



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:35 PM UTC

PDB ID : 2YIC / pdb_00002yic
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

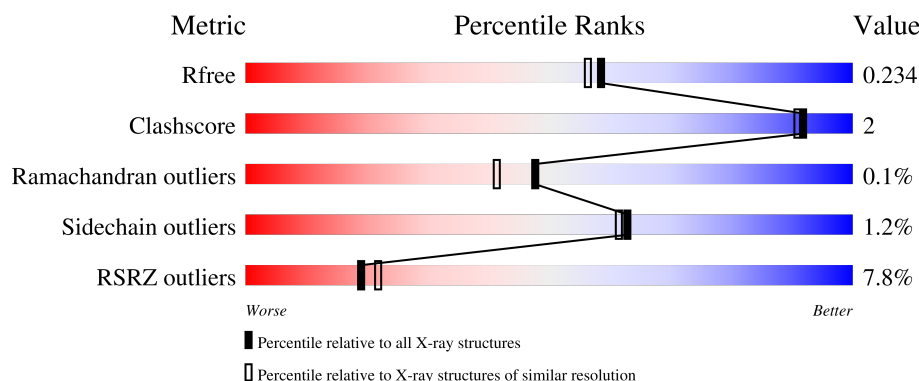
1 Overall quality at a glance

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 of 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	6% 88% 5% 6%
1	B	868	8% 88% 5% 7%
1	C	868	7% 89% • 7%
1	D	868	9% 87% 6% 7%

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.

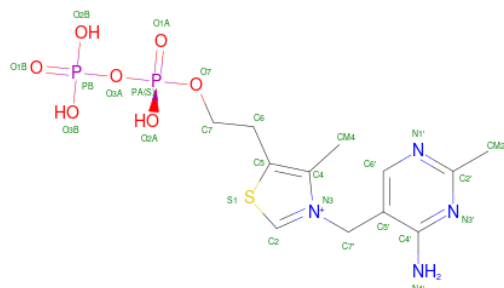
- Molecule 1 is a protein called 2-OXOGLUTARATE DECARBOXYLASE.

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 (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

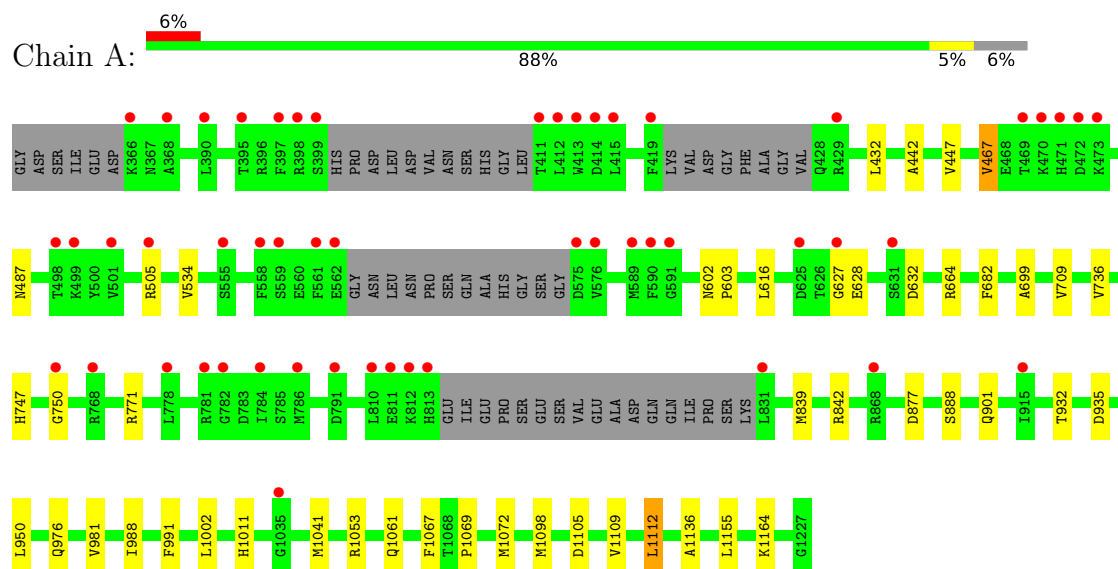
- Molecule 5 is water.

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

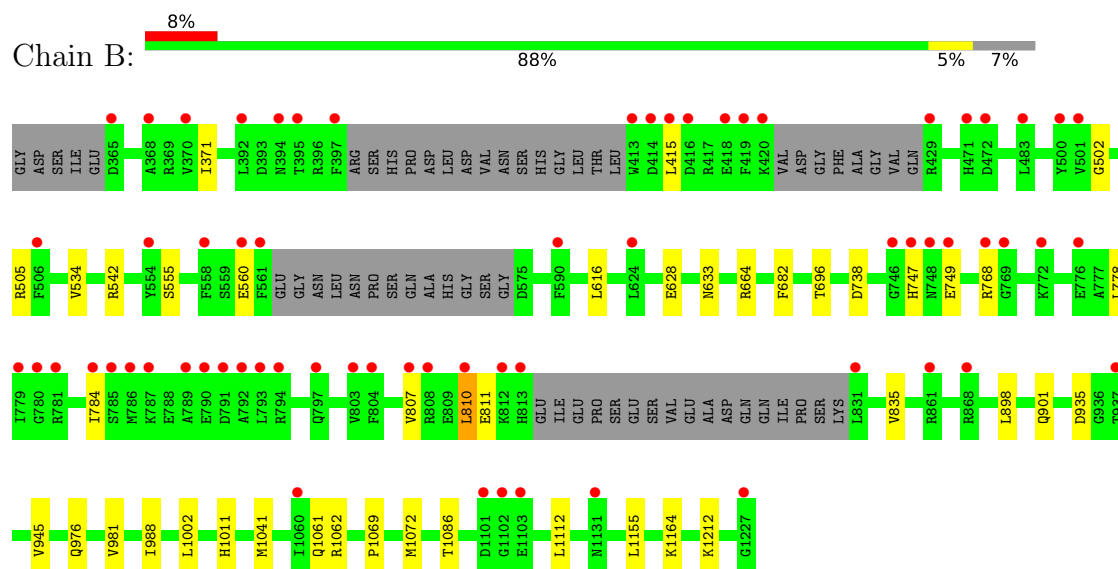
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

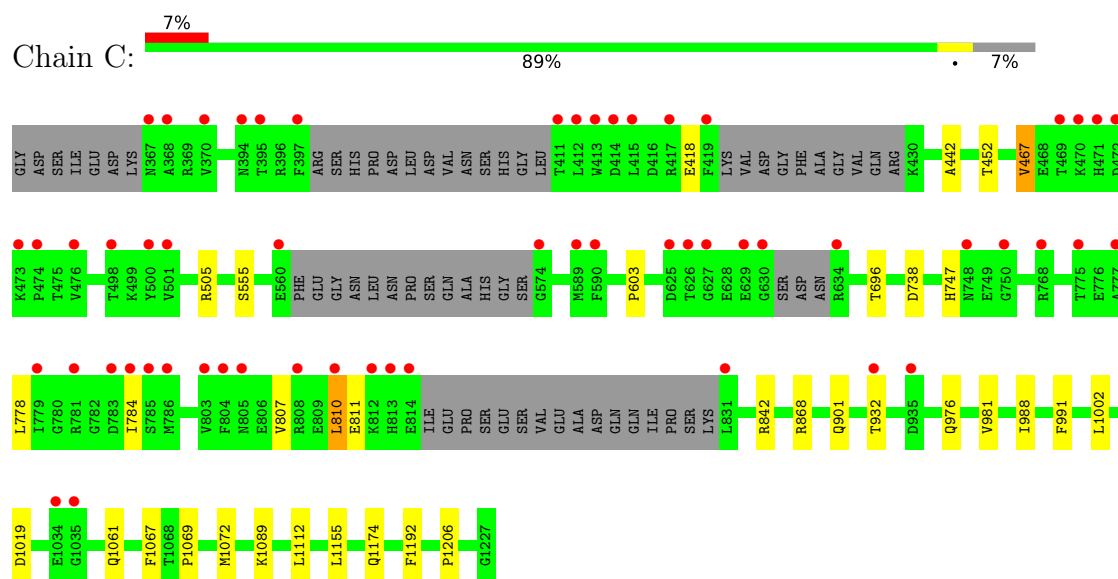
• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



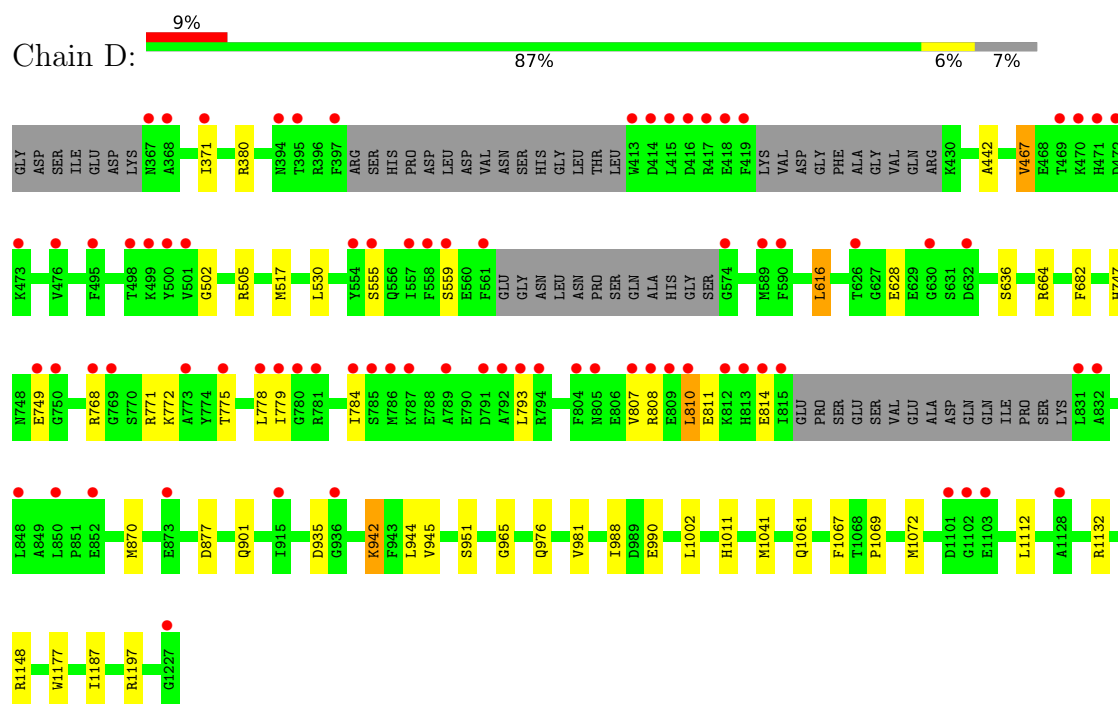
• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



• 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 39.20 – 1.96	Depositor EDS
% Data completeness (in resolution range)	95.2 (39.20-1.96) 94.0 (39.20-1.96)	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 (4.79%)	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)	0.36 , 53.8	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: TPP, MG, CA

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	0.86	2/6425 (0.0%)	1.14	10/8715 (0.1%)
1	B	0.85	0/6371	1.15	3/8645 (0.0%)
1	C	0.85	0/6381	1.13	1/8650 (0.0%)
1	D	0.85	2/6367 (0.0%)	1.15	5/8640 (0.1%)
All	All	0.85	4/25544 (0.0%)	1.14	19/34650 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	870	MET	SD-CE	-6.00	1.64	1.79
1	D	517	MET	SD-CE	-5.83	1.65	1.79
1	A	839	MET	SD-CE	-5.23	1.66	1.79
1	A	1098	MET	SD-CE	-5.16	1.66	1.79

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	682	PHE	CA-CB-CG	6.11	119.91	113.80
1	A	935	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	627	GLY	CA-C-N	5.66	128.17	120.54
1	A	627	GLY	C-N-CA	5.66	128.17	120.54
1	B	935	ASP	CA-CB-CG	5.47	118.07	112.60
1	D	935	ASP	CA-CB-CG	5.39	117.99	112.60
1	D	877	ASP	CA-CB-CG	5.33	117.92	112.60
1	A	1067	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	602	ASN	N-CA-C	5.24	112.94	108.22
1	B	768	ARG	N-CA-C	-5.21	102.03	110.32
1	A	750	GLY	CA-C-N	5.20	128.16	120.82
1	A	750	GLY	C-N-CA	5.20	128.16	120.82
1	C	1067	PHE	CA-CB-CG	-5.18	108.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1105	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	877	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	779	ILE	CA-C-N	5.12	125.77	120.03
1	D	779	ILE	C-N-CA	5.12	125.77	120.03
1	B	633	ASN	CA-CB-CG	5.08	117.68	112.60
1	D	768	ARG	N-CA-C	-5.06	102.27	110.32

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	6295	0	6066	18	0
1	B	6241	0	6017	20	0
1	C	6256	0	6055	16	0
1	D	6238	0	6009	27	0
2	A	26	0	16	1	0
2	B	26	0	16	1	0
2	C	26	0	16	1	0
2	D	26	0	16	1	0
3	A	1	0	0	0	0
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	0	0
5	B	275	0	0	2	0
5	C	338	0	0	0	0
5	D	243	0	0	0	0
All	All	26363	0	24211	79	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 (79) 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: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
1:B:502:GLY:HA2	1:B:749:GLU:CD	2.39	0.47
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:B:1041[B]:MET:HE2	5:B:3246:HOH:O	2.13	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
1:D:502:GLY:HA2	1:D:749:GLU:CD	2.41	0.46
2:A:2001:TPP:H6'	1:B:901:GLN:OE1	2.15	0.46
1:D:749:GLU:CD	1:D:749:GLU:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:555:SER:HA	1:B:810:LEU:HG	2.00	0.43
1:B:1155:LEU:HD13	1:B:1164:LYS:HE2	1.99	0.43
1:A:487:ASN:OD1	1:A:771:ARG:HD2	2.18	0.43
1:B:749:GLU:CD	1:B:749:GLU:H	2.27	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
1:B:696:THR:HG21	1:B:738:ASP:HB2	2.01	0.42
1:B:1011:HIS:HD2	1:B:1041[B]:MET:HE1	1.83	0.42
1:D:807:VAL:O	1:D:811:GLU:HG3	2.18	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:D:1011:HIS:HD2	1:D:1041[A]:MET:HE1	1.85	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
1:A:505:ARG:HA	1:A:747:HIS:O	2.21	0.41
1:A:1011:HIS:HD2	1:A:1041[A]:MET:HE1	1.85	0.41
1:C:1019:ASP:OD1	1:D:990:GLU:OE1	2.39	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: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: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%)	43	36
1	C	794/868 (92%)	778 (98%)	16 (2%)	0	100	100
1	D	800/868 (92%)	783 (98%)	16 (2%)	1 (0%)	48	41
All	All	3200/3472 (92%)	3136 (98%)	61 (2%)	3 (0%)	48	41

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 [i](#)

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%)	641 (99%)	6 (1%)	70	70
1	B	637/726 (88%)	630 (99%)	7 (1%)	65	64
1	C	645/726 (89%)	638 (99%)	7 (1%)	65	64
1	D	640/726 (88%)	629 (98%)	11 (2%)	53	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2569/2904 (88%)	2538 (99%)	31 (1%)	63 61

All (31) 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	950	LEU
1	A	976	GLN
1	A	1112	LEU
1	B	371	ILE
1	B	542	ARG
1	B	560	GLU
1	B	810	LEU
1	B	976	GLN
1	B	1112	LEU
1	B	1212	LYS
1	C	418	GLU
1	C	467	VAL
1	C	810	LEU
1	C	868	ARG
1	C	976	GLN
1	C	1089	LYS
1	C	1112	LEU
1	D	371	ILE
1	D	467	VAL
1	D	616	LEU
1	D	808	ARG
1	D	810	LEU
1	D	942	LYS
1	D	945	VAL
1	D	951	SER
1	D	976	GLN
1	D	1112	LEU
1	D	1132	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	ASN

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Mol	Chain	Res	Type
1	A	748	ASN
1	A	1030	GLN
1	A	1107	ASN
1	B	679	GLN
1	B	748	ASN
1	B	904	GLN
1	B	1001	GLN
1	B	1107	ASN
1	B	1219	GLN
1	C	748	ASN
1	C	933	ASN
1	C	1001	GLN
1	C	1107	ASN
1	C	1219	GLN
1	D	503	GLN
1	D	679	GLN
1	D	747	HIS
1	D	805	ASN
1	D	1001	GLN
1	D	1061	GLN
1	D	1107	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	2001	3	26,27,27	1.21	3 (11%)	38,40,40	1.45	7 (18%)
2	TPP	B	2001	3	26,27,27	1.19	2 (7%)	38,40,40	1.66	12 (31%)
2	TPP	C	2001	3	26,27,27	1.23	2 (7%)	38,40,40	1.53	8 (21%)
2	TPP	D	2001	3	26,27,27	1.23	3 (11%)	38,40,40	1.61	10 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	A	2001	3	-	1/17/17/17	0/2/2/2
2	TPP	B	2001	3	-	0/17/17/17	0/2/2/2
2	TPP	C	2001	3	-	1/17/17/17	0/2/2/2
2	TPP	D	2001	3	-	1/17/17/17	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	TPP	C4-N3	-3.09	1.33	1.39
2	D	2001	TPP	C4-N3	-2.99	1.33	1.39
2	A	2001	TPP	PA-O3A	2.97	1.62	1.59
2	C	2001	TPP	C4-N3	-2.84	1.34	1.39
2	A	2001	TPP	C4-N3	-2.76	1.34	1.39
2	C	2001	TPP	PA-O3A	2.74	1.62	1.59
2	D	2001	TPP	C4'-N4'	2.60	1.40	1.34
2	A	2001	TPP	PB-O1B	2.39	1.57	1.50
2	D	2001	TPP	PB-O1B	2.28	1.57	1.50
2	B	2001	TPP	PB-O1B	2.05	1.56	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	TPP	CM4-C4-C5	-3.83	117.92	127.75
2	A	2001	TPP	CM4-C4-C5	-3.82	117.97	127.75
2	C	2001	TPP	CM4-C4-C5	-3.72	118.22	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	TPP	C2-S1-C5	-3.68	88.78	91.22
2	B	2001	TPP	CM4-C4-C5	-3.60	118.52	127.75
2	C	2001	TPP	C6'-N1'-C2'	3.50	121.81	116.07
2	B	2001	TPP	C6'-N1'-C2'	3.30	121.50	116.07
2	B	2001	TPP	N1'-C2'-N3'	-3.11	120.35	125.53
2	D	2001	TPP	C6'-N1'-C2'	3.07	121.12	116.07
2	A	2001	TPP	C7-C6-C5	-2.78	104.00	112.73
2	C	2001	TPP	C7-C6-C5	-2.77	104.03	112.73
2	A	2001	TPP	C6'-N1'-C2'	2.72	120.53	116.07
2	D	2001	TPP	C2-S1-C5	-2.69	89.43	91.22
2	D	2001	TPP	C5'-C6'-N1'	-2.68	119.48	123.83
2	B	2001	TPP	C5'-C6'-N1'	-2.66	119.50	123.83
2	D	2001	TPP	N1'-C2'-N3'	-2.66	121.11	125.53
2	C	2001	TPP	N1'-C2'-N3'	-2.65	121.12	125.53
2	C	2001	TPP	C5'-C6'-N1'	-2.61	119.58	123.83
2	B	2001	TPP	C7-C6-C5	-2.59	104.59	112.73
2	A	2001	TPP	N1'-C2'-N3'	-2.49	121.39	125.53
2	D	2001	TPP	C7-C6-C5	-2.41	105.17	112.73
2	C	2001	TPP	O2A-PA-O3A	2.38	113.70	107.27
2	A	2001	TPP	C5-C4-N3	2.30	115.86	111.67
2	D	2001	TPP	CM4-C4-N3	2.29	125.84	120.57
2	A	2001	TPP	CM4-C4-N3	2.28	125.83	120.57
2	B	2001	TPP	O2A-PA-O3A	2.28	113.43	107.27
2	B	2001	TPP	CM4-C4-N3	2.27	125.81	120.57
2	C	2001	TPP	C5-C4-N3	2.26	115.78	111.67
2	D	2001	TPP	C5-C4-N3	2.24	115.75	111.67
2	D	2001	TPP	O2A-PA-O3A	2.22	113.28	107.27
2	C	2001	TPP	CM4-C4-N3	2.22	125.69	120.57
2	B	2001	TPP	C2'-N3'-C4'	2.14	121.39	118.10
2	D	2001	TPP	C2'-N3'-C4'	2.14	121.39	118.10
2	B	2001	TPP	CM2-C2'-N3'	2.06	120.22	117.13
2	B	2001	TPP	CM2-C2'-N1'	2.05	119.38	117.20
2	A	2001	TPP	C4-C5-S1	-2.02	107.41	110.56
2	B	2001	TPP	C5-C4-N3	2.01	115.33	111.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

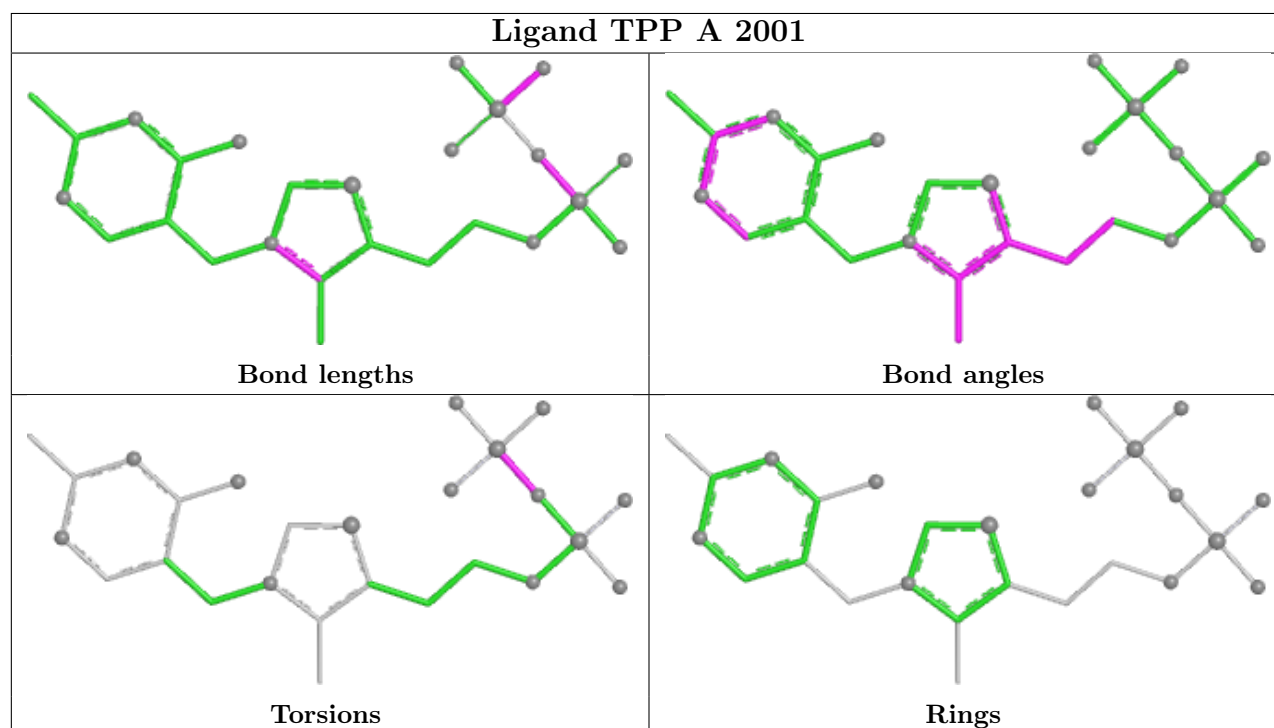
Mol	Chain	Res	Type	Atoms
2	A	2001	TPP	PA-O3A-PB-O3B
2	C	2001	TPP	PA-O3A-PB-O3B
2	D	2001	TPP	PA-O3A-PB-O3B

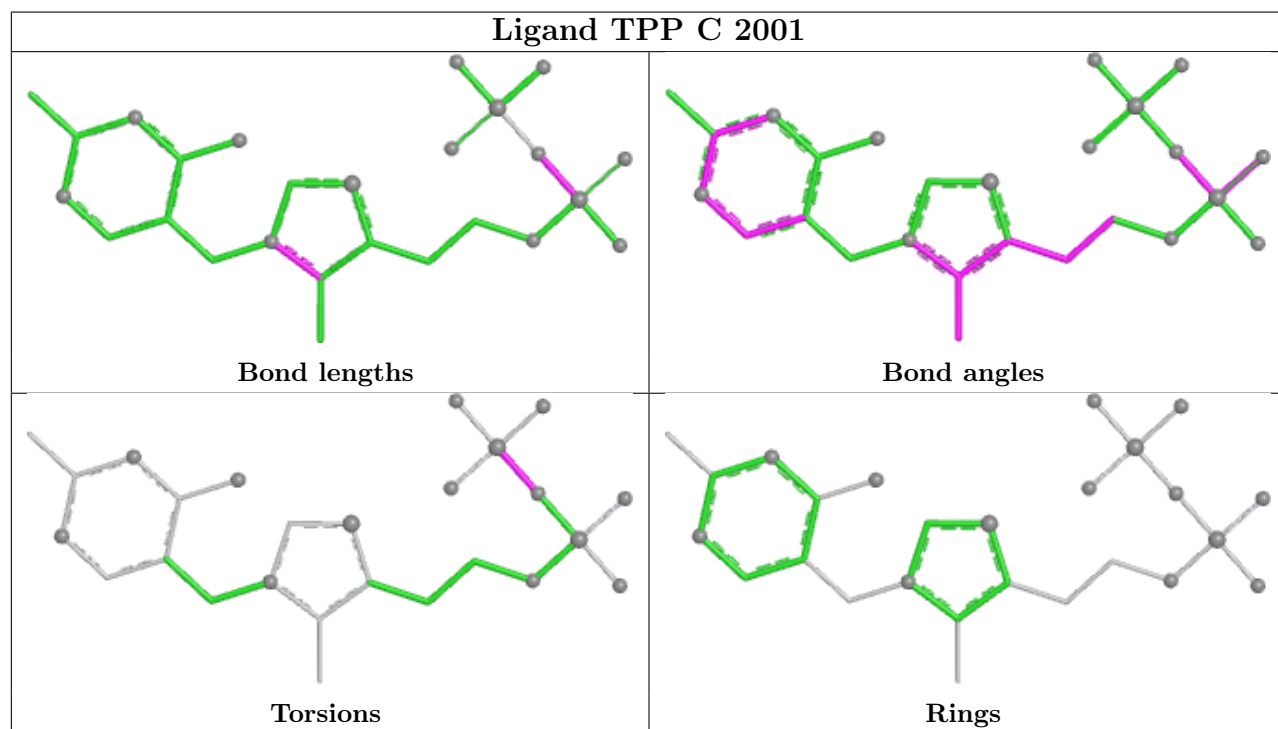
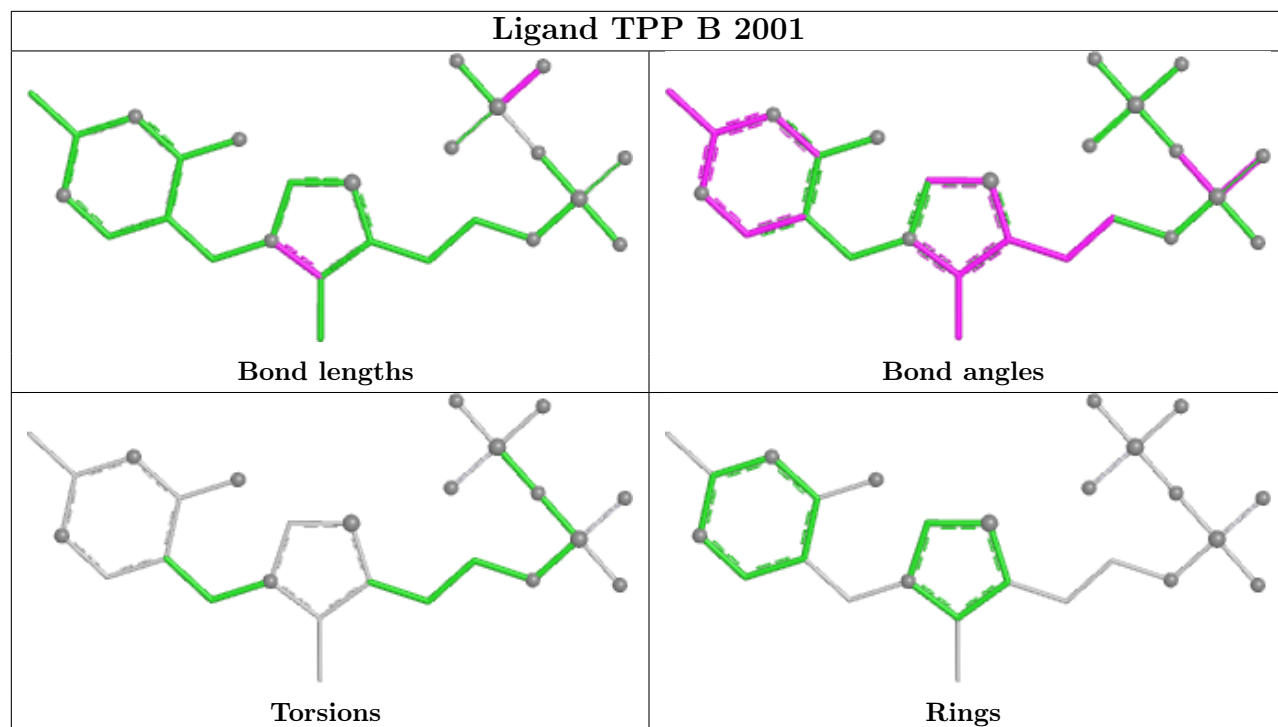
There are no ring outliers.

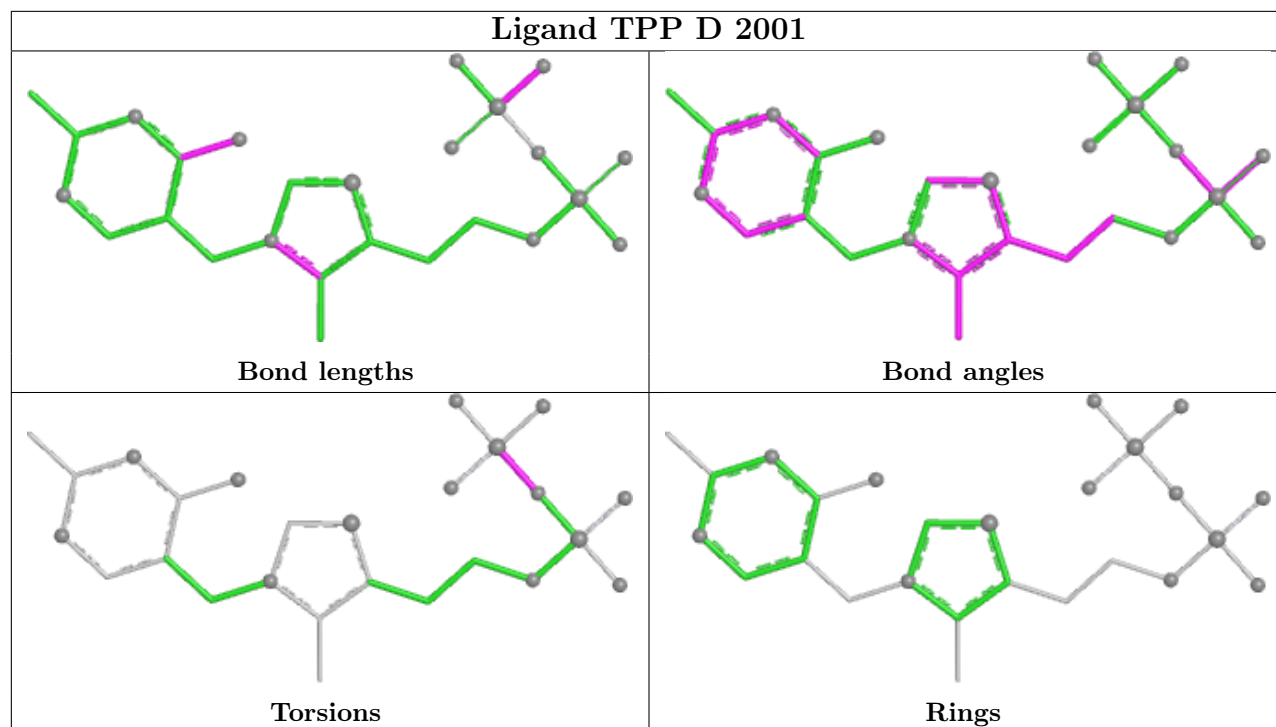
4 monomers are involved in 4 short contacts:

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







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.30	52 (6%)	25 29	10, 24, 52, 90	1 (0%)
1	B	810/868 (93%)	0.48	66 (8%)	18 21	12, 26, 57, 106	1 (0%)
1	C	806/868 (92%)	0.30	57 (7%)	22 25	11, 24, 55, 76	0
1	D	809/868 (93%)	0.58	78 (9%)	13 15	12, 27, 59, 92	1 (0%)
All	All	3239/3472 (93%)	0.42	253 (7%)	19 22	10, 25, 56, 106	3 (0%)

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	397	PHE	9.2
1	D	815	ILE	8.4
1	D	413	TRP	8.2
1	D	414	ASP	8.0
1	A	411	THR	7.8
1	C	630	GLY	6.8
1	C	411	THR	6.7
1	A	413	TRP	6.6
1	B	561	PHE	6.3
1	C	413	TRP	6.3
1	D	394	ASN	6.3
1	C	574	GLY	6.0
1	D	419	PHE	5.7
1	B	397	PHE	5.6
1	B	420	LYS	5.5
1	A	399	SER	5.4
1	D	415	LEU	5.3
1	B	813	HIS	5.2
1	B	394	ASN	5.2
1	D	561	PHE	5.1
1	B	414	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	419	PHE	5.0
1	B	780	GLY	5.0
1	B	416	ASP	4.7
1	B	793	LEU	4.6
1	B	415	LEU	4.5
1	B	501	VAL	4.5
1	B	792	ALA	4.4
1	A	590	PHE	4.3
1	C	627	GLY	4.3
1	B	365	ASP	4.2
1	D	809	GLU	4.2
1	A	412	LEU	4.2
1	C	560	GLU	4.2
1	D	813	HIS	4.1
1	C	626	THR	4.1
1	D	831	LEU	4.1
1	D	1227	GLY	4.1
1	C	590	PHE	4.0
1	D	416	ASP	4.0
1	D	784	ILE	4.0
1	C	397	PHE	4.0
1	D	367	ASN	3.9
1	B	787	LYS	3.9
1	B	395	THR	3.9
1	D	779	ILE	3.8
1	D	499	LYS	3.8
1	B	786	MET	3.8
1	B	831	LEU	3.8
1	A	813	HIS	3.7
1	C	831	LEU	3.6
1	D	559	SER	3.6
1	C	750	GLY	3.6
1	D	775	THR	3.6
1	D	785	SER	3.6
1	D	786	MET	3.6
1	A	499	LYS	3.6
1	B	418	GLU	3.6
1	C	367	ASN	3.5
1	A	750	GLY	3.5
1	B	1227	GLY	3.5
1	D	574	GLY	3.5
1	B	413	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	790	GLU	3.5
1	D	780	GLY	3.5
1	D	793	LEU	3.5
1	D	473	LYS	3.5
1	B	560	GLU	3.4
1	B	791	ASP	3.4
1	C	412	LEU	3.4
1	D	472	ASP	3.4
1	B	781	ARG	3.4
1	D	501	VAL	3.4
1	D	792	ALA	3.4
1	A	831	LEU	3.4
1	B	794	ARG	3.4
1	D	371	ILE	3.4
1	A	562	GLU	3.3
1	A	561	PHE	3.3
1	D	469	THR	3.3
1	B	785	SER	3.3
1	B	747	HIS	3.3
1	B	789	ALA	3.3
1	D	471	HIS	3.2
1	A	368	ALA	3.2
1	D	804	PHE	3.2
1	B	779	ILE	3.2
1	A	471	HIS	3.2
1	C	471	HIS	3.2
1	D	1103	GLU	3.2
1	D	769	GLY	3.1
1	B	1102	GLY	3.1
1	D	807	VAL	3.1
1	B	558	PHE	3.1
1	D	590	PHE	3.1
1	C	368	ALA	3.1
1	D	368	ALA	3.1
1	C	625	ASP	3.1
1	A	470	LYS	3.1
1	B	429	ARG	3.1
1	D	810	LEU	3.0
1	C	589	MET	3.0
1	C	629	GLU	3.0
1	B	810	LEU	3.0
1	D	395	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	812	LYS	3.0
1	D	1128	ALA	3.0
1	D	500	TYR	2.9
1	D	812	LYS	2.9
1	A	591	GLY	2.9
1	A	786	MET	2.9
1	A	472	ASP	2.9
1	D	778	LEU	2.9
1	D	749	GLU	2.9
1	C	501	VAL	2.9
1	C	777	ALA	2.8
1	B	1103	GLU	2.8
1	A	397	PHE	2.8
1	A	631	SER	2.8
1	C	785	SER	2.8
1	D	418	GLU	2.8
1	B	590	PHE	2.8
1	A	415	LEU	2.8
1	D	873	GLU	2.8
1	B	769	GLY	2.7
1	C	634	ARG	2.7
1	D	808	ARG	2.7
1	A	812	LYS	2.7
1	C	469	THR	2.7
1	D	417	ARG	2.7
1	D	470	LYS	2.7
1	C	500	TYR	2.7
1	D	750	GLY	2.7
1	D	1101	ASP	2.7
1	B	807	VAL	2.7
1	B	500	TYR	2.6
1	B	776	GLU	2.6
1	A	625	ASP	2.6
1	B	808	ARG	2.6
1	B	768	ARG	2.6
1	D	791	ASP	2.6
1	C	414	ASP	2.6
1	B	370	VAL	2.6
1	D	555	SER	2.6
1	B	861	ARG	2.5
1	D	554	TYR	2.5
1	C	786	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1034	GLU	2.5
1	B	772	LYS	2.5
1	C	394	ASN	2.5
1	A	395	THR	2.5
1	B	937	THR	2.5
1	C	775	THR	2.5
1	D	781	ARG	2.5
1	C	814	GLU	2.5
1	A	419	PHE	2.5
1	A	558	PHE	2.5
1	C	779	ILE	2.5
1	B	368	ALA	2.5
1	D	832	ALA	2.5
1	A	501	VAL	2.5
1	D	589	MET	2.5
1	C	810	LEU	2.5
1	D	1102	GLY	2.5
1	A	498	THR	2.5
1	C	395	THR	2.5
1	C	935	ASP	2.5
1	C	768	ARG	2.4
1	A	810	LEU	2.4
1	B	804	PHE	2.4
1	C	419	PHE	2.4
1	D	558	PHE	2.4
1	D	557	ILE	2.4
1	C	781	ARG	2.4
1	B	554	TYR	2.4
1	A	366	LYS	2.4
1	A	398	ARG	2.4
1	C	805	ASN	2.4
1	C	804	PHE	2.3
1	B	1060	ILE	2.3
1	D	789	ALA	2.3
1	C	476	VAL	2.3
1	A	414	ASP	2.3
1	D	632	ASP	2.3
1	B	624	LEU	2.3
1	C	784	ILE	2.3
1	D	787	LYS	2.3
1	D	768	ARG	2.3
1	B	803	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	476	VAL	2.3
1	B	471	HIS	2.3
1	B	472	ASP	2.3
1	C	803	VAL	2.3
1	D	848	LEU	2.3
1	A	782	GLY	2.2
1	B	749	GLU	2.2
1	C	783	ASP	2.2
1	C	417	ARG	2.2
1	C	498	THR	2.2
1	C	1035	GLY	2.2
1	B	1101	ASP	2.2
1	C	808	ARG	2.2
1	C	370	VAL	2.2
1	B	392	LEU	2.2
1	A	1035	GLY	2.2
1	A	429	ARG	2.2
1	A	781	ARG	2.2
1	C	748	ASN	2.2
1	A	473	LYS	2.2
1	C	470	LYS	2.2
1	C	812	LYS	2.2
1	D	794	ARG	2.2
1	D	805	ASN	2.1
1	A	576	VAL	2.1
1	A	555	SER	2.1
1	D	630	GLY	2.1
1	B	483	LEU	2.1
1	B	784	ILE	2.1
1	A	469	THR	2.1
1	D	626	THR	2.1
1	A	627	GLY	2.1
1	D	814	GLU	2.1
1	C	415	LEU	2.1
1	B	797	GLN	2.1
1	B	506	PHE	2.1
1	A	784	ILE	2.1
1	A	791	ASP	2.1
1	A	915	ILE	2.1
1	C	472	ASP	2.1
1	A	559	SER	2.1
1	A	868	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	811	GLU	2.1
1	C	932	THR	2.1
1	D	498	THR	2.1
1	D	852	GLU	2.1
1	D	936	GLY	2.1
1	A	589	MET	2.1
1	C	813	HIS	2.1
1	B	748	ASN	2.1
1	B	1131	ASN	2.1
1	A	390	LEU	2.1
1	A	575	ASP	2.1
1	A	505	ARG	2.1
1	A	768	ARG	2.1
1	B	868	ARG	2.1
1	C	473	LYS	2.0
1	C	474	PRO	2.0
1	A	778	LEU	2.0
1	D	850	LEU	2.0
1	D	773	ALA	2.0
1	D	495	PHE	2.0
1	D	915	ILE	2.0
1	B	746	GLY	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 oligosaccharides 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.

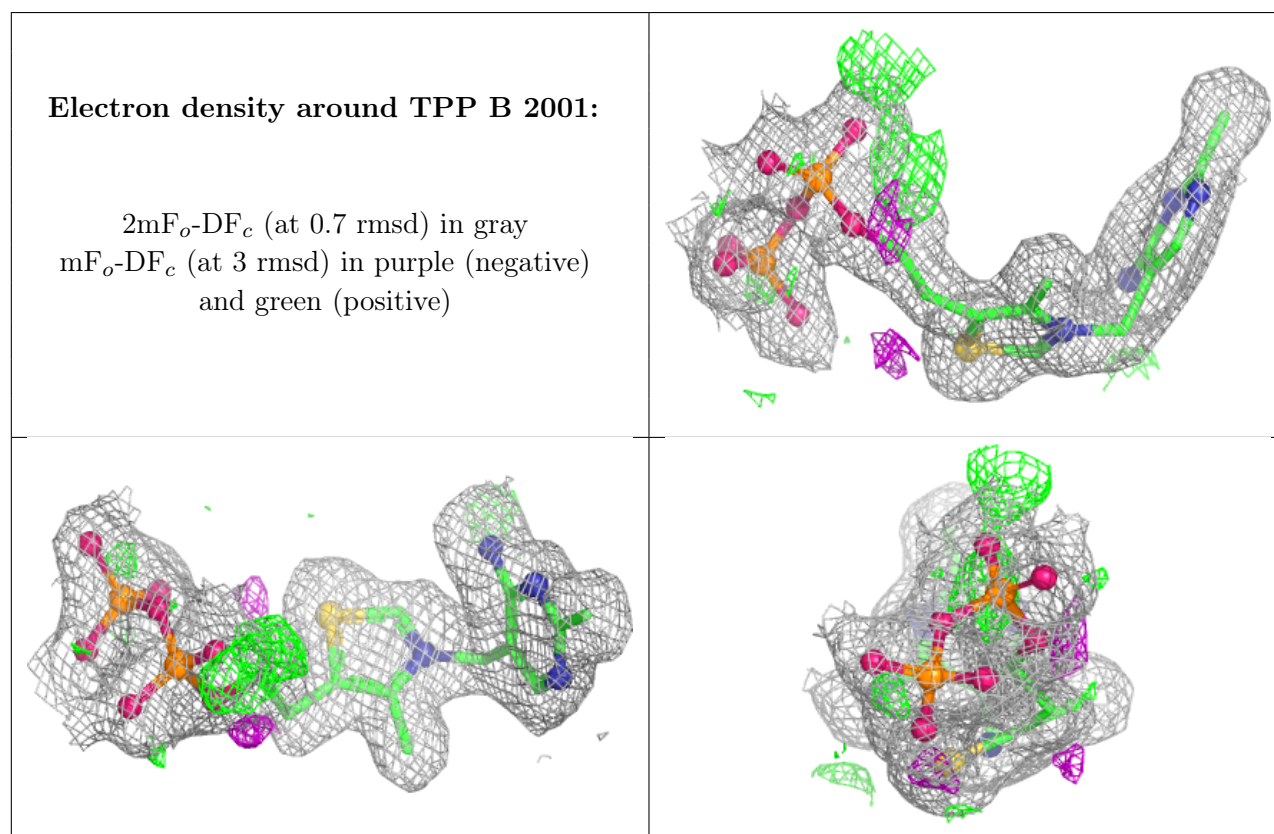
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TPP	B	2001	26/26	0.97	0.07	10,15,19,22	0

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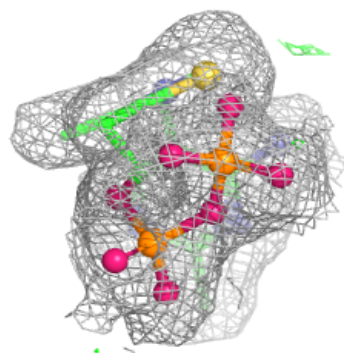
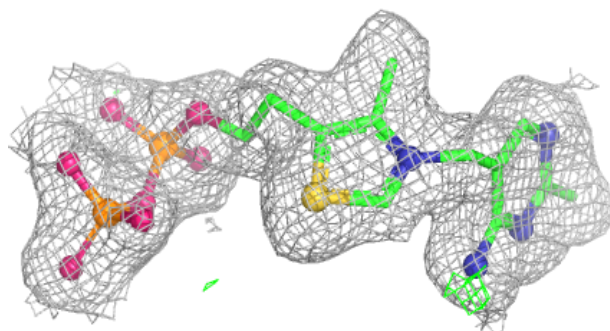
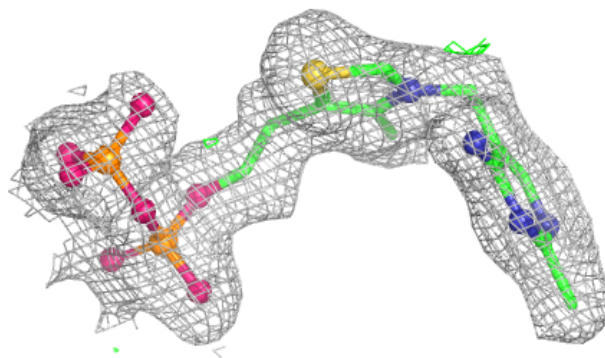
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TPP	A	2001	26/26	0.98	0.05	13,18,20,23	0
2	TPP	C	2001	26/26	0.98	0.06	10,16,20,23	0
2	TPP	D	2001	26/26	0.98	0.05	12,16,20,23	0
3	MG	A	2002	1/1	0.98	0.04	10,10,10,10	0
3	MG	B	2002	1/1	0.98	0.05	11,11,11,11	0
3	MG	C	2002	1/1	0.99	0.04	10,10,10,10	0
3	MG	D	2002	1/1	0.99	0.06	12,12,12,12	0
4	CA	B	2003	1/1	0.99	0.03	23,23,23,23	0
4	CA	C	2003	1/1	0.99	0.03	20,20,20,20	0
4	CA	D	2003	1/1	0.99	0.02	25,25,25,25	0
4	CA	A	2003	1/1	1.00	0.02	20,20,20,20	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.

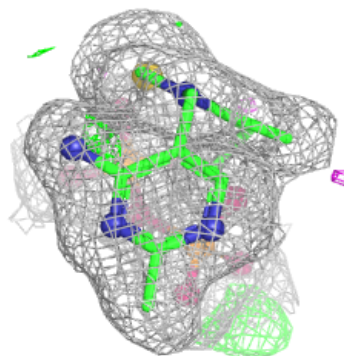
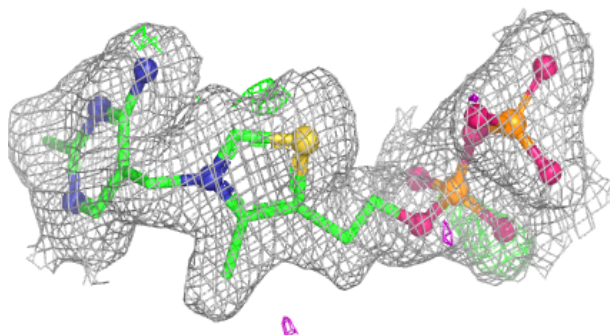
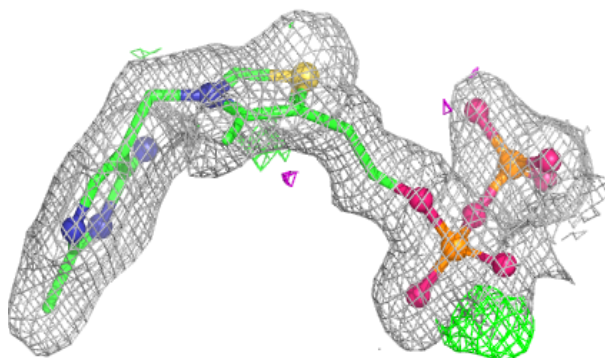


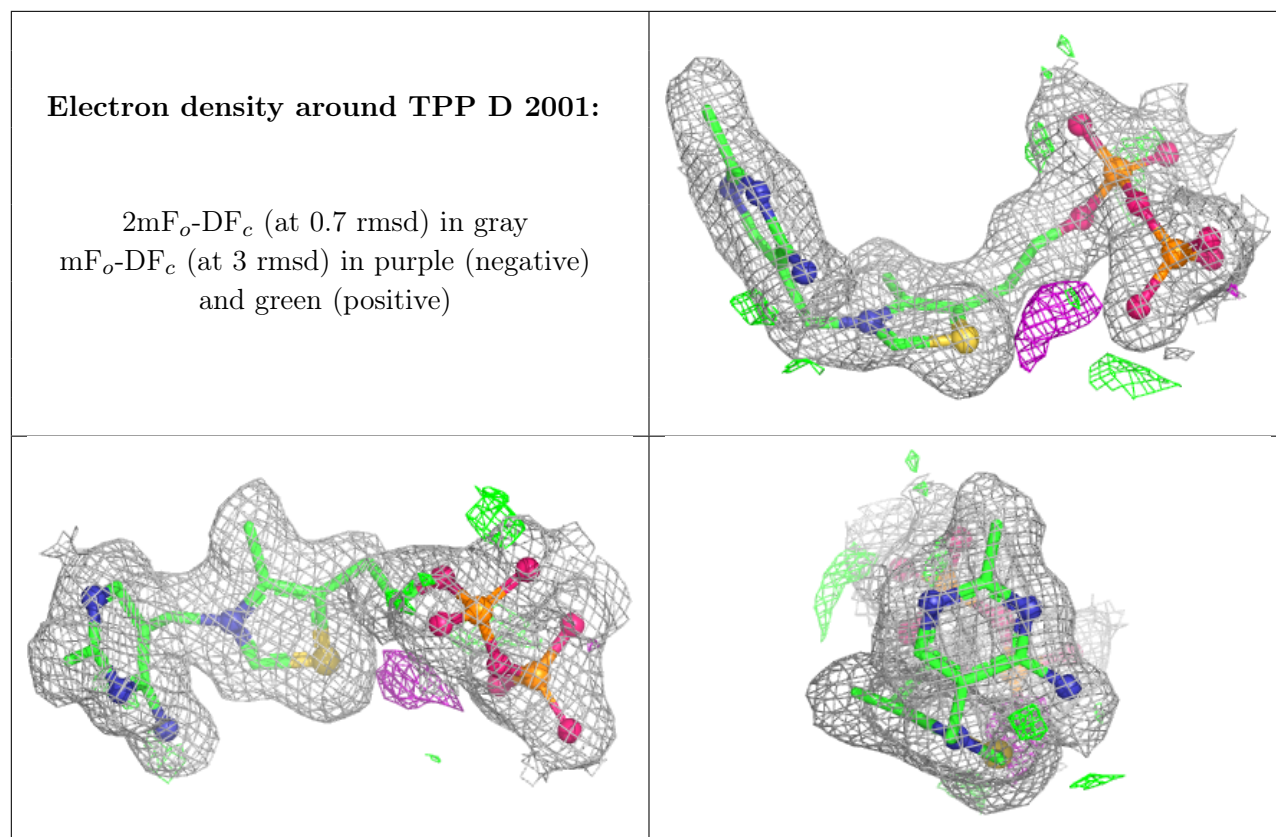
Electron density around TPP A 2001:

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

**Electron density around TPP C 2001:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.