2001	TPP	C2-N3	-2.23	1.31	1.36
2	D	2001	TPP	PB-O1B	2.18	1.57	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	TPP	C6-C5-C4	5.05	131.48	127.43
2	D	2001	TPP	CM4-C4-C5	-4.43	117.92	127.60
2	A	2001	TPP	CM4-C4-C5	-4.40	117.97	127.60
2	C	2001	TPP	CM4-C4-C5	-4.29	118.22	127.60
2	B	2001	TPP	CM4-C4-C5	-4.15	118.52	127.60
2	A	2001	TPP	C5-C4-N3	4.14	115.86	107.57
2	C	2001	TPP	C6-C5-C4	4.14	130.75	127.43
2	C	2001	TPP	C5-C4-N3	4.10	115.78	107.57
2	D	2001	TPP	C5-C4-N3	4.08	115.75	107.57
2	B	2001	TPP	C5-C4-N3	3.88	115.33	107.57
2	C	2001	TPP	C6'-N1'-C2'	3.44	121.81	115.96
2	B	2001	TPP	C6'-N1'-C2'	3.25	121.50	115.96
2	D	2001	TPP	C6-C5-C4	3.22	130.02	127.43
2	D	2001	TPP	C6'-N1'-C2'	3.03	121.12	115.96
2	B	2001	TPP	N1'-C2'-N3'	-3.01	120.35	125.54
2	A	2001	TPP	C7'-N3-C2	-2.91	120.10	125.35
2	D	2001	TPP	C7'-N3-C2	-2.76	120.37	125.35
2	A	2001	TPP	C6'-N1'-C2'	2.69	120.53	115.96
2	D	2001	TPP	C5'-C6'-N1'	-2.61	119.48	123.82
2	D	2001	TPP	CM4-C4-N3	2.60	125.84	122.53
2	B	2001	TPP	C5'-C6'-N1'	-2.59	119.50	123.82
2	A	2001	TPP	CM4-C4-N3	2.59	125.83	122.53
2	B	2001	TPP	CM4-C4-N3	2.58	125.81	122.53
2	D	2001	TPP	N1'-C2'-N3'	-2.57	121.11	125.54
2	C	2001	TPP	N1'-C2'-N3'	-2.57	121.12	125.54
2	B	2001	TPP	C6-C5-C4	2.56	129.48	127.43
2	C	2001	TPP	C5'-C6'-N1'	-2.54	119.58	123.82
2	C	2001	TPP	CM4-C4-N3	2.47	125.69	122.53
2	A	2001	TPP	N1'-C2'-N3'	-2.41	121.39	125.54
2	B	2001	TPP	C7'-N3-C2	-2.39	121.04	125.35
2	B	2001	TPP	C2'-N3'-C4'	2.12	121.39	118.08
2	D	2001	TPP	C2'-N3'-C4'	2.12	121.39	118.08
2	B	2001	TPP	CM2-C2'-N1'	2.04	119.38	117.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

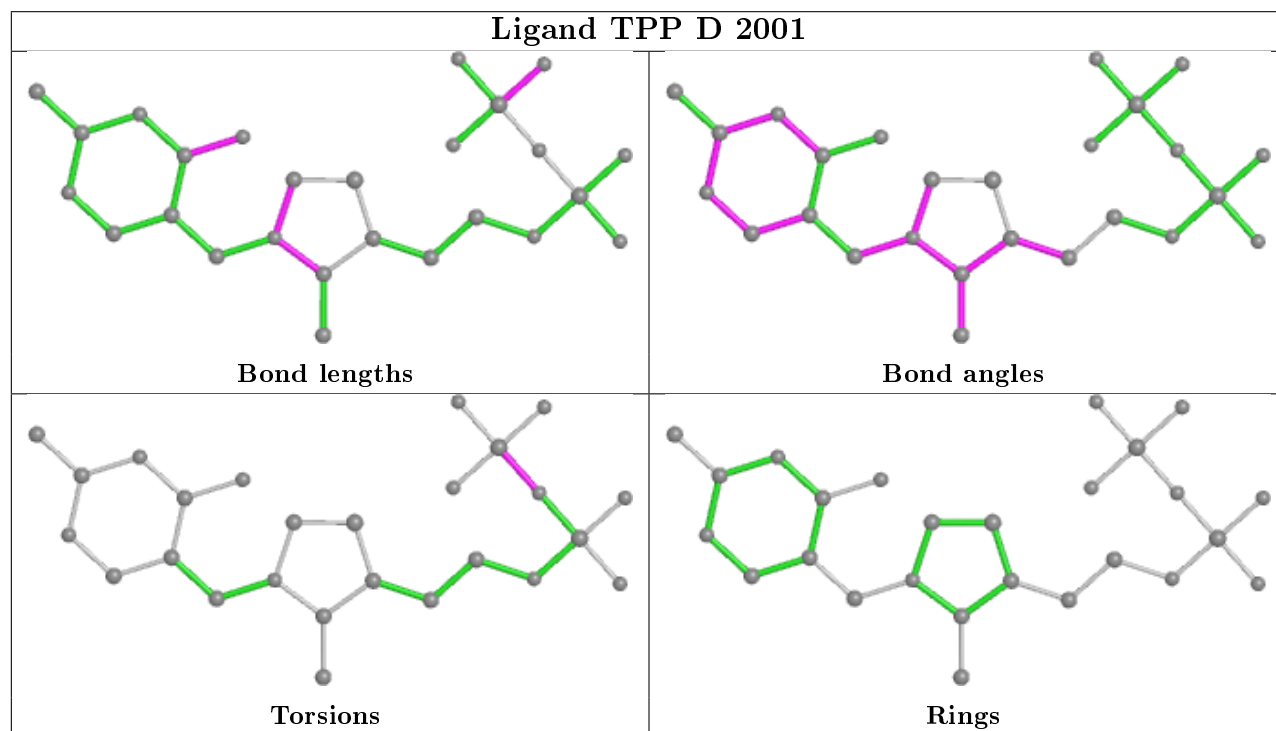
Mol	Chain	Res	Type	Atoms
2	C	2001	TPP	PA-O3A-PB-O3B
2	D	2001	TPP	PA-O3A-PB-O3B
2	A	2001	TPP	PA-O3A-PB-O3B

There are no ring outliers.

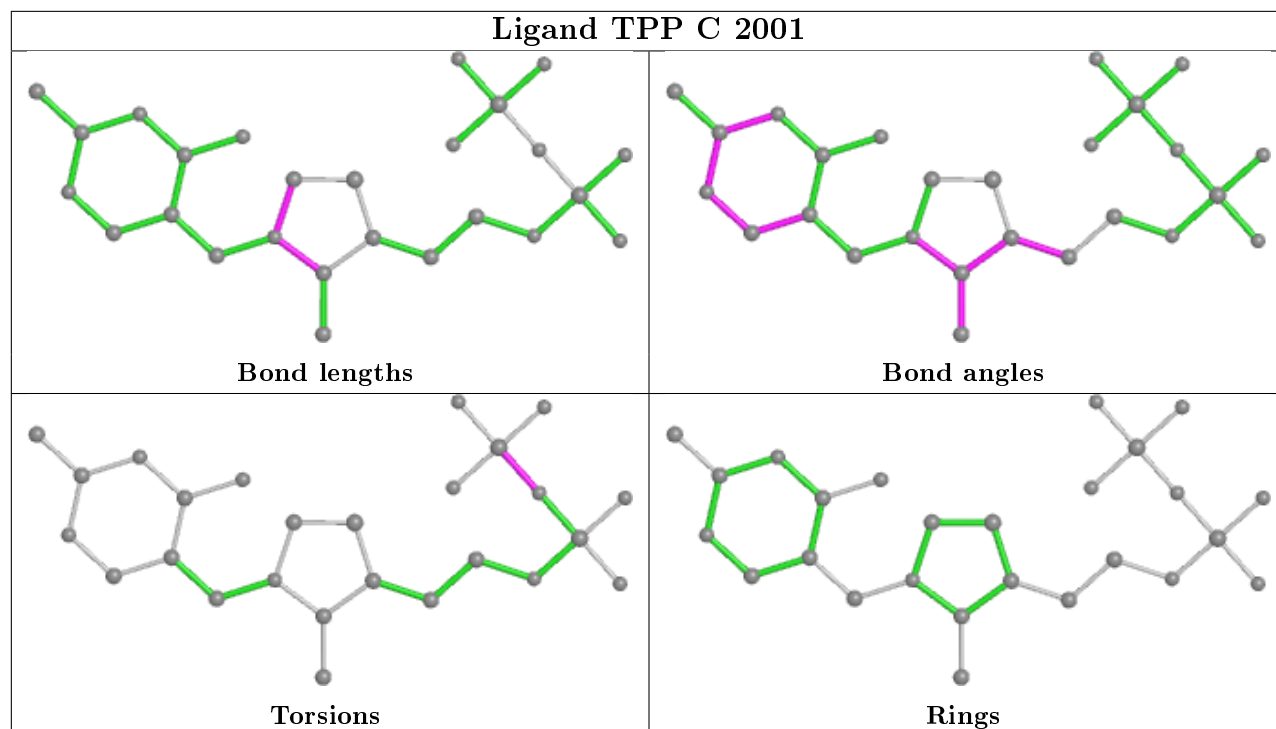
4 monomers are involved in 5 short contacts:

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

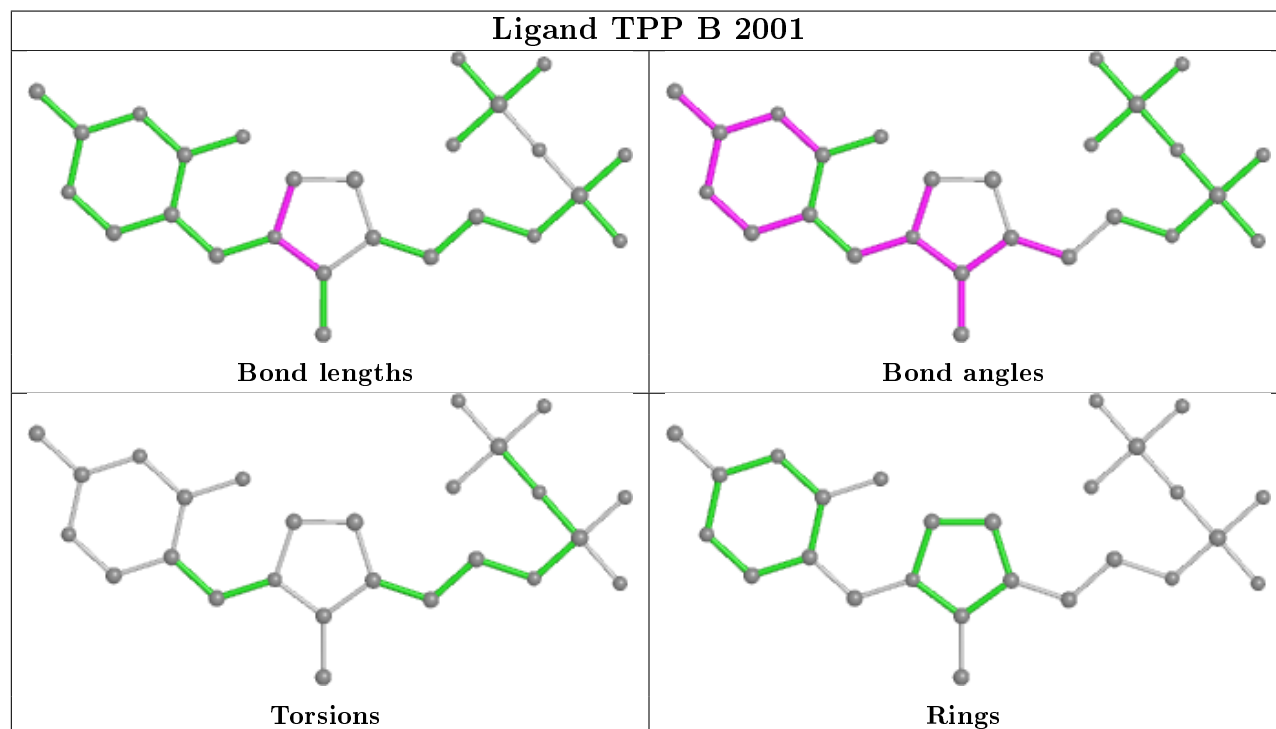
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

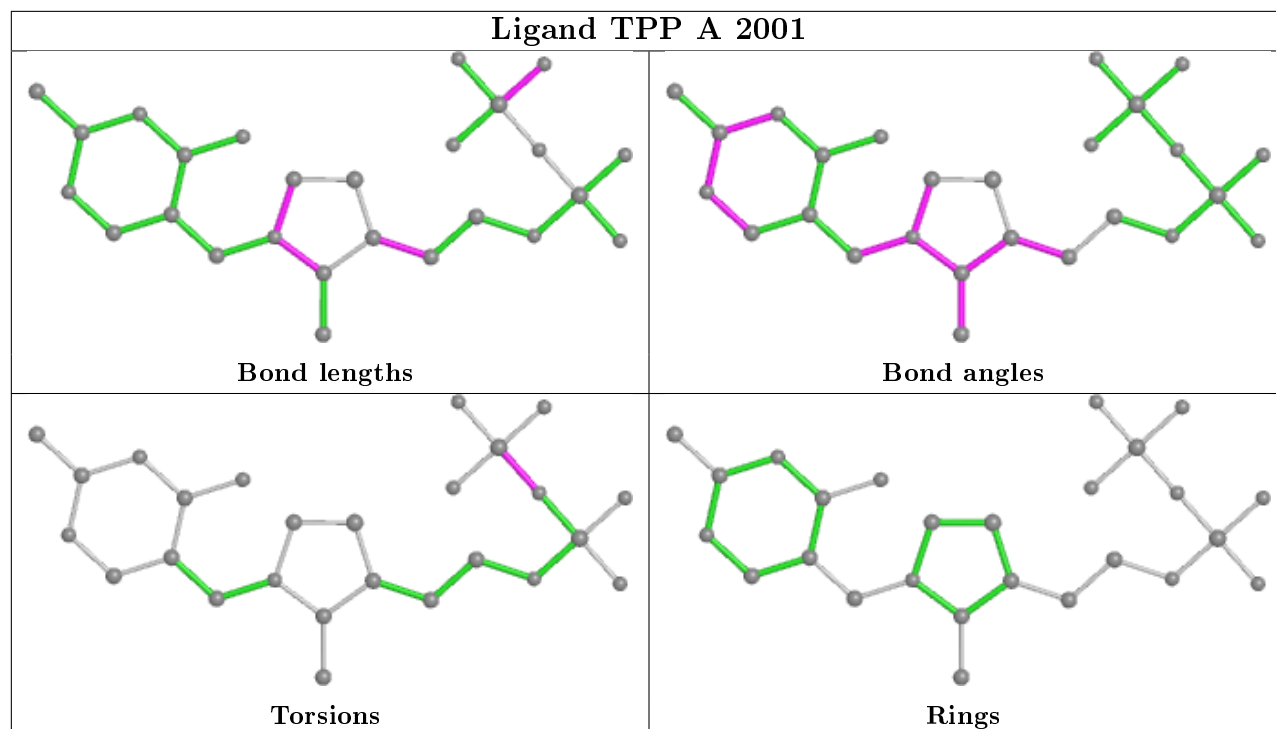


Ligand TPP C 2001



Ligand TPP B 2001





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	814/868 (93%)	-0.04	23 (2%)	53	62	11, 24, 52, 90	0
1	B	810/868 (93%)	0.11	37 (4%)	32	42	12, 26, 57, 106	0
1	C	806/868 (92%)	-0.00	22 (2%)	54	63	11, 24, 55, 76	0
1	D	809/868 (93%)	0.13	40 (4%)	29	39	13, 27, 59, 92	0
All	All	3239/3472 (93%)	0.05	122 (3%)	40	50	11, 25, 56, 106	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	394	ASN	6.5
1	B	394	ASN	5.9
1	B	419	PHE	5.5
1	C	368	ALA	5.4
1	C	779	ILE	5.0
1	B	786	MET	4.8
1	D	395	THR	4.6
1	D	419	PHE	4.6
1	D	371	ILE	4.5
1	B	395	THR	4.5
1	D	810	LEU	4.4
1	B	785	SER	4.4
1	C	590	PHE	4.2
1	A	429	ARG	4.2
1	B	779	ILE	4.2
1	C	785	SER	4.0
1	D	1103	GLU	4.0
1	B	397	PHE	3.8
1	D	780	GLY	3.8
1	B	807	VAL	3.8
1	B	789	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	785	SER	3.7
1	C	630	GLY	3.7
1	B	420	LYS	3.5
1	A	472	ASP	3.5
1	C	750	GLY	3.4
1	D	368	ALA	3.4
1	C	574	GLY	3.3
1	B	368	ALA	3.3
1	C	472	ASP	3.3
1	C	471	HIS	3.2
1	D	574	GLY	3.2
1	B	413	TRP	3.2
1	D	471	HIS	3.2
1	D	953	PHE	3.2
1	B	1102	GLY	3.1
1	A	812	LYS	3.1
1	D	815	ILE	3.1
1	B	1103	GLU	3.1
1	D	936	GLY	3.1
1	D	472	ASP	3.1
1	A	810	LEU	3.0
1	B	561	PHE	3.0
1	B	795	ASP	3.0
1	A	398	ARG	3.0
1	D	473	LYS	2.9
1	C	367	ASN	2.9
1	D	559	SER	2.9
1	B	371	ILE	2.9
1	B	471	HIS	2.9
1	D	784	ILE	2.9
1	D	779	ILE	2.8
1	D	413	TRP	2.8
1	A	935	ASP	2.7
1	A	366	LYS	2.7
1	D	632	ASP	2.7
1	B	812	LYS	2.6
1	D	807	VAL	2.6
1	C	775	THR	2.6
1	D	793	LEU	2.5
1	B	780	GLY	2.5
1	C	476	VAL	2.5
1	C	808	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	368	ALA	2.5
1	C	589	MET	2.5
1	D	630	GLY	2.5
1	D	1102	GLY	2.5
1	B	367	ASN	2.5
1	B	791	ASP	2.5
1	D	791	ASP	2.5
1	A	397	PHE	2.5
1	B	810	LEU	2.5
1	A	394	ASN	2.4
1	A	411	THR	2.4
1	D	501	VAL	2.4
1	D	418	GLU	2.4
1	A	631	SER	2.4
1	D	938	PRO	2.4
1	B	653	VAL	2.4
1	A	412	LEU	2.3
1	B	802	ARG	2.3
1	C	394	ASN	2.3
1	D	805	ASN	2.3
1	B	953	PHE	2.3
1	B	501	VAL	2.3
1	B	432	LEU	2.3
1	C	784	ILE	2.3
1	A	470	LYS	2.2
1	A	625	ASP	2.2
1	A	813	HIS	2.2
1	B	793	LEU	2.2
1	B	804	PHE	2.2
1	C	953	PHE	2.2
1	A	750	GLY	2.2
1	A	633	ASN	2.2
1	A	555	SER	2.2
1	A	419	PHE	2.2
1	D	653	VAL	2.2
1	D	786	MET	2.1
1	A	415	LEU	2.1
1	B	811	GLU	2.1
1	D	750	GLY	2.1
1	A	590	PHE	2.1
1	B	590	PHE	2.1
1	B	781	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	787	LYS	2.1
1	A	934	PRO	2.1
1	C	609	VAL	2.1
1	D	987	ILE	2.1
1	C	810	LEU	2.1
1	B	805	ASN	2.1
1	C	812	LYS	2.1
1	B	365	ASP	2.1
1	D	414	ASP	2.1
1	C	813	HIS	2.1
1	D	831	LEU	2.1
1	B	808	ARG	2.0
1	B	1216	VAL	2.0
1	D	397	PHE	2.0
1	C	988	ILE	2.0
1	D	808	ARG	2.0
1	D	792	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95th 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.

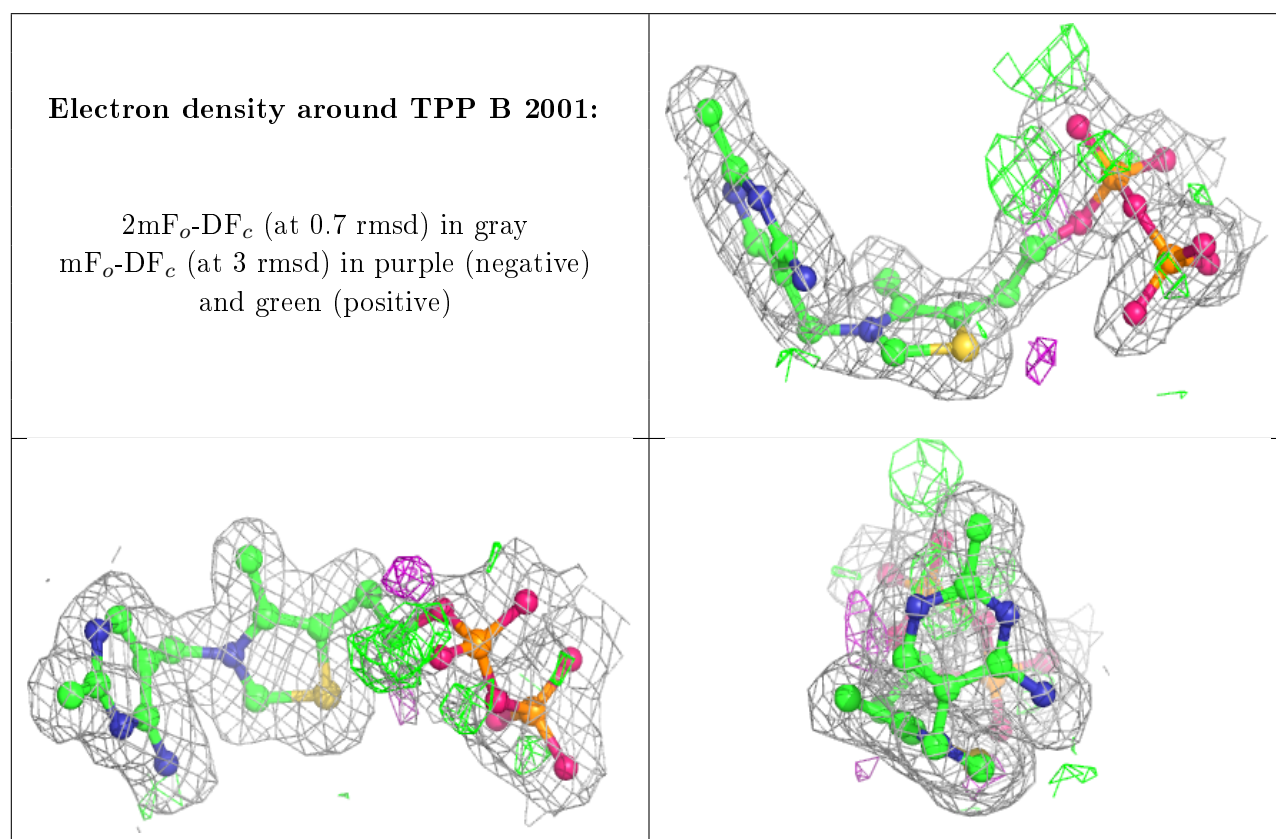
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TPP	B	2001	26/26	0.97	0.13	10,15,19,22	0
2	TPP	C	2001	26/26	0.98	0.14	10,16,20,23	0
3	MG	B	2002	1/1	0.98	0.12	11,11,11,11	0
2	TPP	D	2001	26/26	0.98	0.12	12,16,20,23	0
2	TPP	A	2001	26/26	0.98	0.12	13,18,20,23	0
3	MG	D	2002	1/1	0.99	0.12	12,12,12,12	0

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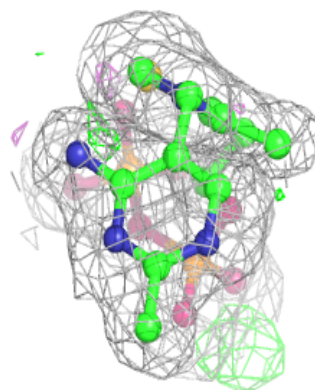
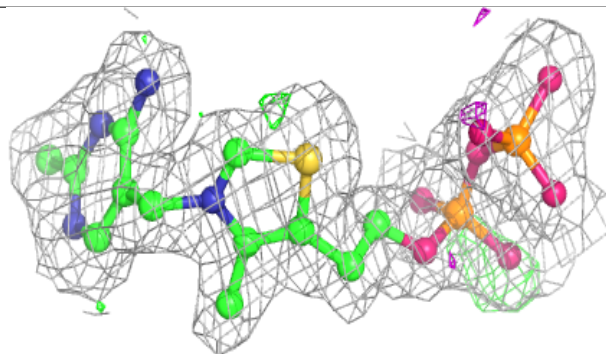
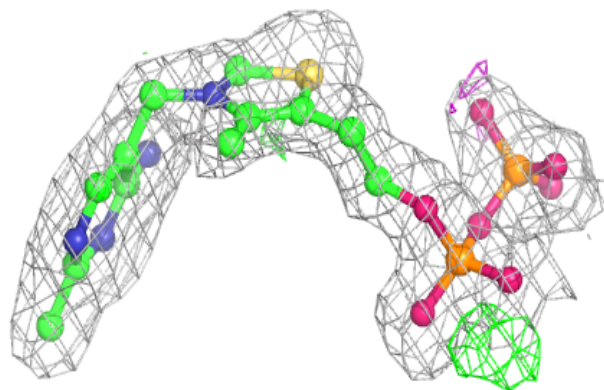
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CA	B	2003	1/1	0.99	0.05	23,23,23,23	0
4	CA	D	2003	1/1	0.99	0.04	25,25,25,25	0
3	MG	A	2002	1/1	0.99	0.11	10,10,10,10	0
4	CA	C	2003	1/1	1.00	0.04	20,20,20,20	0
4	CA	A	2003	1/1	1.00	0.05	20,20,20,20	0
3	MG	C	2002	1/1	1.00	0.12	10,10,10,10	0

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.

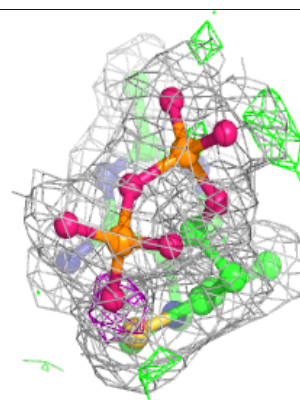
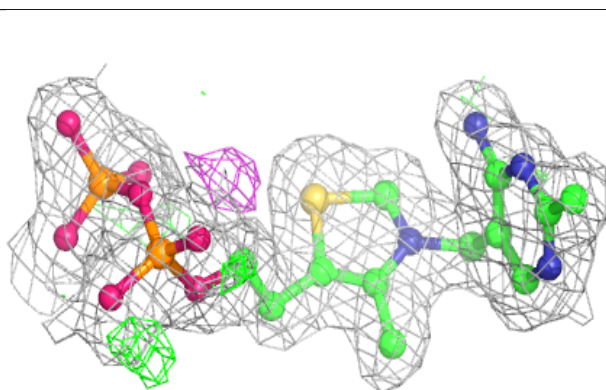
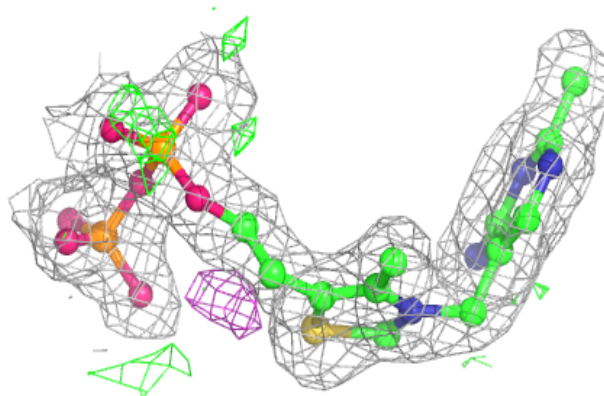


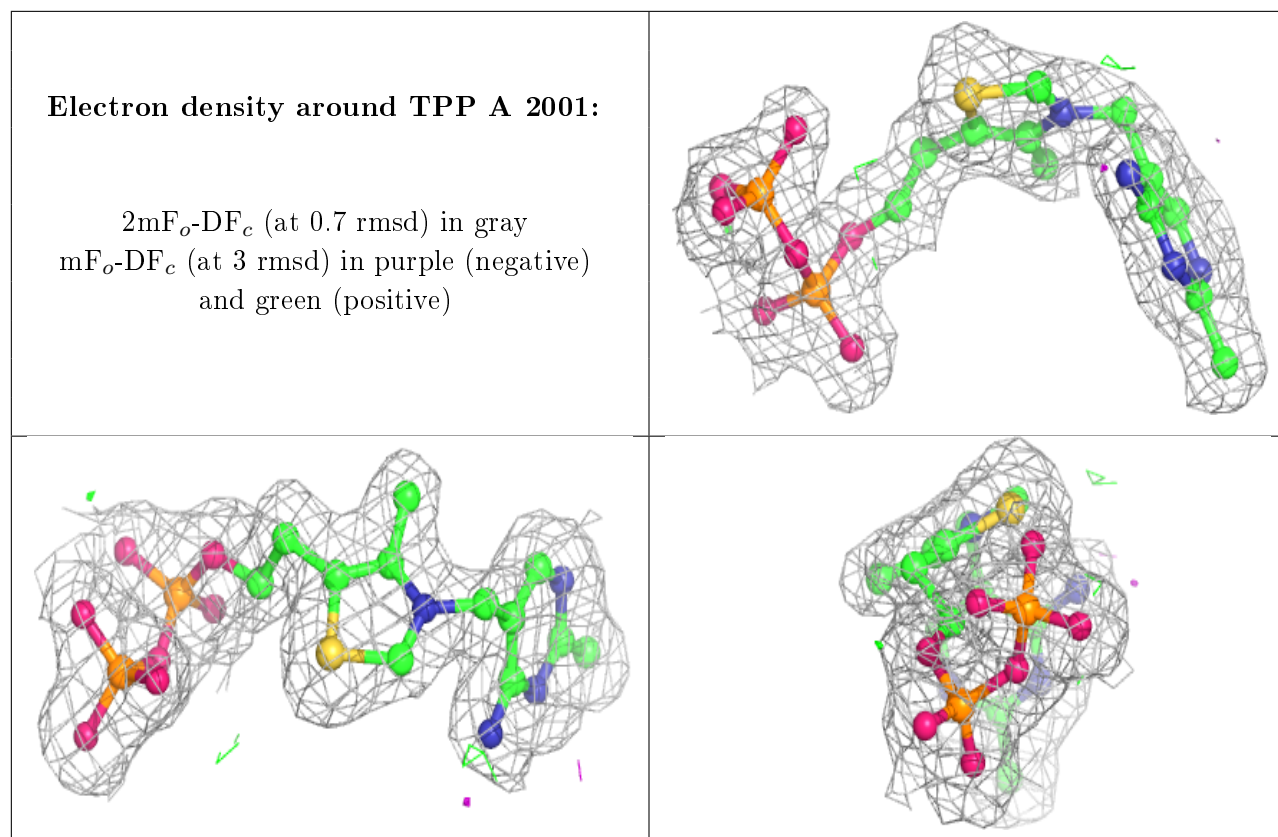
Electron density around TPP C 2001:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.