



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:22 PM UTC

PDB ID : 2XT6 / pdb_00002xt6
Title : Crystal structure of Mycobacterium smegmatis alpha-ketoglutarate decarboxylase homodimer (orthorhombic form)
Authors : Wagner, T.; Bellinzoni, M.; Wehenkel, A.M.; O'Hare, H.M.; Alzari, P.M.
Deposited on : 2010-10-05
Resolution : 2.74 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

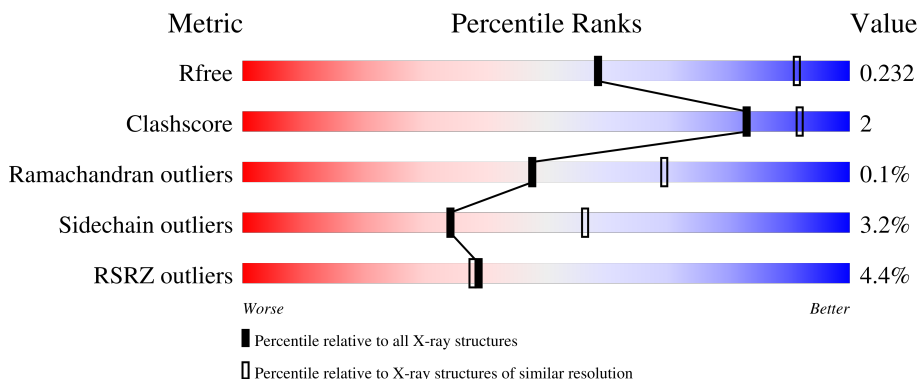
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	1113	 86% 8% • 5%
1	B	1113	 79% 9% • 11%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15902 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.

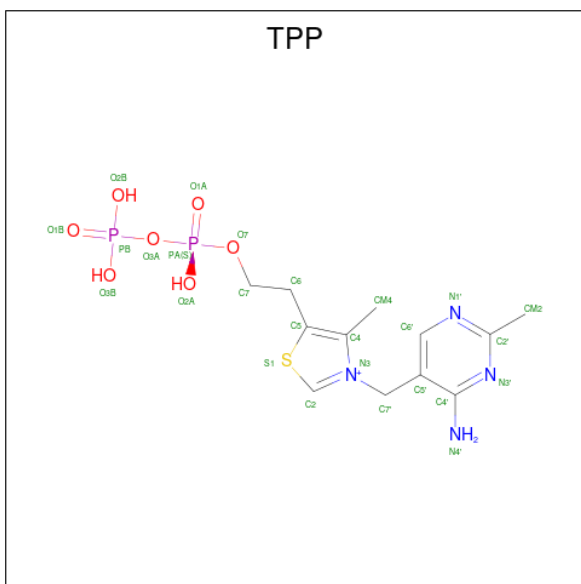
- Molecule 1 is a protein called 2-OXOGLUTARATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1055	8153	5136	1447	1540	30	0	0	0
1	B	989	7574	4776	1342	1429	27	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	GLY	-	expression tag	UNP A0R2B1
B	115	GLY	-	expression tag	UNP A0R2B1

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

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

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

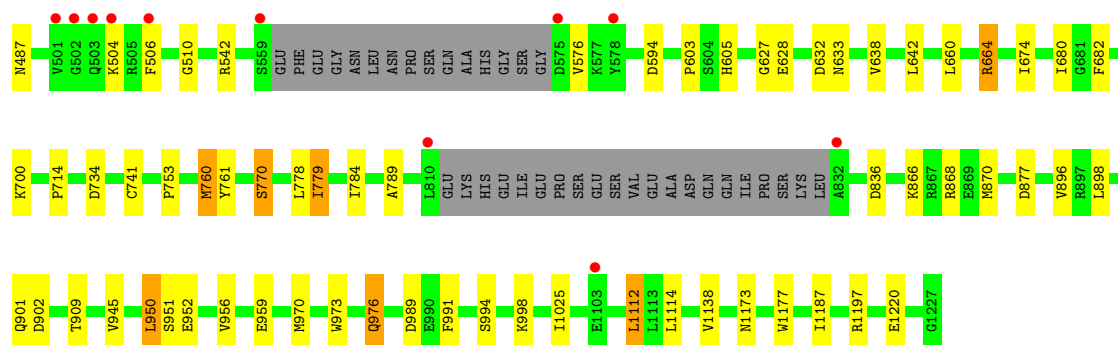
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	63	Total	O	0	0
			63	63		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.99Å 247.72Å 79.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.12 – 2.74 40.12 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.12-2.74) 99.1 (40.12-2.74)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.73Å)	Xtrriage
Refinement program	BUSTER-TNT 2.9.3	Depositor
R, R_{free}	0.185 , 0.224 0.193 , 0.232	Depositor DCC
R_{free} test set	4027 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtrriage
Anisotropy	0.620	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15902	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, TPP, MG

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	2/8319 (0.0%)	1.32	33/11288 (0.3%)
1	B	0.88	2/7721 (0.0%)	1.34	40/10472 (0.4%)
All	All	0.87	4/16040 (0.0%)	1.33	73/21760 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	760	MET	SD-CE	-6.62	1.63	1.79
1	A	384	MET	SD-CE	6.53	1.95	1.79
1	A	760	MET	SD-CE	-5.96	1.64	1.79
1	B	384	MET	SD-CE	5.32	1.92	1.79

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	594	ASP	CA-CB-CG	7.61	120.21	112.60
1	A	306	ILE	N-CA-CB	7.27	119.72	110.99
1	A	836	ASP	CA-CB-CG	6.73	119.33	112.60
1	B	836	ASP	CA-CB-CG	6.53	119.13	112.60
1	A	877	ASP	CA-CB-CG	6.36	118.96	112.60
1	B	329	ILE	CA-C-N	6.28	129.02	120.54
1	B	329	ILE	C-N-CA	6.28	129.02	120.54
1	B	877	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	313	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	989	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	1186	GLU	CA-C-N	6.02	128.15	120.56
1	A	1186	GLU	C-N-CA	6.02	128.15	120.56
1	A	335	ASP	CA-C-N	6.02	128.26	120.44
1	A	335	ASP	C-N-CA	6.02	128.26	120.44
1	A	645	ASP	CA-CB-CG	5.90	118.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	VAL	N-CA-C	5.89	114.31	107.89
1	A	1147	PRO	CA-C-N	5.87	129.63	120.82
1	A	1147	PRO	C-N-CA	5.87	129.63	120.82
1	B	989	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	700	LYS	CA-C-N	5.81	128.33	120.38
1	B	700	LYS	C-N-CA	5.81	128.33	120.38
1	B	638	VAL	N-CA-C	5.75	114.16	107.89
1	B	504	LYS	CA-C-N	5.74	128.54	120.28
1	B	504	LYS	C-N-CA	5.74	128.54	120.28
1	A	700	LYS	CA-C-N	5.72	128.22	120.38
1	A	700	LYS	C-N-CA	5.72	128.22	120.38
1	A	734	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	394	ASN	CA-C-N	5.62	128.58	120.38
1	A	394	ASN	C-N-CA	5.62	128.58	120.38
1	B	336	ASP	CA-C-N	5.55	128.49	120.38
1	B	336	ASP	C-N-CA	5.55	128.49	120.38
1	B	734	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	441	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	594	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	677	ASN	CA-CB-CG	5.48	118.08	112.60
1	B	632	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	1025	ILE	CA-C-N	5.39	128.26	120.38
1	A	1025	ILE	C-N-CA	5.39	128.26	120.38
1	B	1025	ILE	CA-C-N	5.35	128.19	120.38
1	B	1025	ILE	C-N-CA	5.35	128.19	120.38
1	B	195	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	1173	ASN	CA-CB-CG	5.33	117.93	112.60
1	B	458	GLU	CB-CG-CD	5.32	121.64	112.60
1	A	632	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	394	ASN	CA-C-N	5.27	128.08	120.38
1	B	394	ASN	C-N-CA	5.27	128.08	120.38
1	B	1173	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	660	LEU	CA-C-N	5.22	128.66	120.82
1	A	660	LEU	C-N-CA	5.22	128.66	120.82
1	B	386	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	976	GLN	N-CA-C	-5.21	105.50	111.07
1	B	138	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	770	SER	CA-C-N	5.19	127.19	120.44
1	B	770	SER	C-N-CA	5.19	127.19	120.44
1	A	1179	SER	CA-C-N	5.18	127.22	120.28
1	A	1179	SER	C-N-CA	5.18	127.22	120.28
1	A	542	ARG	N-CA-C	5.16	116.59	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	HIS	CA-C-N	5.16	127.19	120.28
1	B	330	HIS	C-N-CA	5.16	127.19	120.28
1	B	542	ARG	N-CA-C	5.15	116.58	111.07
1	A	395	THR	CA-C-N	5.14	127.43	120.38
1	A	395	THR	C-N-CA	5.14	127.43	120.38
1	B	487	ASN	CA-CB-CG	5.14	117.75	112.60
1	B	660	LEU	CA-C-N	5.13	128.52	120.82
1	B	660	LEU	C-N-CA	5.13	128.52	120.82
1	B	976	GLN	N-CA-C	-5.10	105.63	111.14
1	B	779	ILE	CA-C-N	5.07	125.61	119.98
1	B	779	ILE	C-N-CA	5.07	125.61	119.98
1	A	441	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	423	GLY	CA-C-N	5.04	126.99	120.44
1	B	423	GLY	C-N-CA	5.04	126.99	120.44
1	B	627	GLY	CA-C-N	5.01	126.96	120.44
1	B	627	GLY	C-N-CA	5.01	126.96	120.44

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	8153	0	7892	36	0
1	B	7574	0	7289	40	0
2	A	26	0	16	2	0
2	B	26	0	16	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	56	0	0	0	0
5	B	63	0	0	0	0
All	All	15902	0	15213	74	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 (74) 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:779:ILE:HD11	1:B:789:ALA:HB2	1.49	0.94
1:A:779:ILE:HD11	1:A:789:ALA:HB2	1.51	0.92
1:A:642:LEU:HD22	1:A:674:ILE:HB	1.75	0.68
1:B:642:LEU:HD22	1:B:674:ILE:HB	1.75	0.68
1:B:680:ILE:HD12	1:B:760:MET:HE1	1.76	0.67
1:A:416:ASP:CG	1:A:433:ARG:HH12	2.03	0.65
1:A:1095:GLU:OE1	1:A:1106:ARG:NH1	2.30	0.64
1:B:778:LEU:HB3	1:B:784:ILE:HG12	1.80	0.64
1:A:778:LEU:HB3	1:A:784:ILE:HG12	1.80	0.63
1:A:779:ILE:HD11	1:A:789:ALA:CB	2.27	0.63
1:B:779:ILE:HD11	1:B:789:ALA:CB	2.26	0.63
1:A:133:ALA:HB2	1:A:306:ILE:HG13	1.83	0.60
1:A:683:THR:HB	1:B:902:ASP:OD1	2.01	0.60
1:B:225:GLY:H	1:B:345:GLU:HG2	1.65	0.60
1:A:225:GLY:H	1:A:345:GLU:CG	2.18	0.57
1:B:952:GLU:O	1:B:956:VAL:HG23	2.06	0.56
1:A:952:GLU:O	1:A:956:VAL:HG23	2.06	0.55
1:A:523:ASP:OD2	1:A:722:ARG:NH2	2.39	0.55
1:A:225:GLY:H	1:A:345:GLU:HG2	1.72	0.54
1:B:133:ALA:CB	1:B:306:ILE:HD12	2.39	0.52
1:A:1093:VAL:HB	1:A:1150:ARG:HD3	1.92	0.51
1:B:132:PRO:HD2	1:B:330:HIS:NE2	2.26	0.51
1:B:1112:LEU:HD11	1:B:1138:VAL:HG23	1.92	0.51
1:A:603:PRO:HD3	1:A:991:PHE:CZ	2.46	0.51
1:B:603:PRO:HD3	1:B:991:PHE:CZ	2.46	0.51
1:B:680:ILE:HD12	1:B:760:MET:CE	2.41	0.50
1:A:161:LEU:HD21	1:A:308:LEU:HD21	1.92	0.50
1:B:131:ILE:HD12	1:B:308:LEU:HD12	1.93	0.50
1:A:397:PHE:O	1:A:398:ARG:HD2	2.11	0.50
1:B:133:ALA:HB3	1:B:306:ILE:HD12	1.93	0.50
1:B:441:ASP:HA	1:B:445:ARG:HG3	1.93	0.50
1:B:340:ASP:O	1:B:344:ARG:HG2	2.11	0.49
1:B:510:GLY:O	1:B:741:CYS:HB2	2.11	0.49
1:A:901:GLN:OE1	2:B:2001:TPP:H6'	2.13	0.49
1:A:898:LEU:O	1:A:945:VAL:HA	2.13	0.48
2:A:2001:TPP:HM43	1:B:950:LEU:HD11	1.96	0.48
1:B:215:ALA:HB2	1:B:251:VAL:HG22	1.95	0.48
1:A:959:GLU:HG3	1:A:973:TRP:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:GLY:O	1:B:308:LEU:HD23	2.13	0.48
1:A:169:VAL:HG13	1:A:176:ASN:HB2	1.96	0.47
1:B:898:LEU:O	1:B:945:VAL:HA	2.15	0.47
1:B:959:GLU:HG3	1:B:973:TRP:HB2	1.96	0.46
1:B:225:GLY:HA2	1:B:228:ILE:HD12	1.95	0.46
1:B:753:PRO:HB2	1:B:761:TYR:CE2	2.50	0.46
1:A:363:ILE:H	1:A:363:ILE:HD12	1.81	0.46
1:B:363:ILE:H	1:B:363:ILE:HD12	1.80	0.46
1:B:476:VAL:HG12	1:B:480:LYS:HD2	1.97	0.45
1:B:337:ASP:HA	1:B:340:ASP:HB2	1.98	0.45
1:A:460:GLN:NE2	1:B:380:ARG:HH11	2.14	0.44
1:A:446:HIS:ND1	1:A:713:ASP:OD2	2.51	0.44
1:A:994:SER:HB2	1:A:998:LYS:HE2	2.00	0.43
1:B:224:PHE:O	1:B:228:ILE:HG13	2.18	0.43
1:A:753:PRO:HB2	1:A:761:TYR:CE2	2.54	0.43
1:A:225:GLY:H	1:A:345:GLU:HG3	1.84	0.43
1:B:486:LEU:HD11	1:B:714:PRO:HG3	1.99	0.43
1:A:486:LEU:HD11	1:A:714:PRO:HG3	2.01	0.42
1:A:161:LEU:HD11	1:A:308:LEU:HD11	2.00	0.42
1:B:628:GLU:HG2	1:B:664:ARG:O	2.19	0.42
1:A:628:GLU:HG2	1:A:664:ARG:O	2.20	0.42
2:A:2001:TPP:H6'	1:B:901:GLN:OE1	2.20	0.42
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.56	0.41
1:B:896:VAL:HG22	1:B:970:MET:HB3	2.02	0.41
1:A:384:MET:HE2	1:A:384:MET:HB3	1.97	0.41
1:B:129:ARG:NH2	1:B:327:ARG:HD3	2.34	0.41
1:A:539:HIS:CD2	1:A:539:HIS:H	2.37	0.41
1:B:994:SER:HB2	1:B:998:LYS:HE2	2.02	0.41
1:A:950:LEU:HD11	2:B:2001:TPP:HM43	2.03	0.41
1:A:189:ILE:O	1:A:191:PRO:HD3	2.21	0.40
1:A:122:VAL:O	1:A:124:THR:HG23	2.21	0.40
1:B:146:HIS:CD2	1:B:348:ILE:HG12	2.56	0.40
1:B:605:HIS:HA	2:B:2001:TPP:HM23	2.03	0.40
1:B:866:LYS:HE3	1:B:870:MET:HE3	2.03	0.40
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.57	0.40
1:A:1187:ILE:HG22	1:A:1188:LEU:HG	2.03	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	1045/1113 (94%)	1010 (97%)	34 (3%)	1 (0%)	48 69
1	B	973/1113 (87%)	938 (96%)	33 (3%)	2 (0%)	43 62
All	All	2018/2226 (91%)	1948 (96%)	67 (3%)	3 (0%)	48 69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	399	SER
1	A	682	PHE
1	B	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	838/926 (90%)	811 (97%)	27 (3%)	34 56
1	B	767/926 (83%)	742 (97%)	25 (3%)	33 55
All	All	1605/1852 (87%)	1553 (97%)	52 (3%)	34 56

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	THR
1	A	161	LEU
1	A	198	LEU

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Mol	Chain	Res	Type
1	A	233	ASP
1	A	234	ILE
1	A	253	ILE
1	A	293	SER
1	A	295	GLU
1	A	300	LEU
1	A	306	ILE
1	A	308	LEU
1	A	316	ILE
1	A	341	GLU
1	A	394	ASN
1	A	467	VAL
1	A	471	HIS
1	A	664	ARG
1	A	740	LEU
1	A	781	ARG
1	A	805	ASN
1	A	950	LEU
1	A	951	SER
1	A	976	GLN
1	A	1112	LEU
1	A	1114	LEU
1	A	1188	LEU
1	A	1220	GLU
1	B	158	THR
1	B	212	VAL
1	B	228	ILE
1	B	234	ILE
1	B	300	LEU
1	B	341	GLU
1	B	363	ILE
1	B	402	ASP
1	B	427	VAL
1	B	432	LEU
1	B	467	VAL
1	B	506	PHE
1	B	576	VAL
1	B	633	ASN
1	B	664	ARG
1	B	770	SER
1	B	868	ARG
1	B	909	THR

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Mol	Chain	Res	Type
1	B	950	LEU
1	B	951	SER
1	B	976	GLN
1	B	1112	LEU
1	B	1114	LEU
1	B	1187	ILE
1	B	1220	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	GLN
1	A	359	ASN
1	A	379	ASN
1	A	503	GLN
1	A	679	GLN
1	A	757	GLN
1	A	841	GLN
1	A	1001	GLN
1	A	1107	ASN
1	B	359	ASN
1	B	679	GLN
1	B	748	ASN
1	B	1001	GLN
1	B	1030	GLN
1	B	1061	GLN
1	B	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

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TPP	B	2001	3	26,27,27	1.48	4 (15%)	38,40,40	1.69	9 (23%)
2	TPP	A	2001	3	26,27,27	1.41	2 (7%)	38,40,40	1.68	9 (23%)

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	B	2001	3	-	4/17/17/17	0/2/2/2
2	TPP	A	2001	3	-	4/17/17/17	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	TPP	C4-N3	-3.73	1.32	1.39
2	A	2001	TPP	PB-O1B	3.62	1.61	1.50
2	B	2001	TPP	PB-O1B	3.38	1.61	1.50
2	A	2001	TPP	C4-N3	-3.22	1.33	1.39
2	B	2001	TPP	PB-O3B	2.38	1.63	1.54
2	B	2001	TPP	PA-O3A	2.38	1.62	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	TPP	CM2-C2'-N1'	5.54	123.10	117.20
2	A	2001	TPP	CM2-C2'-N1'	5.10	122.63	117.20
2	A	2001	TPP	CM4-C4-C5	-3.90	117.76	127.75
2	B	2001	TPP	CM4-C4-C5	-3.70	118.26	127.75
2	A	2001	TPP	C6'-N1'-C2'	3.21	121.34	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	TPP	C6'-N1'-C2'	2.86	120.77	116.07
2	A	2001	TPP	N1'-C2'-N3'	-2.85	120.78	125.53
2	A	2001	TPP	C5-C4-N3	2.85	116.86	111.67
2	B	2001	TPP	N1'-C2'-N3'	-2.68	121.07	125.53
2	B	2001	TPP	C5'-C6'-N1'	-2.58	119.63	123.83
2	B	2001	TPP	C2'-N3'-C4'	2.52	121.98	118.10
2	B	2001	TPP	C2-S1-C5	-2.49	89.56	91.22
2	B	2001	TPP	C5-C4-N3	2.45	116.12	111.67
2	A	2001	TPP	C5'-C6'-N1'	-2.35	120.01	123.83
2	A	2001	TPP	C2'-N3'-C4'	2.20	121.49	118.10
2	B	2001	TPP	CM4-C4-N3	2.19	125.62	120.57
2	A	2001	TPP	C2-S1-C5	-2.18	89.77	91.22
2	A	2001	TPP	CM4-C4-N3	2.05	125.31	120.57

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	TPP	C7-O7-PA-O1A
2	A	2001	TPP	PA-O3A-PB-O2B
2	B	2001	TPP	C7-O7-PA-O1A
2	B	2001	TPP	PA-O3A-PB-O2B
2	A	2001	TPP	PA-O3A-PB-O3B
2	B	2001	TPP	PA-O3A-PB-O3B
2	A	2001	TPP	PA-O3A-PB-O1B
2	B	2001	TPP	PA-O3A-PB-O1B

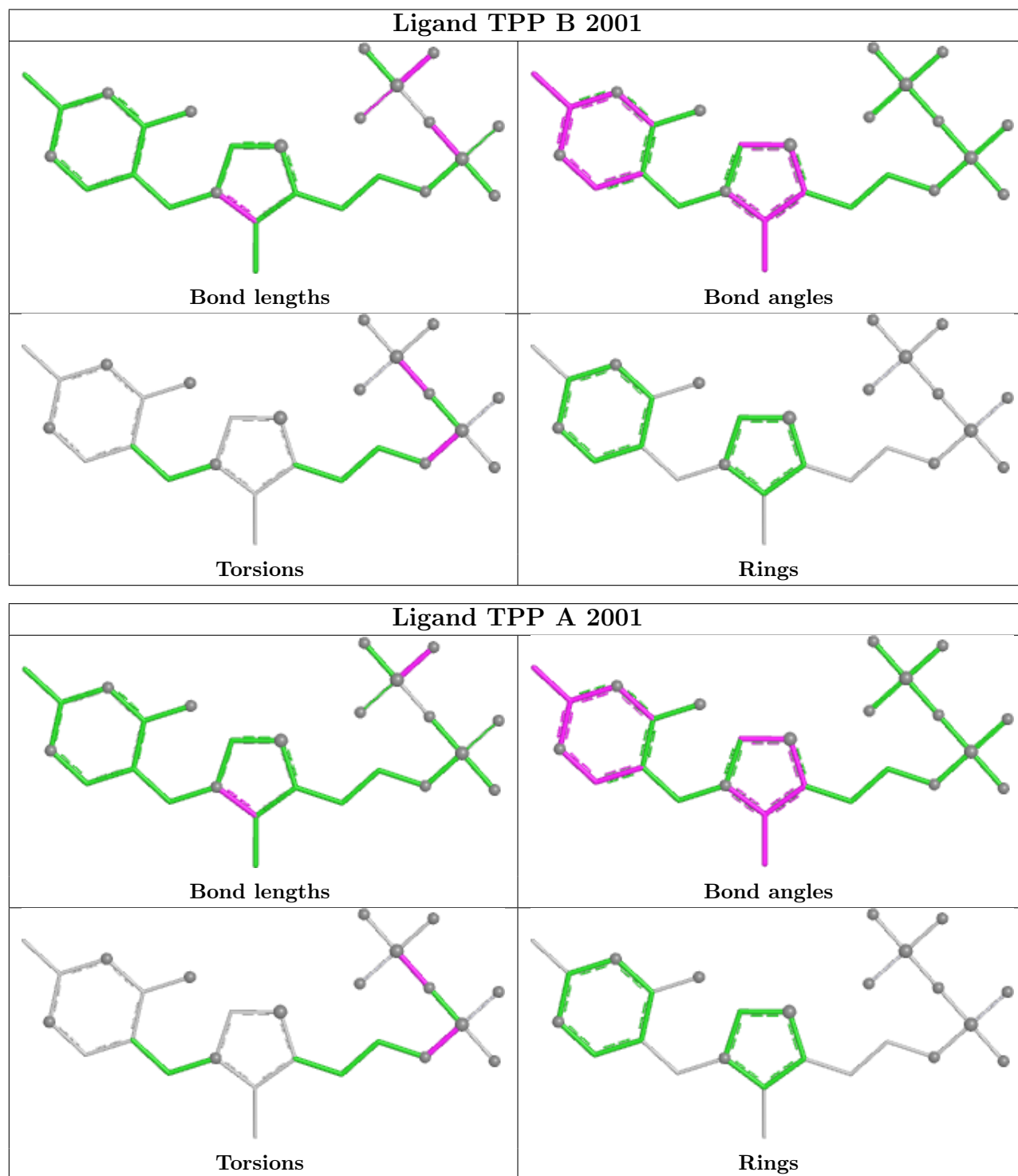
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	TPP	3	0
2	A	2001	TPP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	1055/1113 (94%)	-0.12	12 (1%) 78 77	39, 65, 102, 140	0
1	B	989/1113 (88%)	0.16	77 (7%) 19 19	41, 65, 140, 173	0
All	All	2044/2226 (91%)	0.02	89 (4%) 39 38	39, 65, 115, 173	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	VAL	6.1
1	A	200	ILE	5.8
1	B	256	THR	5.1
1	B	501	VAL	4.8
1	B	325	PHE	4.7
1	B	293	SER	4.7
1	B	213	VAL	4.4
1	B	302	ILE	4.3
1	B	503	GLN	4.2
1	A	814	GLU	4.0
1	B	319	GLY	3.9
1	B	278	ILE	3.9
1	B	502	GLY	3.9
1	B	233	ASP	3.9
1	B	282	ALA	3.8
1	B	284	GLU	3.7
1	B	810	LEU	3.6
1	B	136	MET	3.6
1	B	214	ALA	3.5
1	B	245	ALA	3.4
1	B	504	LYS	3.4
1	B	220	GLU	3.4
1	B	244	THR	3.3
1	B	164	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	472	ASP	3.3
1	B	310	SER	3.2
1	B	297	ILE	3.2
1	B	305	LEU	3.2
1	B	1103	GLU	3.2
1	B	303	GLY	3.2
1	A	258	PRO	3.1
1	A	561	PHE	3.1
1	B	199	ALA	3.0
1	B	128	VAL	3.0
1	B	194	THR	2.8
1	B	332	LEU	2.8
1	B	234	ILE	2.8
1	B	160	LEU	2.8
1	B	306	ILE	2.7
1	B	323	GLY	2.6
1	B	328	THR	2.6
1	B	363	ILE	2.6
1	B	280	ALA	2.6
1	A	363	ILE	2.6
1	A	831	LEU	2.6
1	B	326	LEU	2.6
1	A	476	VAL	2.6
1	B	355	TRP	2.5
1	B	296	ARG	2.5
1	B	559	SER	2.5
1	B	132	PRO	2.5
1	B	394	ASN	2.5
1	B	236	ARG	2.5
1	B	472	ASP	2.5
1	B	165	ILE	2.4
1	B	216	ILE	2.4
1	A	122	VAL	2.4
1	B	238	ALA	2.4
1	A	785	SER	2.4
1	B	294	GLU	2.4
1	B	134	LYS	2.3
1	B	425	ALA	2.3
1	B	578	TYR	2.3
1	B	249	SER	2.3
1	B	330	HIS	2.3
1	B	130	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	506	PHE	2.3
1	A	770	SER	2.2
1	B	243	LEU	2.2
1	B	239	ARG	2.2
1	B	255	LEU	2.2
1	B	231	TYR	2.2
1	B	283	MET	2.2
1	B	424	PHE	2.2
1	B	307	THR	2.2
1	B	327	ARG	2.2
1	B	331	GLN	2.2
1	B	253	ILE	2.2
1	B	329	ILE	2.1
1	B	575	ASP	2.1
1	B	157	PHE	2.1
1	A	288	GLU	2.1
1	B	240	ASP	2.1
1	B	304	LYS	2.1
1	B	832	ALA	2.0
1	B	333	LEU	2.0
1	B	471	HIS	2.0
1	B	301	GLY	2.0
1	B	295	GLU	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](#)

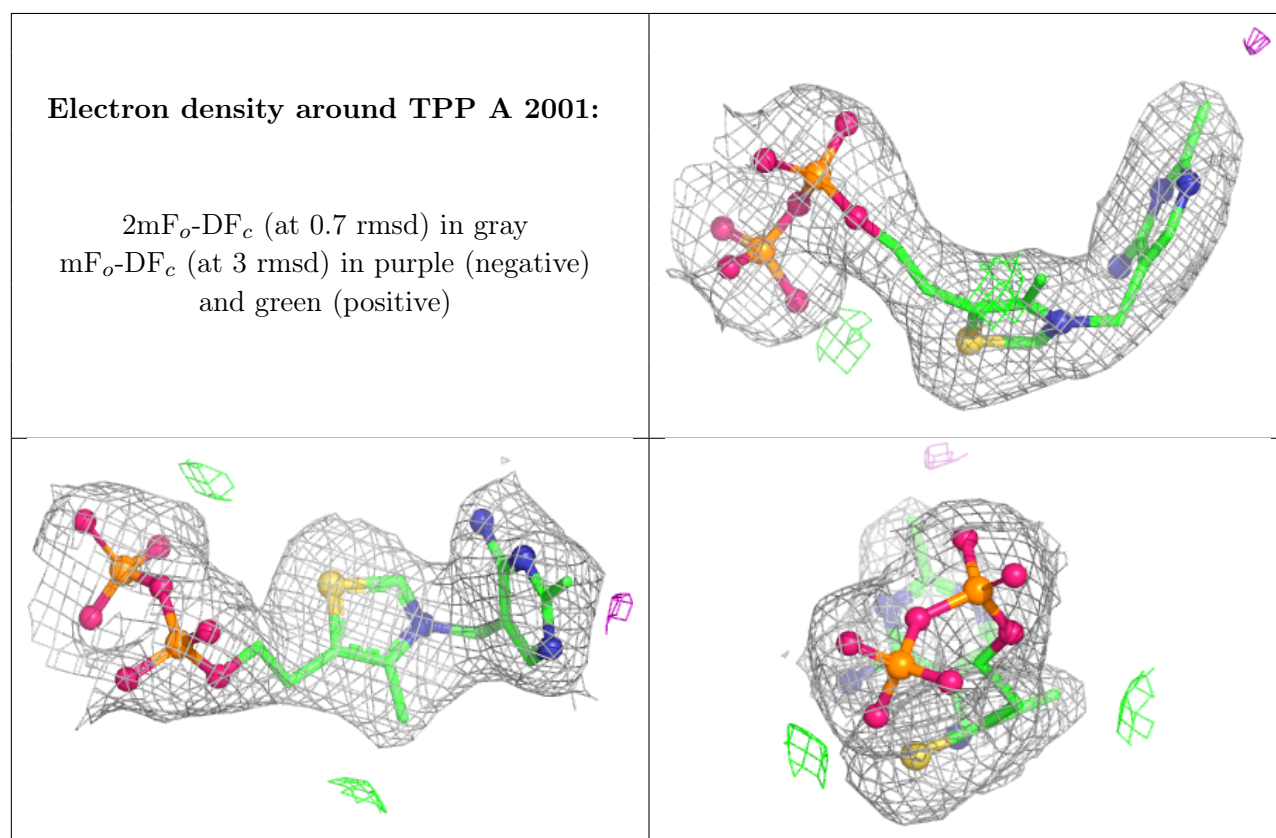
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

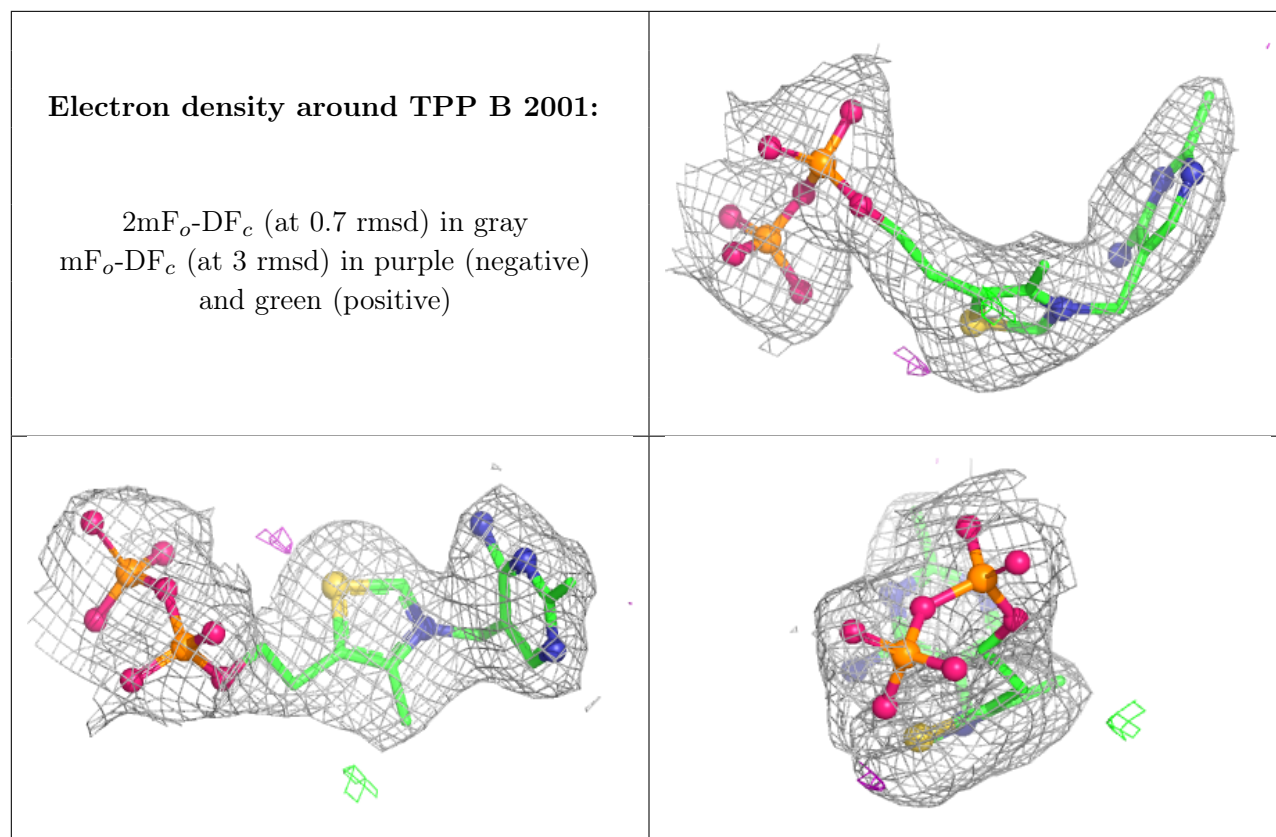
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TPP	A	2001	26/26	0.98	0.06	35,51,66,74	0
2	TPP	B	2001	26/26	0.98	0.06	23,41,70,73	0
4	CA	A	2003	1/1	0.98	0.04	72,72,72,72	0
4	CA	B	2003	1/1	0.99	0.04	67,67,67,67	0
3	MG	A	2002	1/1	1.00	0.03	41,41,41,41	0
3	MG	B	2002	1/1	1.00	0.06	32,32,32,32	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.