



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:14 PM UTC

PDB ID : 3ZHQ / pdb_00003zhq
Title : Crystal structure of the H747A mutant of the SucA domain of Mycobacterium smegmatis KGD
Authors : Wagner, T.; Barilone, N.; Bellinzoni, M.; Alzari, P.M.
Deposited on : 2012-12-24
Resolution : 2.50 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

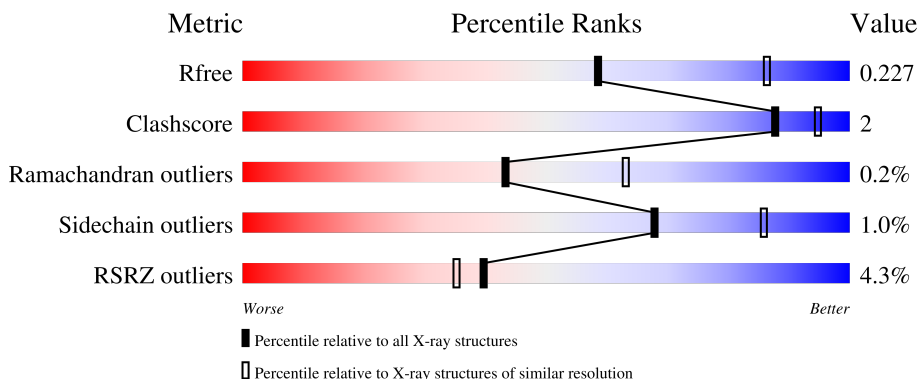
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	3% 87% 7% 7%
1	B	868	4% 85% 7% 7%
1	C	868	4% 87% 6% 6%
1	D	868	5% 88% 6% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25781 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.

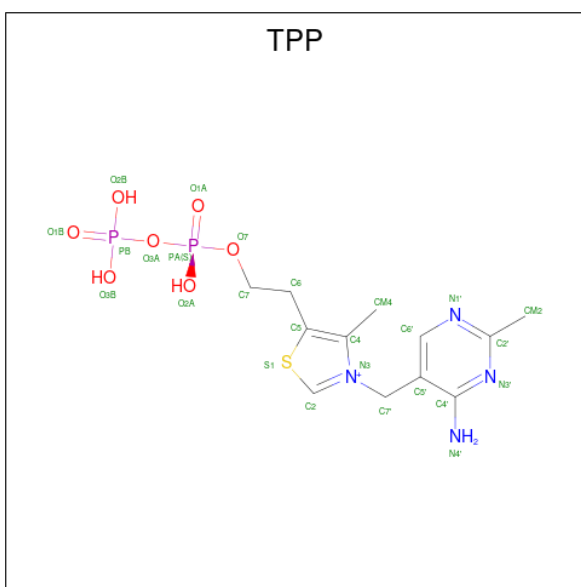
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	811	Total	C	N	O	S	0	1	0
			6283	3959	1108	1194	22			
1	B	808	Total	C	N	O	S	0	0	0
			6208	3913	1103	1168	24			
1	C	812	Total	C	N	O	S	0	0	0
			6301	3971	1110	1197	23			
1	D	810	Total	C	N	O	S	0	0	0
			6234	3933	1097	1180	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	expression tag	UNP A0R2B1
A	747	ALA	HIS	engineered mutation	UNP A0R2B1
B	360	GLY	-	expression tag	UNP A0R2B1
B	747	ALA	HIS	engineered mutation	UNP A0R2B1
C	360	GLY	-	expression tag	UNP A0R2B1
C	747	ALA	HIS	engineered mutation	UNP A0R2B1
D	360	GLY	-	expression tag	UNP A0R2B1
D	747	ALA	HIS	engineered mutation	UNP A0R2B1

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



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

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

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

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

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

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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

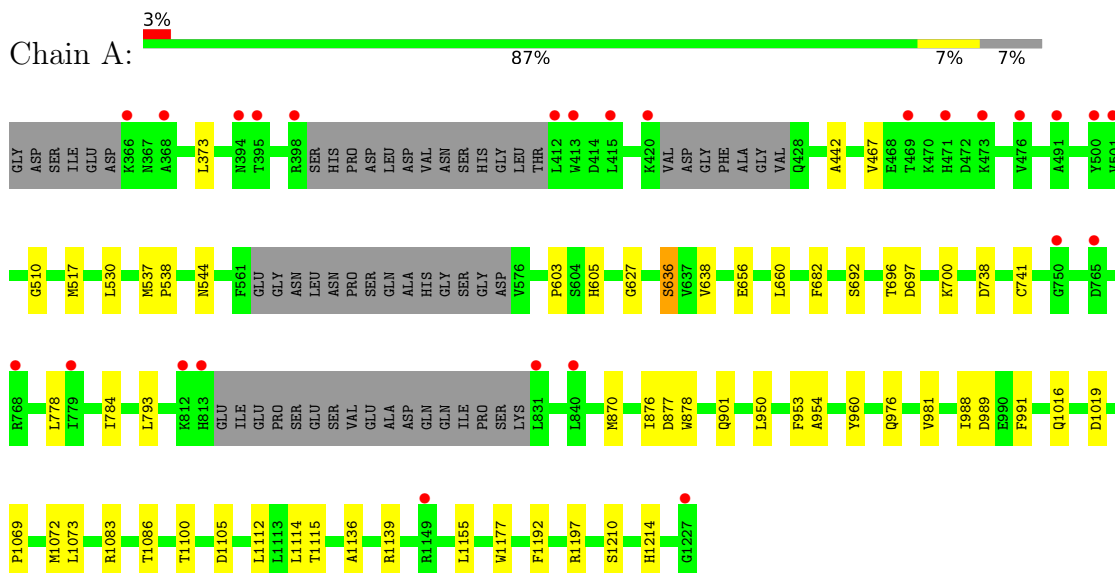
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	197	Total 197	O 197	0	0
5	B	154	Total 154	O 154	0	0
5	C	165	Total 165	O 165	0	0
5	D	127	Total 127	O 127	0	0

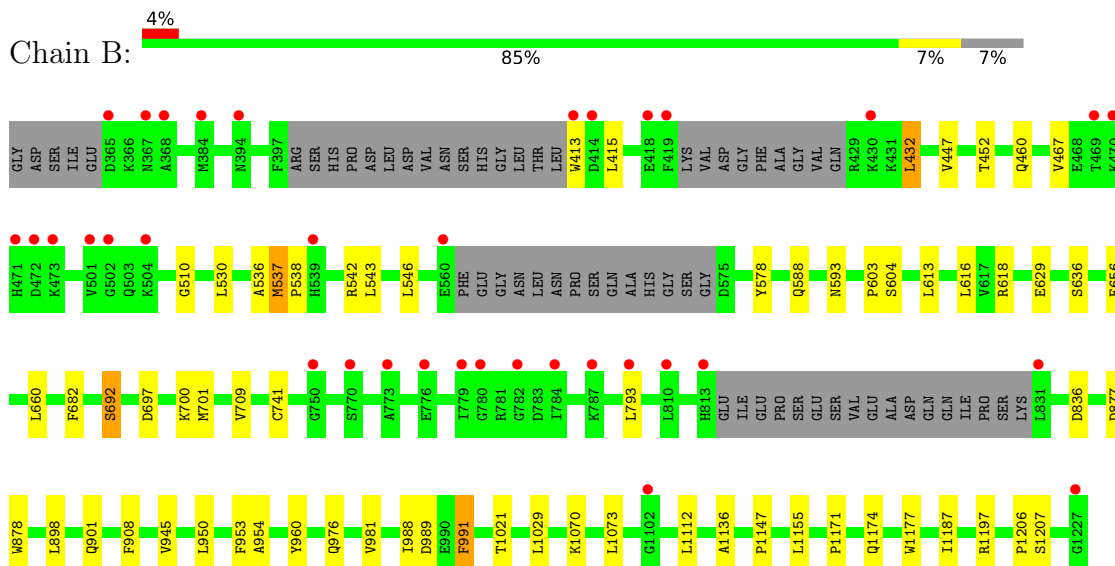
3 Residue-property plots [i](#)

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.

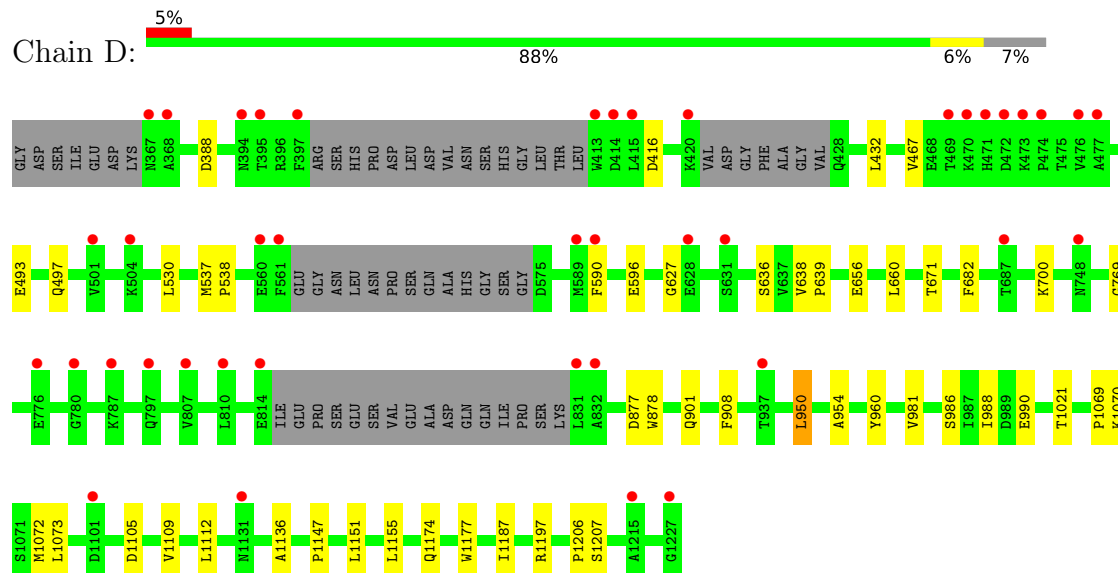
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.67Å 83.74Å 159.58Å 99.86° 98.95° 100.44°	Depositor
Resolution (Å)	48.97 – 2.50 48.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.97-2.50) 96.8 (48.97-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.194 , 0.223 (Not available) , 0.227	Depositor DCC
R_{free} test set	6718 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25781	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.98% 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

5.1 Standard geometry

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	0.86	2/6411 (0.0%)	1.29	17/8699 (0.2%)
1	B	0.87	0/6335	1.30	24/8600 (0.3%)
1	C	0.85	0/6427	1.31	18/8712 (0.2%)
1	D	0.87	0/6359	1.30	15/8625 (0.2%)
All	All	0.86	2/25532 (0.0%)	1.30	74/34636 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	544	ASN	C-N	5.13	1.40	1.33
1	A	517	MET	SD-CE	-5.09	1.66	1.79

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	836	ASP	CA-CB-CG	8.10	120.70	112.60
1	D	590	PHE	CA-CB-CG	7.00	120.80	113.80
1	B	537	MET	N-CA-C	6.71	114.26	108.22
1	A	700	LYS	CA-C-N	6.70	130.17	120.38
1	A	700	LYS	C-N-CA	6.70	130.17	120.38
1	D	416	ASP	N-CA-C	-6.58	104.82	112.92
1	D	537	MET	N-CA-C	6.49	114.06	108.22
1	C	700	LYS	CA-C-N	6.40	129.14	120.38
1	C	700	LYS	C-N-CA	6.40	129.14	120.38
1	A	877	ASP	CA-CB-CG	6.36	118.96	112.60
1	B	700	LYS	CA-C-N	6.27	129.54	120.38
1	B	700	LYS	C-N-CA	6.27	129.54	120.38
1	D	700	LYS	CA-C-N	6.17	129.39	120.38
1	D	700	LYS	C-N-CA	6.17	129.39	120.38
1	A	627	GLY	CA-C-N	5.95	128.18	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	627	GLY	C-N-CA	5.95	128.18	120.44
1	B	1147	PRO	CA-C-N	5.80	128.37	120.54
1	B	1147	PRO	C-N-CA	5.80	128.37	120.54
1	A	660	LEU	CA-C-N	5.78	128.30	120.38
1	A	660	LEU	C-N-CA	5.78	128.30	120.38
1	C	537	MET	N-CA-C	5.65	113.30	108.22
1	C	1087	GLU	CB-CG-CD	5.60	122.11	112.60
1	C	877	ASP	CA-CB-CG	5.58	118.17	112.60
1	C	1147	PRO	CA-C-N	5.57	128.06	120.54
1	C	1147	PRO	C-N-CA	5.57	128.06	120.54
1	B	991	PHE	CA-C-N	5.50	127.49	120.56
1	B	991	PHE	C-N-CA	5.50	127.49	120.56
1	D	627	GLY	CA-C-N	5.50	127.65	120.28
1	D	627	GLY	C-N-CA	5.50	127.65	120.28
1	A	989	ASP	CA-CB-CG	5.46	118.06	112.60
1	C	487	ASN	CA-CB-CG	5.44	118.04	112.60
1	A	1105	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	953	PHE	CA-CB-CG	5.39	119.19	113.80
1	B	877	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	692	SER	CA-C-N	5.37	127.79	120.54
1	B	692	SER	C-N-CA	5.37	127.79	120.54
1	C	976	GLN	N-CA-C	-5.34	105.36	111.07
1	A	960	TYR	CA-C-N	5.32	125.89	119.98
1	A	960	TYR	C-N-CA	5.32	125.89	119.98
1	A	537	MET	N-CA-C	5.31	113.00	108.22
1	C	953	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	638	VAL	N-CA-C	5.28	113.68	107.77
1	D	660	LEU	CA-C-N	5.27	128.07	120.38
1	D	660	LEU	C-N-CA	5.27	128.07	120.38
1	D	638	VAL	N-CA-C	5.22	113.61	107.77
1	D	877	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	953	PHE	CA-CB-CG	5.21	119.01	113.80
1	B	660	LEU	CA-C-N	5.20	127.97	120.38
1	B	660	LEU	C-N-CA	5.20	127.97	120.38
1	B	1029	LEU	CA-C-N	5.20	127.67	120.29
1	B	1029	LEU	C-N-CA	5.20	127.67	120.29
1	B	960	TYR	CA-C-N	5.19	125.74	119.98
1	B	960	TYR	C-N-CA	5.19	125.74	119.98
1	B	1171	PRO	CA-C-N	5.18	127.94	120.38
1	B	1171	PRO	C-N-CA	5.18	127.94	120.38
1	B	976	GLN	N-CA-C	-5.17	105.54	111.07
1	B	989	ASP	CA-CB-CG	5.15	117.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	976	GLN	N-CA-C	-5.11	105.60	111.07
1	A	1214	HIS	CA-C-N	5.09	127.09	120.28
1	A	1214	HIS	C-N-CA	5.09	127.09	120.28
1	C	1105	ASP	CA-CB-CG	5.08	117.69	112.60
1	C	769	GLY	CA-C-N	5.08	127.09	120.28
1	C	769	GLY	C-N-CA	5.08	127.09	120.28
1	C	678	ASN	CA-CB-CG	5.07	117.67	112.60
1	C	660	LEU	CA-C-N	5.06	127.77	120.38
1	C	660	LEU	C-N-CA	5.06	127.77	120.38
1	D	960	TYR	CA-C-N	5.05	125.59	119.98
1	D	960	TYR	C-N-CA	5.05	125.59	119.98
1	C	627	GLY	CA-C-N	5.04	126.99	120.44
1	C	627	GLY	C-N-CA	5.04	126.99	120.44
1	B	413	TRP	CA-C-N	5.04	129.99	122.74
1	B	413	TRP	C-N-CA	5.04	129.99	122.74
1	D	1105	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	388	ASP	CA-CB-CG	5.03	117.63	112.60

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	6283	0	6051	24	0
1	B	6208	0	5963	28	0
1	C	6301	0	6108	27	0
1	D	6234	0	6017	23	0
2	A	26	0	16	1	0
2	B	26	0	16	1	0
2	C	26	0	16	2	0
2	D	26	0	16	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	197	0	0	2	0
5	B	154	0	0	2	0
5	C	165	0	0	0	0
5	D	127	0	0	4	0
All	All	25781	0	24203	99	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 (99) 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:C:705:PRO:HG2	1:C:735:VAL:HG13	1.69	0.73
1:C:373:LEU:CD1	1:C:436:LEU:HD21	2.20	0.71
1:C:692:SER:HB2	1:C:697:ASP:OD2	1.93	0.67
1:C:373:LEU:HD11	1:C:436:LEU:CD2	2.27	0.65
1:A:692:SER:HB2	1:A:697:ASP:OD2	1.98	0.63
1:C:373:LEU:HD11	1:C:436:LEU:HD21	1.82	0.62
1:C:373:LEU:CD1	1:C:436:LEU:CD2	2.78	0.61
1:C:373:LEU:HD12	1:C:436:LEU:HD21	1.84	0.57
1:A:530:LEU:HD22	1:A:636:SER:HA	1.88	0.56
1:A:901:GLN:OE1	2:B:2001:TPP:H6'	2.07	0.55
1:D:1174:GLN:OE1	1:D:1206:PRO:HA	2.07	0.55
1:B:542:ARG:HD3	1:B:578:TYR:HA	1.90	0.53
1:C:1112:LEU:HD12	1:C:1136:ALA:HB3	1.91	0.53
1:D:1069:PRO:HB3	1:D:1072:MET:HB3	1.91	0.53
1:A:442:ALA:HB1	1:A:467:VAL:HG12	1.91	0.52
1:B:603:PRO:HD3	1:B:991:PHE:CZ	2.45	0.52
1:C:898:LEU:O	1:C:945:VAL:HA	2.09	0.52
1:A:603:PRO:HD3	1:A:991:PHE:CZ	2.45	0.51
1:D:1112:LEU:HD12	1:D:1136:ALA:HB3	1.93	0.51
1:B:1112:LEU:HD12	1:B:1136:ALA:HB3	1.92	0.51
1:C:901:GLN:OE1	2:D:2001:TPP:H6'	2.11	0.51
1:A:1112:LEU:HD12	1:A:1136:ALA:HB3	1.92	0.50
1:B:618:ARG:HH21	1:B:629:GLU:HG2	1.77	0.49
1:C:441:ASP:HA	1:C:445:ARG:HG3	1.94	0.49
1:D:639:PRO:HB2	1:D:671:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:LEU:HD22	1:B:636:SER:HA	1.93	0.49
1:C:1148:ARG:HG3	1:C:1187:ILE:HD12	1.94	0.49
2:C:2001:TPP:H6'	1:D:901:GLN:OE1	2.12	0.49
1:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.94	0.49
1:D:538:PRO:HB2	5:D:3019:HOH:O	2.13	0.49
1:D:493:GLU:O	1:D:497:GLN:HG2	2.13	0.48
1:B:536:ALA:HB3	1:B:613:LEU:HD22	1.94	0.48
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.95	0.48
1:A:1086:THR:O	1:C:1157:ARG:NH2	2.41	0.48
1:B:452:THR:HA	1:B:460:GLN:NE2	2.29	0.48
1:D:1147:PRO:O	1:D:1151:LEU:HB2	2.13	0.48
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.96	0.47
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.96	0.47
1:A:878:TRP:HB3	1:A:1073:LEU:HD23	1.95	0.47
1:B:510:GLY:O	1:B:741:CYS:HB2	2.15	0.47
1:C:603:PRO:HD3	1:C:991:PHE:CZ	2.51	0.46
1:A:1112:LEU:HD21	1:A:1155:LEU:HD22	1.98	0.46
1:D:986:SER:O	1:D:990:GLU:HB2	2.16	0.46
1:C:1069:PRO:HB2	1:C:1072:MET:HB3	1.97	0.46
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.51	0.46
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.51	0.46
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.96	0.46
2:C:2001:TPP:HM42	1:D:950:LEU:CD2	2.46	0.46
1:A:538:PRO:HD2	5:A:3028:HOH:O	2.15	0.46
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.51	0.45
1:C:1069:PRO:CB	1:C:1072:MET:HB3	2.47	0.45
1:C:1174:GLN:OE1	1:C:1206:PRO:HA	2.17	0.45
1:B:898:LEU:O	1:B:945:VAL:HA	2.17	0.45
1:C:510:GLY:O	1:C:741:CYS:HB2	2.16	0.45
1:A:692:SER:HB3	1:B:701:MET:O	2.16	0.45
1:A:1083:ARG:HA	1:A:1086:THR:OG1	2.16	0.44
1:D:530:LEU:HD22	1:D:636:SER:HA	1.98	0.44
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.53	0.44
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.52	0.44
1:A:870:MET:HB3	1:A:876:ILE:HG12	2.00	0.44
1:B:538:PRO:HB2	5:B:3018:HOH:O	2.18	0.44
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.53	0.44
1:D:596:GLU:HG3	5:D:3029:HOH:O	2.17	0.44
1:B:692:SER:HB2	1:B:697:ASP:OD2	2.18	0.44
1:D:878:TRP:HB3	1:D:1073:LEU:HD23	2.00	0.44
1:C:554:TYR:HD2	1:C:806:GLU:OE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1069:PRO:CB	1:D:1072:MET:HB3	2.48	0.43
1:B:878:TRP:HB3	1:B:1073:LEU:HD23	2.01	0.43
1:B:1112:LEU:HD21	1:B:1155:LEU:HD22	2.00	0.43
1:C:682:PHE:HD1	1:C:683:THR:HG23	1.83	0.43
1:B:447:VAL:HG22	1:B:709:VAL:HG23	2.00	0.43
1:A:1016:GLN:NE2	5:A:3143:HOH:O	2.22	0.43
1:D:656:GLU:HB3	1:D:954:ALA:HB2	2.01	0.43
1:C:950:LEU:CD2	2:D:2001:TPP:HM42	2.49	0.42
1:B:1174:GLN:OE1	1:B:1206:PRO:HA	2.18	0.42
1:A:656:GLU:HB3	1:A:954:ALA:HB2	2.01	0.42
1:B:656:GLU:HB3	1:B:954:ALA:HB2	2.02	0.42
1:A:696:THR:HG21	1:A:738:ASP:HB2	2.01	0.42
2:A:2001:TPP:H6'	1:B:901:GLN:OE1	2.18	0.42
1:B:543:LEU:HA	1:B:546:LEU:HD12	2.01	0.42
1:A:1069:PRO:HG3	1:A:1072:MET:HE2	2.01	0.42
1:A:778:LEU:HB3	1:A:784:ILE:HG12	2.01	0.41
1:D:1021:THR:HG21	1:D:1207:SER:HB3	2.02	0.41
1:B:536:ALA:CB	1:B:613:LEU:HD22	2.50	0.41
1:A:1155:LEU:HD11	1:A:1192:PHE:CZ	2.55	0.41
1:B:415:LEU:HA	1:B:432:LEU:HB3	2.02	0.41
1:C:656:GLU:HB3	1:C:954:ALA:HB2	2.02	0.41
1:D:596:GLU:CG	5:D:3029:HOH:O	2.68	0.41
1:D:769:GLY:HA3	5:D:3009:HOH:O	2.21	0.41
1:B:1021:THR:HG21	1:B:1207:SER:HB3	2.03	0.41
1:B:537:MET:HE3	5:B:3019:HOH:O	2.20	0.41
1:D:1112:LEU:HD21	1:D:1155:LEU:HD22	2.01	0.41
1:A:510:GLY:O	1:A:741:CYS:HB2	2.21	0.41
1:B:588:GLN:OE1	1:B:593:ASN:HB2	2.21	0.41
1:C:603:PRO:HG3	1:C:990:GLU:HB3	2.03	0.40
1:C:1021:THR:HG21	1:C:1207:SER:HB3	2.03	0.40
1:A:1115:THR:O	1:A:1139:ARG:HA	2.21	0.40
1:A:1019:ASP:CB	1:B:604:SER:HB2	2.51	0.40
1:D:1109:VAL:HG21	1:D:1136:ALA:HB2	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	802/868 (92%)	779 (97%)	20 (2%)	3 (0%)	30	49
1	B	798/868 (92%)	779 (98%)	18 (2%)	1 (0%)	48	68
1	C	802/868 (92%)	779 (97%)	21 (3%)	2 (0%)	43	63
1	D	800/868 (92%)	777 (97%)	22 (3%)	1 (0%)	48	68
All	All	3202/3472 (92%)	3114 (97%)	81 (2%)	7 (0%)	43	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	605	HIS
1	A	605	HIS
1	A	636	SER
1	A	682	PHE
1	B	682	PHE
1	C	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	645/725 (89%)	639 (99%)	6 (1%)	70	87
1	B	629/725 (87%)	623 (99%)	6 (1%)	68	86
1	C	651/725 (90%)	642 (99%)	9 (1%)	59	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	637/725 (88%)	633 (99%)	4 (1%)	78	91
All	All	2562/2900 (88%)	2537 (99%)	25 (1%)	68	86

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	LEU
1	A	793	LEU
1	A	950	LEU
1	A	1100	THR
1	A	1114	LEU
1	A	1210	SER
1	B	432	LEU
1	B	467	VAL
1	B	616	LEU
1	B	793	LEU
1	B	950	LEU
1	B	1187	ILE
1	C	373	LEU
1	C	467	VAL
1	C	501	VAL
1	C	793	LEU
1	C	927	LEU
1	C	930	LEU
1	C	950	LEU
1	C	1083	ARG
1	C	1187	ILE
1	D	432	LEU
1	D	467	VAL
1	D	950	LEU
1	D	1187	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	548	ASN
1	A	933	ASN
1	A	1030	GLN
1	A	1061	GLN
1	A	1219	GLN

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Mol	Chain	Res	Type
1	B	797	GLN
1	B	1107	ASN
1	B	1219	GLN
1	C	497	GLN
1	C	503	GLN
1	C	912	HIS
1	C	1219	GLN
1	D	460	GLN
1	D	556	GLN
1	D	912	HIS
1	D	933	ASN
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	C	2001	3	26,27,27	1.36	3 (11%)	38,40,40	1.56	8 (21%)

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	2 (7%)	38,40,40	1.52	9 (23%)
2	TPP	D	2001	3	26,27,27	1.30	2 (7%)	38,40,40	1.49	7 (18%)
2	TPP	B	2001	3	26,27,27	1.38	2 (7%)	38,40,40	1.52	7 (18%)

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	C	2001	3	-	5/17/17/17	0/2/2/2
2	TPP	A	2001	3	-	3/17/17/17	0/2/2/2
2	TPP	D	2001	3	-	2/17/17/17	0/2/2/2
2	TPP	B	2001	3	-	2/17/17/17	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	TPP	PB-O1B	3.82	1.62	1.50
2	D	2001	TPP	PB-O1B	3.74	1.62	1.50
2	D	2001	TPP	C4-N3	-3.25	1.33	1.39
2	C	2001	TPP	C4-N3	-3.21	1.33	1.39
2	B	2001	TPP	C4-N3	-3.19	1.33	1.39
2	C	2001	TPP	PB-O1B	3.15	1.60	1.50
2	A	2001	TPP	PB-O1B	2.81	1.59	1.50
2	C	2001	TPP	PA-O3A	2.38	1.62	1.59
2	A	2001	TPP	C4-N3	-2.27	1.35	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	TPP	CM4-C4-C5	-3.87	117.84	127.75
2	B	2001	TPP	CM4-C4-C5	-3.73	118.19	127.75
2	C	2001	TPP	CM4-C4-C5	-3.57	118.59	127.75
2	C	2001	TPP	C6'-N1'-C2'	3.40	121.66	116.07
2	D	2001	TPP	CM4-C4-C5	-3.37	119.11	127.75
2	D	2001	TPP	C6'-N1'-C2'	3.12	121.20	116.07
2	B	2001	TPP	C2-S1-C5	-3.11	89.15	91.22
2	B	2001	TPP	C6'-N1'-C2'	3.03	121.05	116.07
2	A	2001	TPP	CM2-C2'-N1'	2.86	120.24	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	TPP	C2-S1-C5	-2.85	89.33	91.22
2	C	2001	TPP	N1'-C2'-N3'	-2.80	120.87	125.53
2	B	2001	TPP	C7-C6-C5	-2.68	104.33	112.73
2	D	2001	TPP	C5'-C6'-N1'	-2.64	119.53	123.83
2	D	2001	TPP	C7-C6-C5	-2.62	104.51	112.73
2	A	2001	TPP	C7-C6-C5	-2.62	104.52	112.73
2	C	2001	TPP	C7-C6-C5	-2.61	104.53	112.73
2	B	2001	TPP	CM4-C4-N3	2.59	126.55	120.57
2	A	2001	TPP	C6'-N1'-C2'	2.56	120.27	116.07
2	A	2001	TPP	N1'-C2'-N3'	-2.50	121.37	125.53
2	C	2001	TPP	CM4-C4-N3	2.43	126.17	120.57
2	A	2001	TPP	C5-C4-N3	2.41	116.06	111.67
2	D	2001	TPP	CM4-C4-N3	2.41	126.14	120.57
2	C	2001	TPP	CM2-C2'-N1'	2.33	119.68	117.20
2	A	2001	TPP	CM4-C4-N3	2.32	125.93	120.57
2	B	2001	TPP	N1'-C2'-N3'	-2.32	121.66	125.53
2	B	2001	TPP	C5'-C6'-N1'	-2.27	120.14	123.83
2	A	2001	TPP	C4-C5-S1	-2.24	107.06	110.56
2	C	2001	TPP	C4-C5-S1	-2.24	107.08	110.56
2	A	2001	TPP	C2'-N3'-C4'	2.22	121.51	118.10
2	D	2001	TPP	N1'-C2'-N3'	-2.11	122.01	125.53
2	C	2001	TPP	C7'-N3-C2	-2.00	119.30	123.48

There are no chirality outliers.

All (12) torsion outliers are listed below:

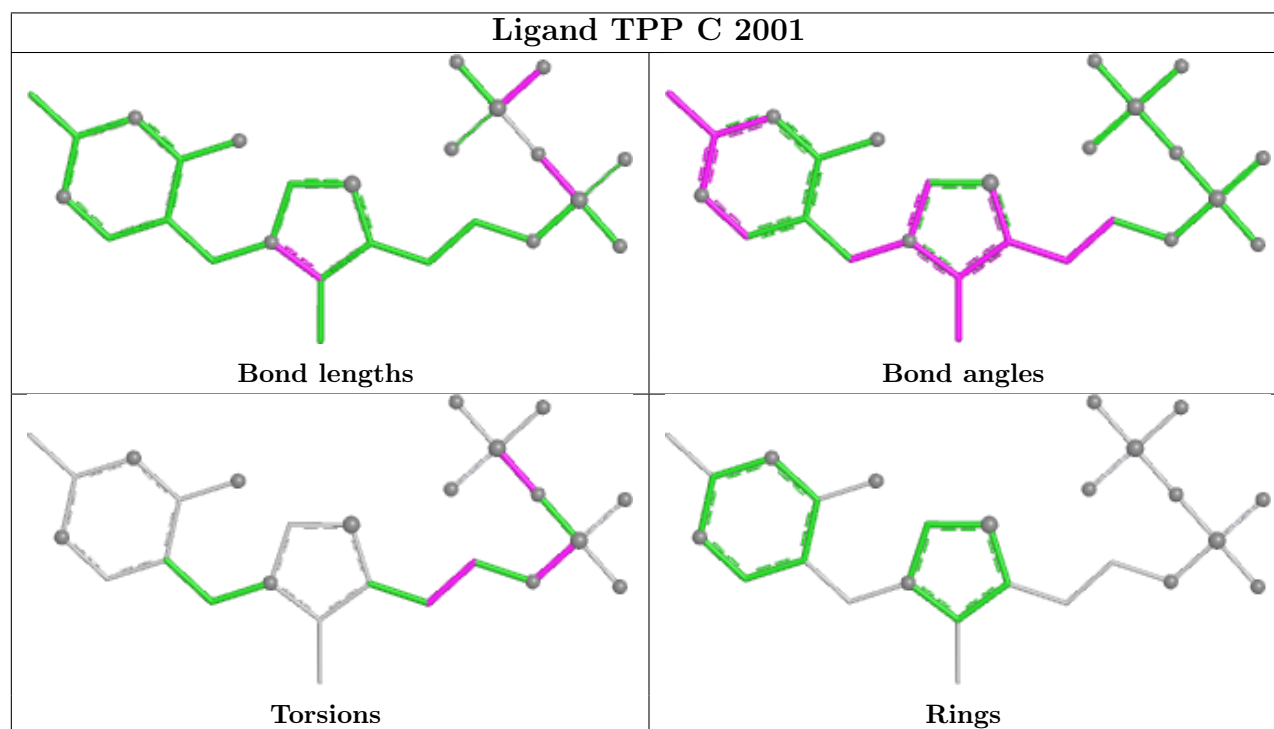
Mol	Chain	Res	Type	Atoms
2	A	2001	TPP	C7-O7-PA-O1A
2	B	2001	TPP	C7-O7-PA-O1A
2	C	2001	TPP	C7-O7-PA-O1A
2	D	2001	TPP	C7-O7-PA-O1A
2	C	2001	TPP	PA-O3A-PB-O2B
2	C	2001	TPP	PA-O3A-PB-O3B
2	C	2001	TPP	C5-C6-C7-O7
2	C	2001	TPP	C7-O7-PA-O3A
2	A	2001	TPP	PA-O3A-PB-O3B
2	A	2001	TPP	C5-C6-C7-O7
2	B	2001	TPP	C5-C6-C7-O7
2	D	2001	TPP	C5-C6-C7-O7

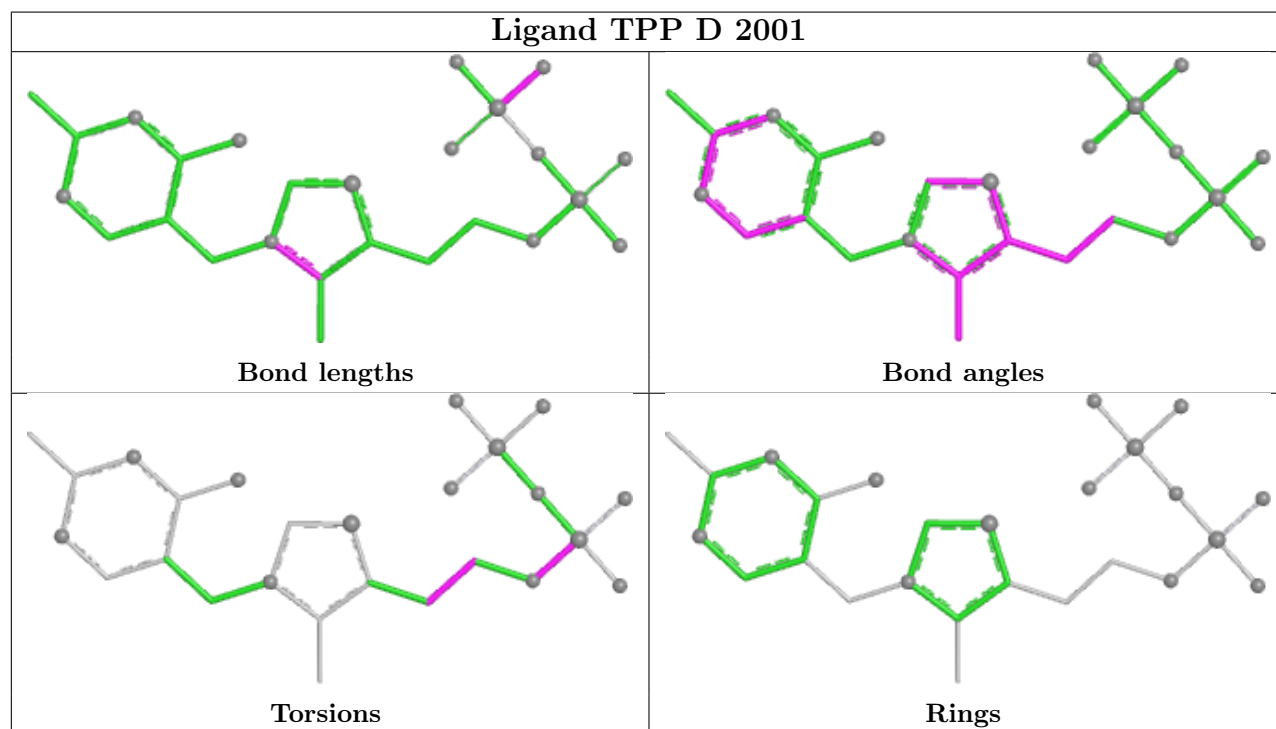
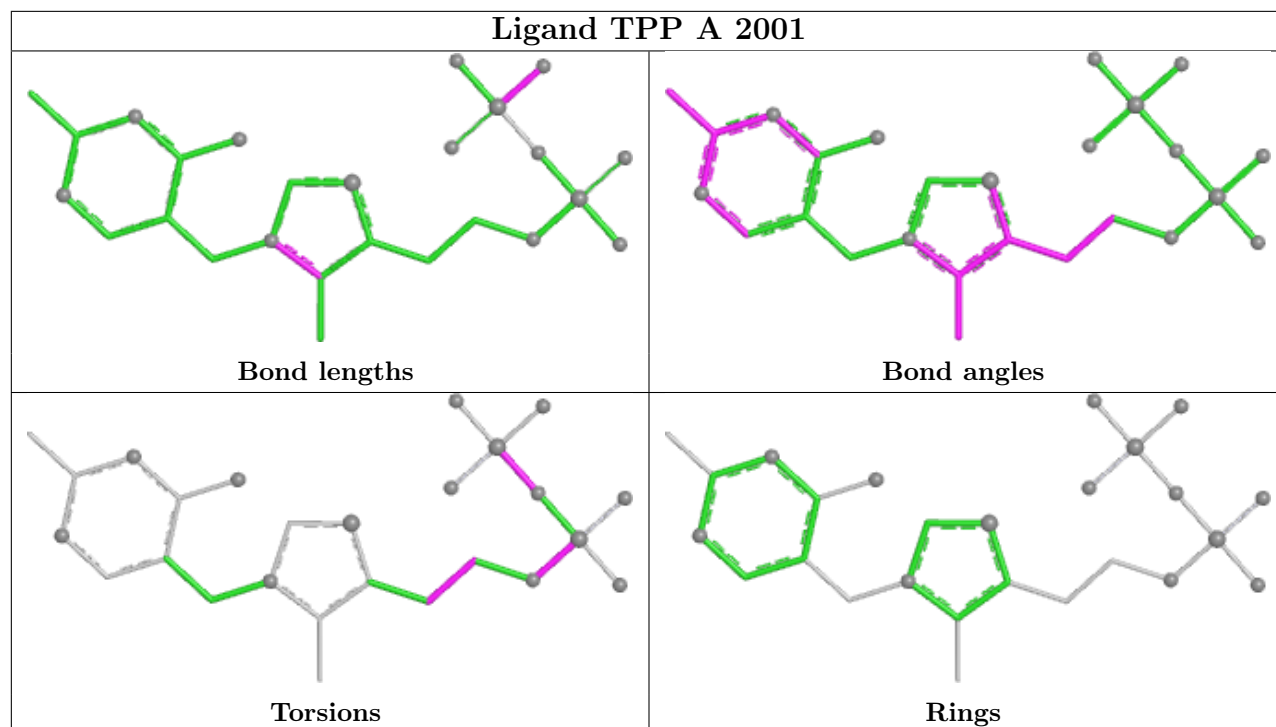
There are no ring outliers.

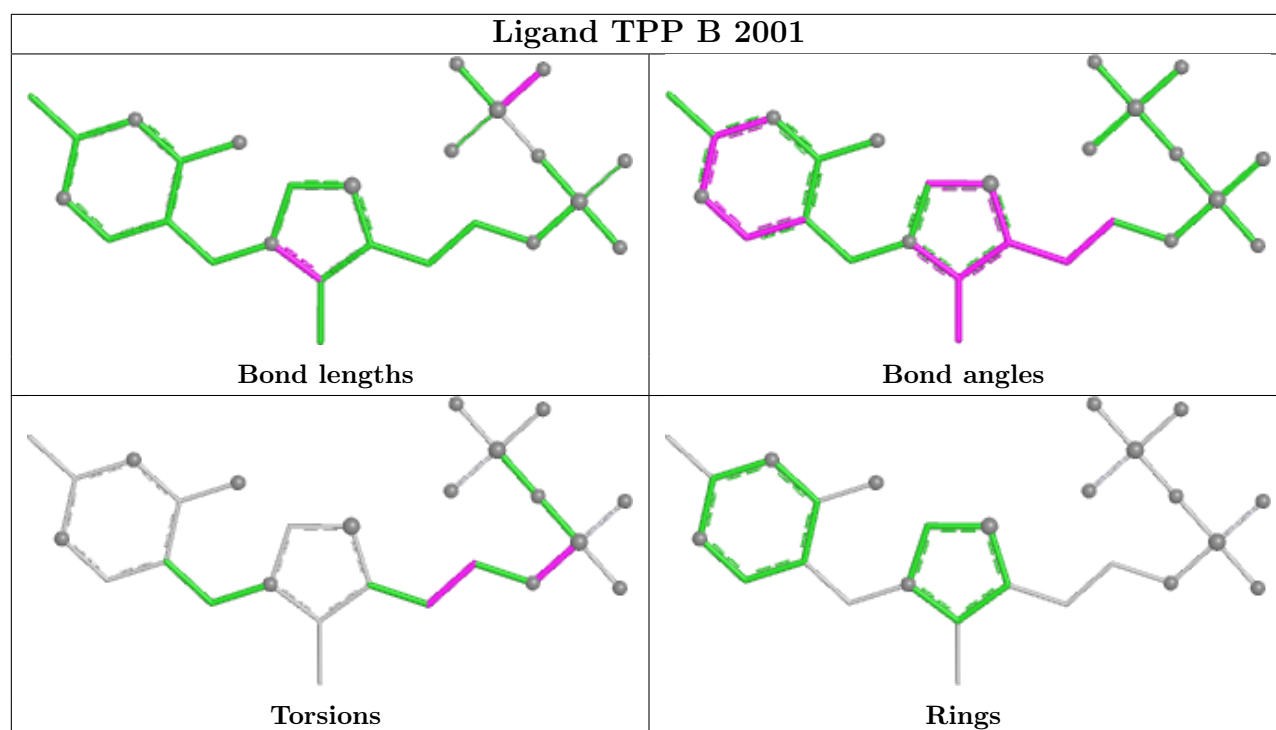
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	TPP	2	0
2	A	2001	TPP	1	0
2	D	2001	TPP	2	0
2	B	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	811/868 (93%)	0.28	26 (3%)	50	46	20, 38, 68, 97	1 (0%)
1	B	808/868 (93%)	0.37	35 (4%)	40	35	20, 40, 75, 103	0
1	C	812/868 (93%)	0.49	36 (4%)	39	34	22, 42, 74, 98	0
1	D	810/868 (93%)	0.44	41 (5%)	33	29	22, 42, 75, 114	0
All	All	3241/3472 (93%)	0.40	138 (4%)	40	35	20, 41, 73, 114	1 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	398	ARG	6.3
1	D	472	ASP	6.0
1	B	413	TRP	5.4
1	D	814	GLU	5.4
1	B	472	ASP	5.0
1	D	471	HIS	4.9
1	C	411	THR	4.8
1	B	365	ASP	4.8
1	D	470	LYS	4.6
1	A	813	HIS	4.5
1	A	412	LEU	4.5
1	D	473	LYS	4.5
1	A	398	ARG	4.5
1	D	590	PHE	4.4
1	D	414	ASP	4.4
1	D	413	TRP	4.3
1	A	469	THR	4.3
1	D	420	LYS	4.3
1	D	367	ASN	4.3
1	B	560	GLU	4.2
1	C	784	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	415	LEU	4.0
1	A	368	ALA	3.9
1	B	368	ALA	3.9
1	B	470	LYS	3.9
1	C	831	LEU	3.6
1	C	561	PHE	3.5
1	B	473	LYS	3.5
1	A	420	LYS	3.5
1	C	629	GLU	3.4
1	C	814	GLU	3.4
1	C	632	ASP	3.4
1	C	394	ASN	3.4
1	B	501	VAL	3.4
1	D	831	LEU	3.3
1	A	1227	GLY	3.2
1	C	413	TRP	3.1
1	B	810	LEU	3.1
1	A	471	HIS	3.1
1	C	939	THR	3.1
1	B	367	ASN	3.1
1	D	1227	GLY	3.0
1	B	779	ILE	3.0
1	C	779	ILE	3.0
1	D	474	PRO	3.0
1	B	793	LEU	3.0
1	A	473	LYS	3.0
1	C	1227	GLY	3.0
1	C	412	LEU	2.9
1	C	421	VAL	2.9
1	A	831	LEU	2.9
1	B	782	GLY	2.9
1	C	633	ASN	2.9
1	C	744	ARG	2.9
1	C	628	GLU	2.9
1	C	539	HIS	2.8
1	C	786	MET	2.8
1	B	776	GLU	2.8
1	B	813	HIS	2.8
1	D	469	THR	2.8
1	D	628	GLU	2.8
1	D	561	PHE	2.8
1	C	627	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	779	ILE	2.8
1	B	394	ASN	2.8
1	A	366	LYS	2.8
1	B	419	PHE	2.8
1	A	394	ASN	2.8
1	D	368	ALA	2.8
1	D	589	MET	2.8
1	C	471	HIS	2.8
1	A	413	TRP	2.7
1	B	831	LEU	2.7
1	B	471	HIS	2.7
1	D	748	ASN	2.7
1	B	784	ILE	2.6
1	D	476	VAL	2.6
1	A	1149	ARG	2.6
1	D	810	LEU	2.6
1	C	631	SER	2.6
1	D	501	VAL	2.6
1	D	394	ASN	2.5
1	C	368	ALA	2.5
1	B	469	THR	2.5
1	A	501	VAL	2.5
1	B	414	ASP	2.5
1	D	1131	ASN	2.5
1	D	631	SER	2.5
1	D	687	THR	2.5
1	B	539	HIS	2.4
1	D	560	GLU	2.4
1	C	592	ASP	2.4
1	B	430	LYS	2.4
1	C	560	GLU	2.4
1	B	1227	GLY	2.3
1	A	765	ASP	2.3
1	D	397	PHE	2.3
1	B	504	LYS	2.3
1	B	773	ALA	2.3
1	C	369	ARG	2.3
1	D	807	VAL	2.3
1	C	559	SER	2.3
1	D	776	GLU	2.3
1	A	768	ARG	2.3
1	C	634	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	395	THR	2.3
1	B	502	GLY	2.3
1	C	415	LEU	2.2
1	C	420	LYS	2.2
1	A	415	LEU	2.2
1	B	418	GLU	2.2
1	D	797	GLN	2.2
1	D	1101	ASP	2.2
1	C	429	ARG	2.2
1	C	626	THR	2.2
1	A	812	LYS	2.2
1	B	384	MET	2.1
1	D	477	ALA	2.1
1	B	750	GLY	2.1
1	D	937	THR	2.1
1	B	770	SER	2.1
1	B	787	LYS	2.1
1	A	840	LEU	2.1
1	C	506	PHE	2.1
1	A	476	VAL	2.1
1	D	832	ALA	2.1
1	A	750	GLY	2.1
1	A	500	TYR	2.1
1	D	504	LYS	2.1
1	B	1102	GLY	2.1
1	C	813	HIS	2.1
1	A	491	ALA	2.0
1	B	780	GLY	2.0
1	D	395	THR	2.0
1	C	792	ALA	2.0
1	D	1215	ALA	2.0
1	D	780	GLY	2.0
1	D	787	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

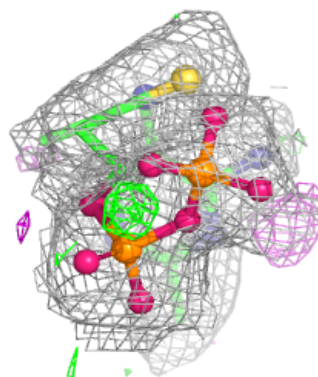
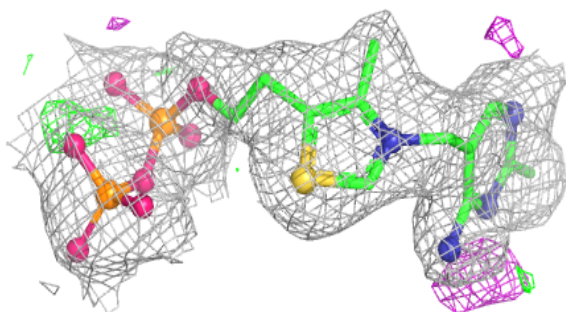
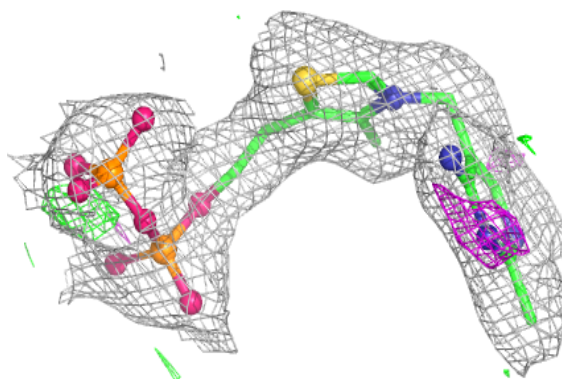
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	2001	26/26	0.96	0.08	16,26,33,34	0
2	TPP	B	2001	26/26	0.96	0.08	20,31,37,38	0
2	TPP	D	2001	26/26	0.96	0.09	23,33,36,38	0
4	CA	B	2003	1/1	0.96	0.04	38,38,38,38	0
2	TPP	C	2001	26/26	0.97	0.08	23,34,39,40	0
3	MG	D	2002	1/1	0.98	0.07	23,23,23,23	0
3	MG	A	2002	1/1	0.98	0.09	20,20,20,20	0
4	CA	C	2003	1/1	0.98	0.04	42,42,42,42	0
4	CA	A	2003	1/1	0.99	0.03	32,32,32,32	0
3	MG	C	2002	1/1	0.99	0.06	15,15,15,15	0
3	MG	B	2002	1/1	0.99	0.03	18,18,18,18	0
4	CA	D	2003	1/1	0.99	0.03	40,40,40,40	0

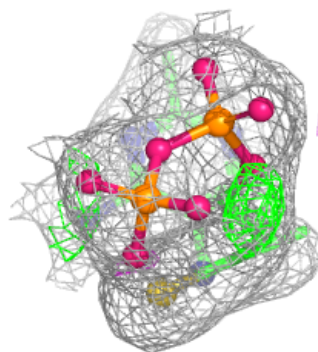
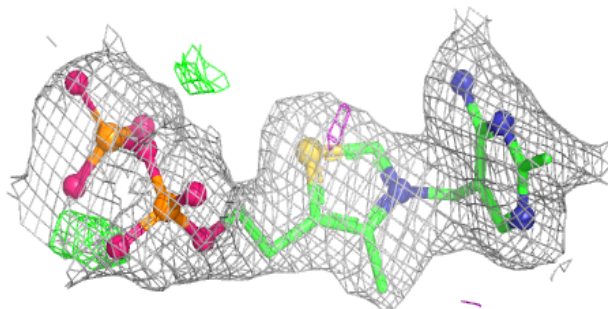
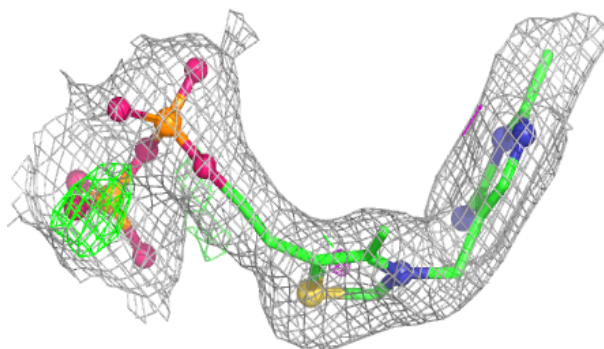
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

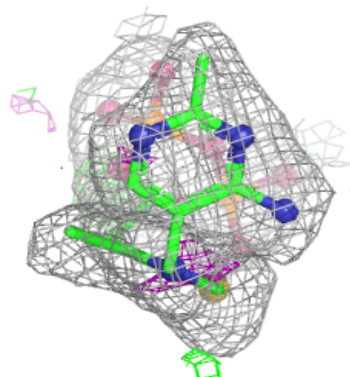
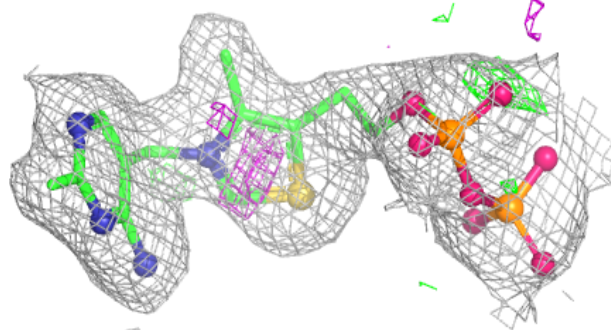
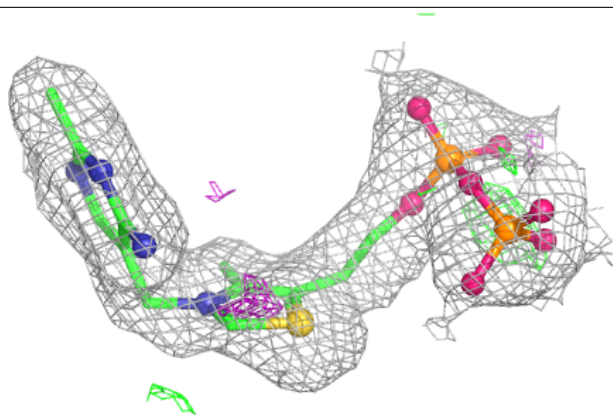
**Electron density around TPP B 2001:**

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

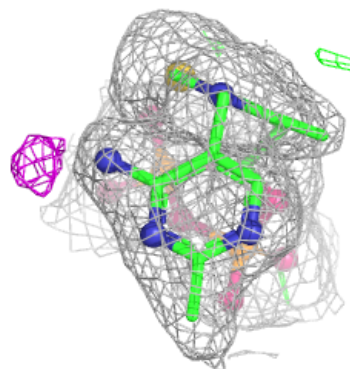
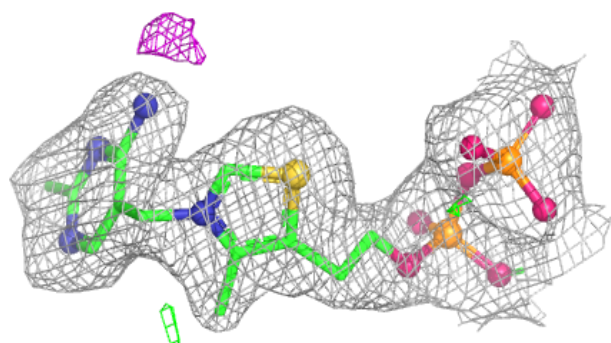
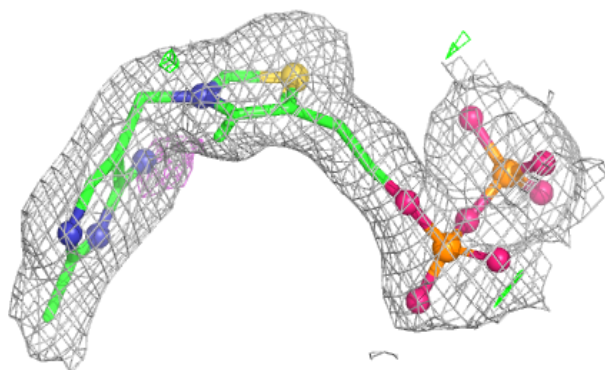


Electron density around TPP D 2001:

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

**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.