



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:57 PM UTC

PDB ID : 3ZHR / pdb_00003zhr
Title : Crystal structure of the H747A mutant of the SucA domain of Mycobacterium smegmatis KGD showing the active site lid closed
Authors : Wagner, T.; Barilone, N.; Bellinzoni, M.; Alzari, P.M.
Deposited on : 2012-12-24
Resolution : 2.10 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

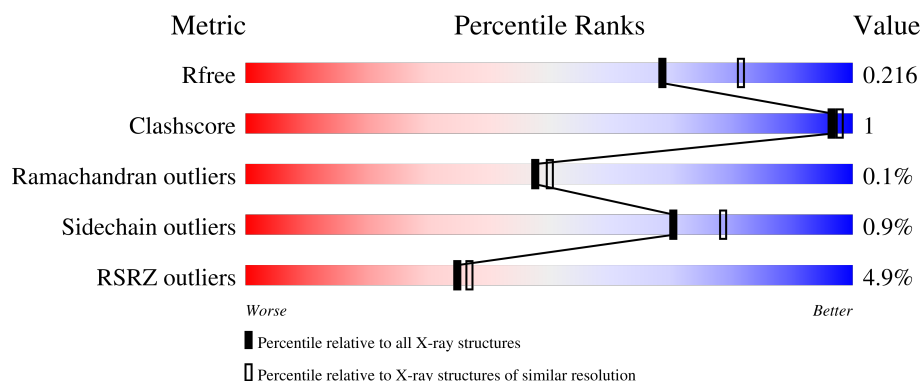
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	4% 90% 5%
1	B	868	5% 91% 5%
1	C	868	4% 91% 6%
1	D	868	6% 91% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26675 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.

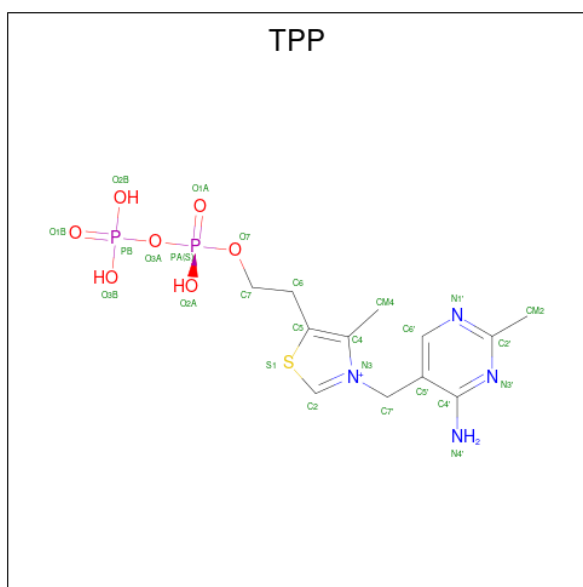
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	2	0
			6376	4017	1124	1210	25			
1	B	823	Total	C	N	O	S	0	2	0
			6371	4010	1130	1205	26			
1	C	813	Total	C	N	O	S	0	1	0
			6307	3973	1116	1193	25			
1	D	823	Total	C	N	O	S	0	1	0
			6302	3971	1109	1197	25			

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: $C_{12}H_{19}N_4O_7P_2S$).



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).

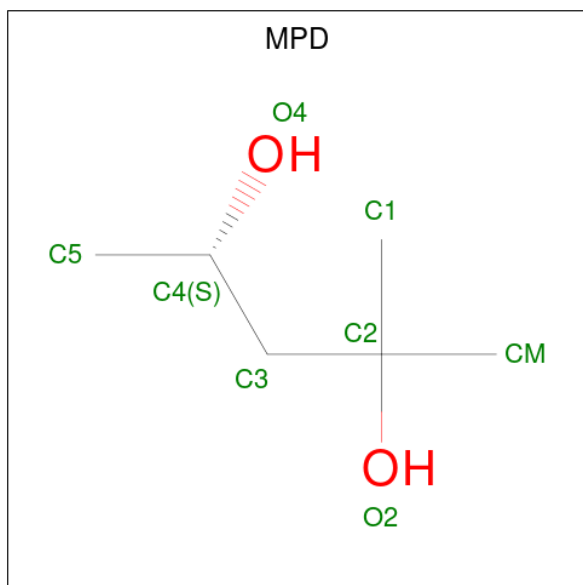
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	C	1	Total	C	O	0	0
			8	6	2		
5	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	339	Total	O	0	0
			339	339		
6	B	259	Total	O	0	0
			259	259		

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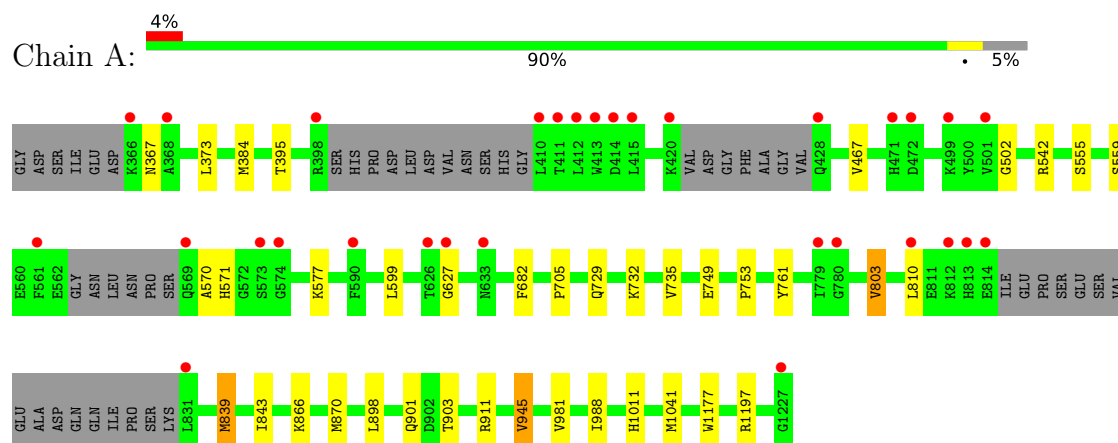
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	326	Total 326	O 326	0	0
6	D	251	Total 251	O 251	0	0

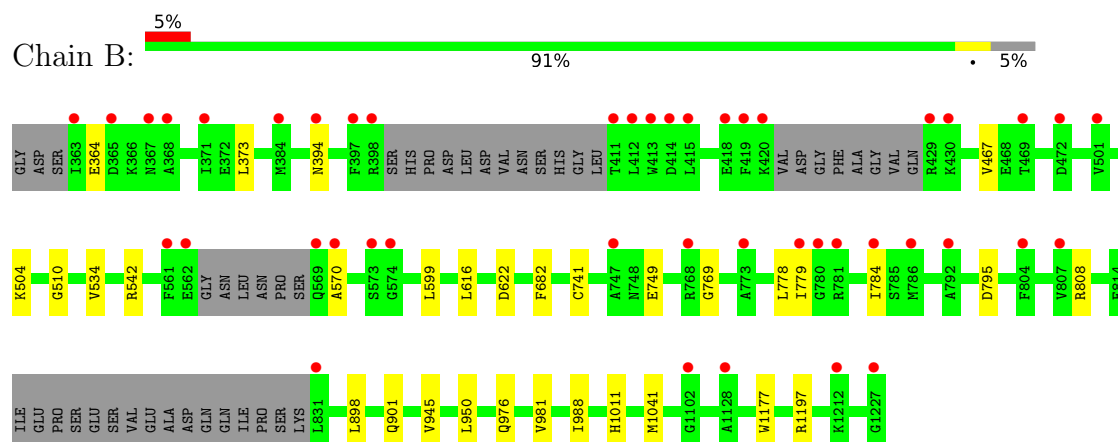
3 Residue-property plots [i](#)

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.

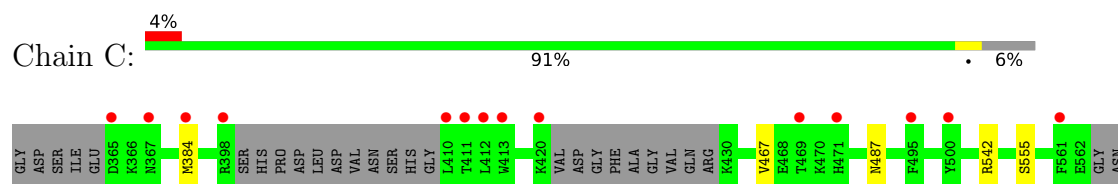
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

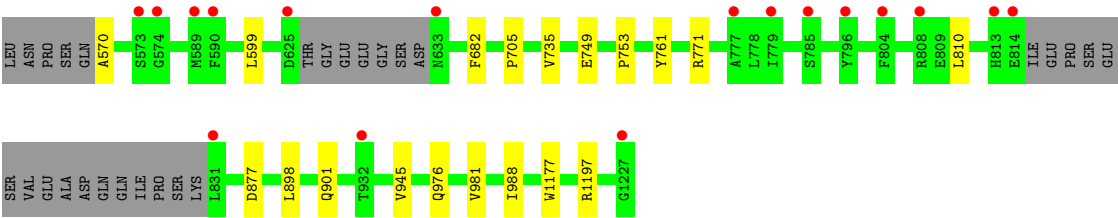


• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

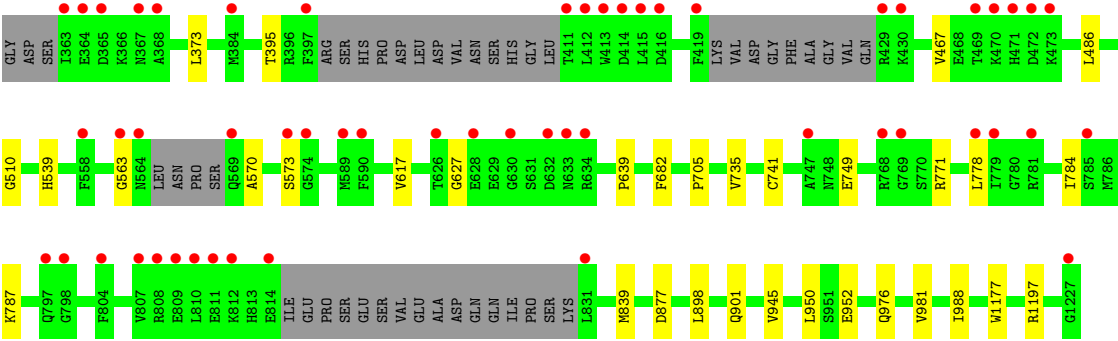
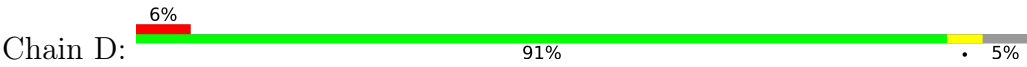


• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME





• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.97Å 83.45Å 159.67Å 99.64° 98.82° 100.98°	Depositor
Resolution (Å)	30.75 – 2.10 30.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.75-2.10) 96.8 (30.75-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.180 , 0.202 0.193 , 0.216	Depositor DCC
R_{free} test set	11124 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26675	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.34% 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: MG, TPP, CA, MPD

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	1/6511 (0.0%)	1.19	5/8828 (0.1%)
1	B	0.84	0/6501	1.18	2/8812 (0.0%)
1	C	0.85	0/6436	1.17	1/8724 (0.0%)
1	D	0.86	1/6431 (0.0%)	1.19	8/8725 (0.1%)
All	All	0.85	2/25879 (0.0%)	1.18	16/35089 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	839	MET	SD-CE	-7.75	1.60	1.79
1	D	839	MET	SD-CE	-6.36	1.63	1.79

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	627	GLY	CA-C-N	6.69	129.57	120.54
1	D	627	GLY	C-N-CA	6.69	129.57	120.54
1	A	627	GLY	CA-C-N	6.61	129.47	120.54
1	A	627	GLY	C-N-CA	6.61	129.47	120.54
1	A	803	VAL	N-CA-CB	6.13	117.72	110.55
1	D	563	GLY	CA-C-N	5.96	132.42	121.70
1	D	563	GLY	C-N-CA	5.96	132.42	121.70
1	B	622	ASP	CA-CB-CG	5.23	117.83	112.60
1	C	877	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	795	ASP	N-CA-C	-5.20	105.29	111.69
1	D	952	GLU	N-CA-C	-5.20	106.07	112.72
1	D	877	ASP	CA-CB-CG	5.14	117.74	112.60
1	D	395	THR	CA-C-N	5.10	127.07	120.44
1	D	395	THR	C-N-CA	5.10	127.07	120.44
1	A	395	THR	CA-C-N	5.05	127.01	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	THR	C-N-CA	5.05	127.01	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	6376	0	6164	17	0
1	B	6371	0	6158	11	0
1	C	6307	0	6102	10	0
1	D	6302	0	6048	11	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	8	0	14	0	0
5	B	8	0	14	0	0
5	C	8	0	14	0	0
5	D	8	0	14	0	0
6	A	339	0	0	1	0
6	B	259	0	0	1	0
6	C	326	0	0	0	0
6	D	251	0	0	0	0
All	All	26675	0	24592	49	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 1.

All (49) 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:A:570:ALA:HA	1:A:749:GLU:HB2	1.81	0.62
1:B:542:ARG:NE	1:B:599:LEU:HD21	2.17	0.59
1:C:570:ALA:HA	1:C:749:GLU:HB2	1.87	0.56
1:D:570:ALA:HA	1:D:749:GLU:HB2	1.88	0.56
1:A:705:PRO:HG2	1:A:735:VAL:HG13	1.93	0.51
1:B:534:VAL:HG11	1:B:616:LEU:HD22	1.94	0.50
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.93	0.50
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.95	0.49
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.94	0.49
1:A:1011:HIS:HD2	1:A:1041[B]:MET:HE1	1.77	0.49
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.95	0.48
1:A:559:SER:O	1:A:577:LYS:NZ	2.45	0.48
1:A:901:GLN:OE1	2:B:2001:TPP:H6'	2.15	0.47
1:A:571:HIS:HE1	6:A:3056:HOH:O	1.98	0.47
1:A:898:LEU:O	1:A:945:VAL:HA	2.15	0.46
1:B:570:ALA:HA	1:B:749:GLU:HB2	1.98	0.46
1:B:1011:HIS:HD2	1:B:1041[B]:MET:HE1	1.80	0.46
1:A:542:ARG:NE	1:A:599:LEU:HD21	2.30	0.46
1:D:617:VAL:HG11	1:D:639:PRO:HG3	1.98	0.45
1:C:898:LEU:O	1:C:945:VAL:HA	2.15	0.45
1:D:510:GLY:O	1:D:741:CYS:HB2	2.15	0.45
2:A:2001:TPP:H6'	1:B:901:GLN:OE1	2.16	0.45
1:A:866:LYS:HG3	1:A:870:MET:HE2	1.97	0.45
1:C:901:GLN:OE1	2:D:2001:TPP:H6'	2.16	0.45
1:D:539:HIS:HE1	1:D:573:SER:HB2	1.81	0.45
1:B:898:LEU:O	1:B:945:VAL:HA	2.18	0.44
2:C:2001:TPP:H6'	1:D:901:GLN:OE1	2.17	0.44
1:D:898:LEU:O	1:D:945:VAL:HA	2.18	0.44
1:C:542:ARG:NE	1:C:599:LEU:HD21	2.33	0.44
1:B:510:GLY:O	1:B:741:CYS:HB2	2.18	0.43
1:B:778:LEU:HB3	1:B:784:ILE:HG12	2.00	0.43
1:D:705:PRO:HG2	1:D:735:VAL:HG13	2.00	0.43
1:A:555:SER:HA	1:A:810:LEU:HD22	2.01	0.43
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.55	0.42
1:C:555:SER:HA	1:C:810:LEU:HD22	2.01	0.42
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.55	0.42
1:D:778:LEU:HB3	1:D:784:ILE:HG12	2.01	0.42
1:A:729:GLN:O	1:A:732:LYS:HE3	2.19	0.42
1:C:487:ASN:OD1	1:C:771:ARG:HD2	2.20	0.42
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:GLY:HA3	6:B:3024:HOH:O	2.20	0.41
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.55	0.41
1:C:753:PRO:HB2	1:C:761:TYR:CE1	2.56	0.41
1:D:486:LEU:HD13	1:D:771:ARG:HA	2.02	0.41
1:A:502:GLY:HA2	1:A:749:GLU:HG3	2.03	0.41
1:A:753:PRO:HB2	1:A:761:TYR:CE1	2.57	0.40
1:A:903:THR:O	1:A:911:ARG:HD2	2.22	0.40
1:C:705:PRO:HG2	1:C:735:VAL:HG13	2.02	0.40
1:A:839:MET:HE2	1:A:843:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	814/868 (94%)	797 (98%)	16 (2%)	1 (0%)	48	50
1	B	815/868 (94%)	798 (98%)	16 (2%)	1 (0%)	48	50
1	C	802/868 (92%)	789 (98%)	12 (2%)	1 (0%)	48	50
1	D	814/868 (94%)	793 (97%)	20 (2%)	1 (0%)	48	50
All	All	3245/3472 (94%)	3177 (98%)	64 (2%)	4 (0%)	48	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	682	PHE
1	B	682	PHE
1	C	682	PHE
1	D	682	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	657/725 (91%)	651 (99%)	6 (1%)	70	78
1	B	653/725 (90%)	644 (99%)	9 (1%)	59	67
1	C	649/725 (90%)	646 (100%)	3 (0%)	81	88
1	D	639/725 (88%)	634 (99%)	5 (1%)	73	81
All	All	2598/2900 (90%)	2575 (99%)	23 (1%)	70	78

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	373	LEU
1	A	384	MET
1	A	467	VAL
1	A	803	VAL
1	A	945	VAL
1	B	364	GLU
1	B	373	LEU
1	B	394	ASN
1	B	467	VAL
1	B	504	LYS
1	B	779	ILE
1	B	808	ARG
1	B	950	LEU
1	B	976	GLN
1	C	384	MET
1	C	467	VAL
1	C	976	GLN
1	D	373	LEU
1	D	467	VAL
1	D	787	LYS
1	D	950	LEU
1	D	976	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	548	ASN
1	A	593	ASN
1	A	1030	GLN
1	A	1061	GLN
1	B	548	ASN
1	B	985	GLN
1	B	1020	HIS
1	B	1061	GLN
1	B	1107	ASN
1	C	593	ASN
1	C	1219	GLN
1	D	503	GLN
1	D	548	ASN
1	D	757	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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TPP	D	2001	3	26,27,27	1.29	3 (11%)	38,40,40	1.66	12 (31%)
5	MPD	D	2228	-	7,7,7	0.58	0	9,10,10	0.45	0
5	MPD	A	2228	-	7,7,7	0.64	0	9,10,10	0.43	0
2	TPP	B	2001	3	26,27,27	1.34	3 (11%)	38,40,40	1.55	9 (23%)
2	TPP	C	2001	3	26,27,27	1.32	3 (11%)	38,40,40	1.60	9 (23%)
5	MPD	B	2228	-	7,7,7	0.60	0	9,10,10	0.43	0
2	TPP	A	2001	3	26,27,27	1.26	3 (11%)	38,40,40	1.54	9 (23%)
5	MPD	C	2228	-	7,7,7	0.61	0	9,10,10	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	D	2001	3	-	2/17/17/17	0/2/2/2
5	MPD	D	2228	-	-	1/5/5/5	-
5	MPD	A	2228	-	-	1/5/5/5	-
2	TPP	B	2001	3	-	0/17/17/17	0/2/2/2
2	TPP	C	2001	3	-	2/17/17/17	0/2/2/2
5	MPD	B	2228	-	-	1/5/5/5	-
2	TPP	A	2001	3	-	1/17/17/17	0/2/2/2
5	MPD	C	2228	-	-	1/5/5/5	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	TPP	PB-O1B	3.31	1.60	1.50
2	D	2001	TPP	C4-N3	-3.28	1.33	1.39
2	C	2001	TPP	PA-O3A	3.21	1.63	1.59
2	B	2001	TPP	C4-N3	-3.01	1.33	1.39
2	A	2001	TPP	PB-O1B	2.92	1.59	1.50
2	C	2001	TPP	C4-N3	-2.77	1.34	1.39
2	D	2001	TPP	PB-O1B	2.75	1.59	1.50
2	C	2001	TPP	PB-O1B	2.73	1.59	1.50
2	A	2001	TPP	C4-N3	-2.65	1.34	1.39
2	A	2001	TPP	PA-O3A	2.29	1.62	1.59
2	B	2001	TPP	PA-O3A	2.13	1.61	1.59
2	D	2001	TPP	C4'-N4'	2.08	1.39	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	TPP	CM4-C4-C5	-4.07	117.33	127.75
2	D	2001	TPP	C6'-N1'-C2'	3.88	122.45	116.07
2	A	2001	TPP	CM4-C4-C5	-3.81	117.97	127.75
2	B	2001	TPP	CM4-C4-C5	-3.53	118.71	127.75
2	D	2001	TPP	CM4-C4-C5	-3.35	119.16	127.75
2	B	2001	TPP	C6'-N1'-C2'	3.33	121.55	116.07
2	C	2001	TPP	C6'-N1'-C2'	3.27	121.45	116.07
2	D	2001	TPP	N1'-C2'-N3'	-3.26	120.11	125.53
2	A	2001	TPP	C6'-N1'-C2'	3.21	121.34	116.07
2	B	2001	TPP	N1'-C2'-N3'	-3.00	120.54	125.53
2	A	2001	TPP	N1'-C2'-N3'	-2.99	120.56	125.53
2	C	2001	TPP	N1'-C2'-N3'	-2.82	120.84	125.53
2	D	2001	TPP	C5'-C6'-N1'	-2.76	119.34	123.83
2	C	2001	TPP	C7-C6-C5	-2.74	104.13	112.73
2	D	2001	TPP	C2-S1-C5	-2.69	89.43	91.22
2	C	2001	TPP	C4-C5-S1	-2.68	106.38	110.56
2	C	2001	TPP	CM4-C4-N3	2.62	126.61	120.57
2	A	2001	TPP	CM4-C4-N3	2.51	126.37	120.57
2	B	2001	TPP	C5'-C6'-N1'	-2.49	119.78	123.83
2	A	2001	TPP	C7-C6-C5	-2.47	104.98	112.73
2	B	2001	TPP	C7-C6-C5	-2.40	105.20	112.73
2	D	2001	TPP	C7-C6-C5	-2.34	105.39	112.73
2	D	2001	TPP	O2A-PA-O3A	2.32	113.54	107.27
2	B	2001	TPP	C2'-N3'-C4'	2.31	121.66	118.10
2	C	2001	TPP	C5-C4-N3	2.30	115.85	111.67
2	D	2001	TPP	C2'-N3'-C4'	2.29	121.62	118.10
2	A	2001	TPP	CM2-C2'-N1'	2.28	119.63	117.20
2	C	2001	TPP	C7'-N3-C2	-2.24	118.81	123.48
2	B	2001	TPP	CM2-C2'-N1'	2.20	119.55	117.20
2	A	2001	TPP	C4-C5-S1	-2.19	107.15	110.56
2	B	2001	TPP	C5-C4-N3	2.18	115.64	111.67
2	D	2001	TPP	CM2-C2'-N3'	2.16	120.37	117.13
2	A	2001	TPP	O2A-PA-O3A	2.16	113.11	107.27
2	D	2001	TPP	CM2-C2'-N1'	2.14	119.47	117.20
2	C	2001	TPP	C5'-C6'-N1'	-2.10	120.41	123.83
2	A	2001	TPP	C5-C4-N3	2.10	115.49	111.67
2	B	2001	TPP	CM4-C4-N3	2.08	125.36	120.57
2	D	2001	TPP	CM4-C4-N3	2.06	125.31	120.57
2	D	2001	TPP	C5-C4-N3	2.01	115.33	111.67

There are no chirality outliers.

All (9) torsion outliers are listed below:

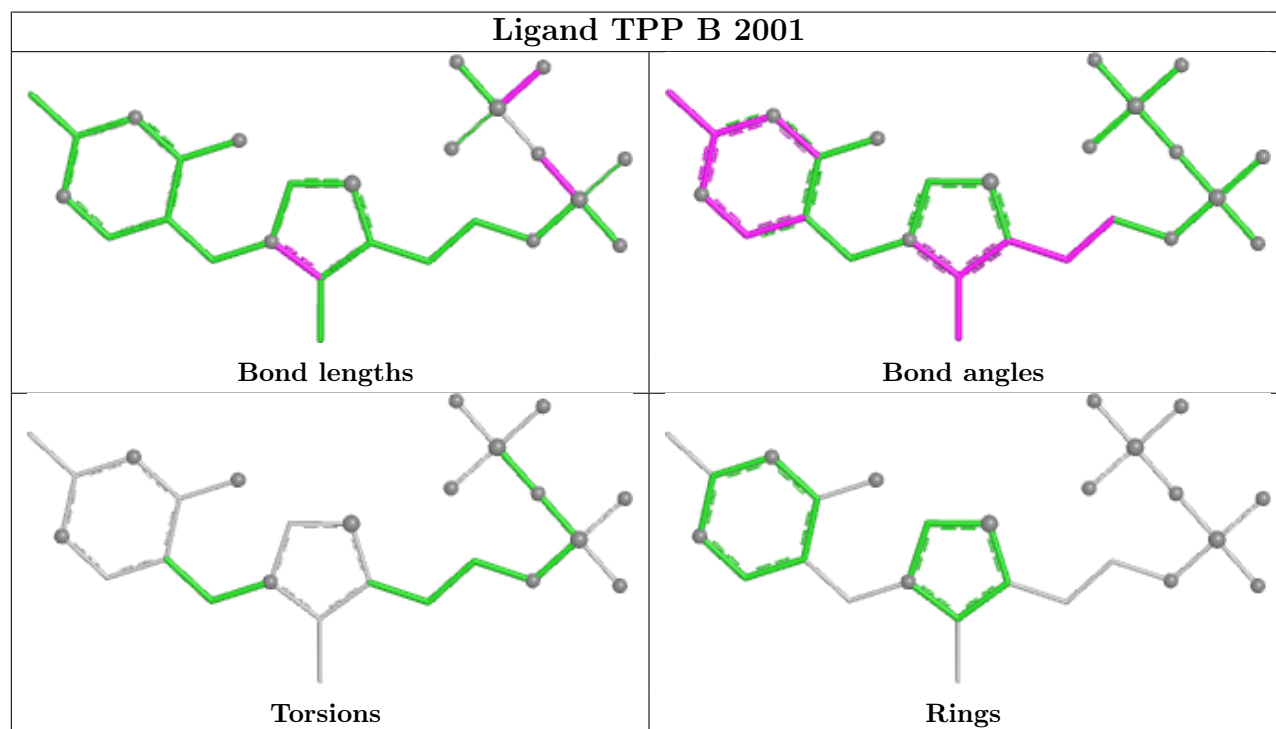
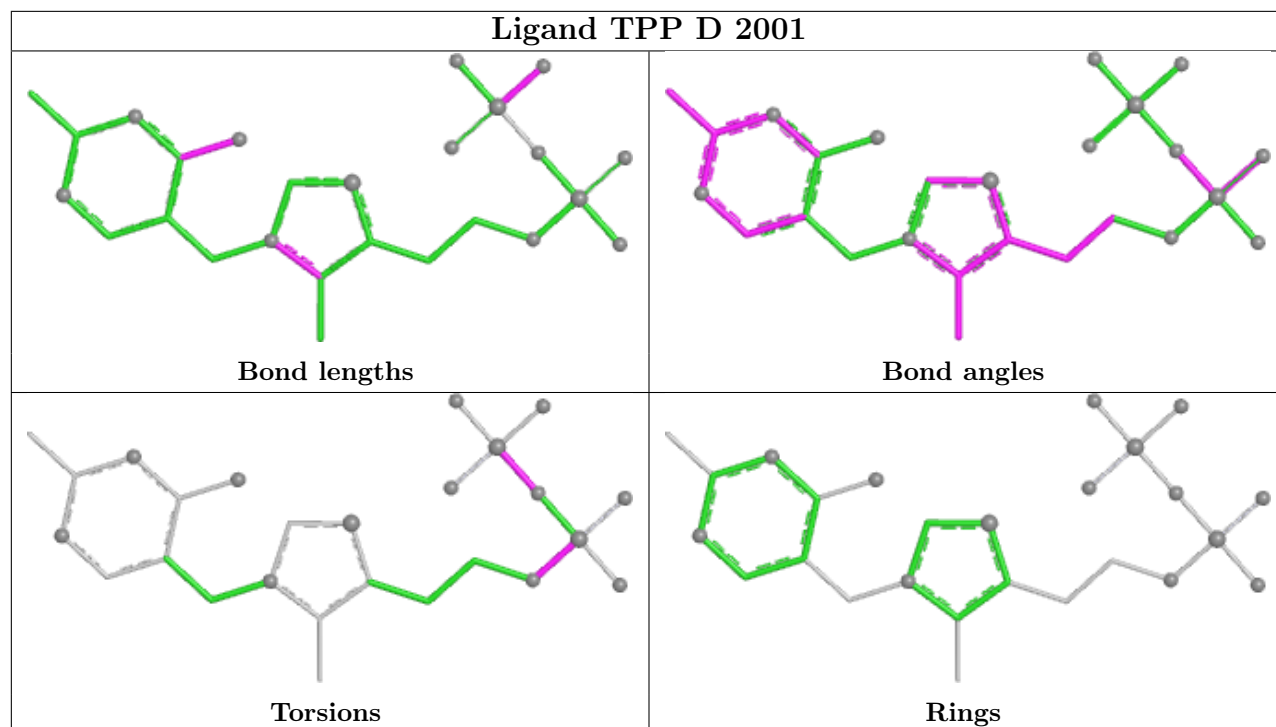
Mol	Chain	Res	Type	Atoms
5	B	2228	MPD	O2-C2-C3-C4
5	D	2228	MPD	O2-C2-C3-C4
2	A	2001	TPP	C7-O7-PA-O1A
2	C	2001	TPP	C7-O7-PA-O1A
2	D	2001	TPP	C7-O7-PA-O1A
2	C	2001	TPP	PA-O3A-PB-O3B
2	D	2001	TPP	PA-O3A-PB-O3B
5	A	2228	MPD	O2-C2-C3-C4
5	C	2228	MPD	O2-C2-C3-C4

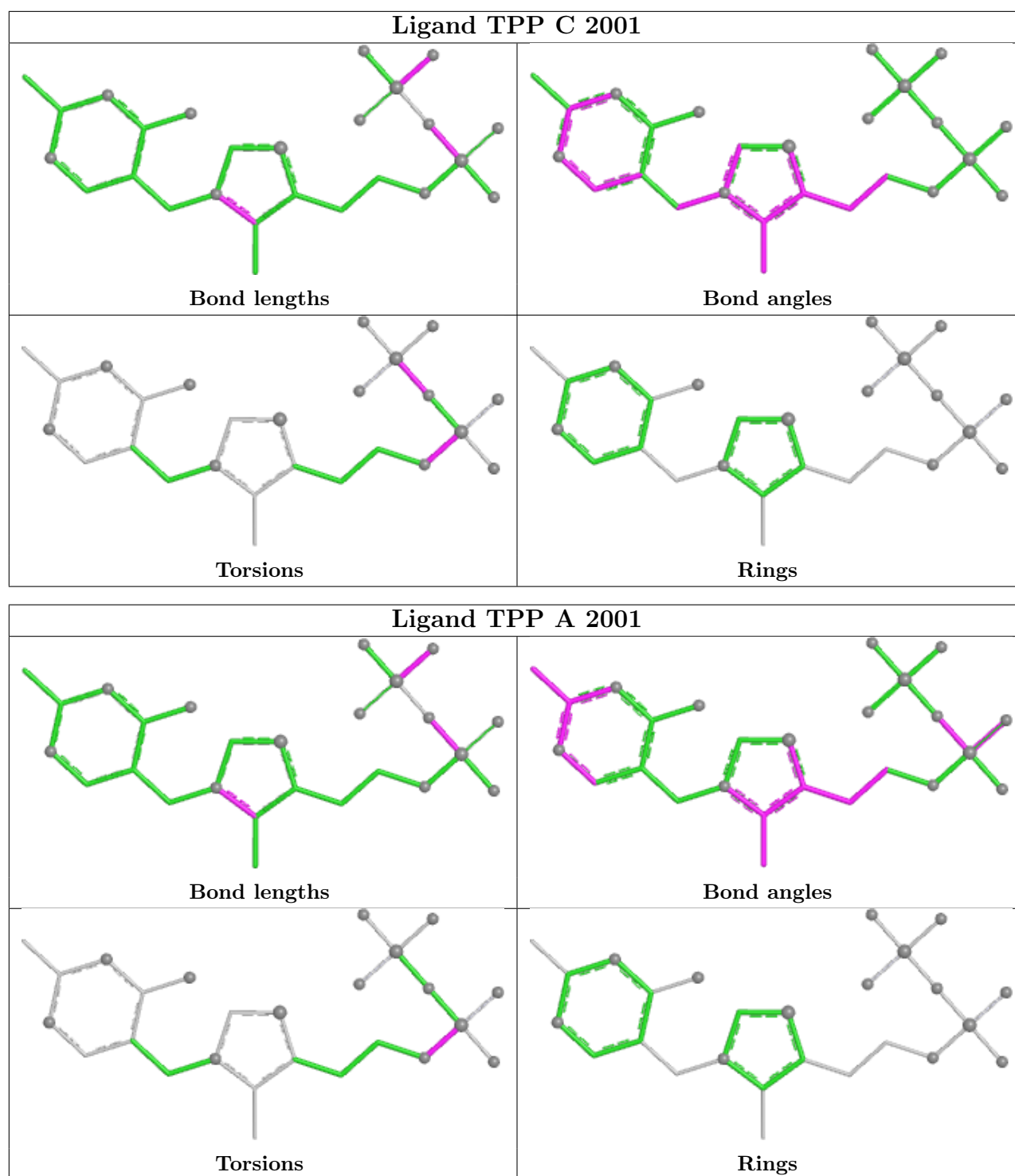
There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	822/868 (94%)	0.13	31 (3%)	44	46	18, 35, 68, 99	2 (0%)
1	B	823/868 (94%)	0.19	44 (5%)	32	34	14, 35, 73, 121	2 (0%)
1	C	813/868 (93%)	0.11	31 (3%)	44	46	16, 33, 68, 108	1 (0%)
1	D	823/868 (94%)	0.22	54 (6%)	24	26	16, 35, 74, 104	1 (0%)
All	All	3281/3472 (94%)	0.16	160 (4%)	35	37	14, 35, 71, 121	6 (0%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	574	GLY	12.5
1	D	564	ASN	7.1
1	B	574	GLY	5.8
1	C	573	SER	5.3
1	B	363	ILE	5.3
1	C	420	LYS	5.2
1	B	411	THR	5.2
1	D	397	PHE	5.1
1	A	398	ARG	5.1
1	D	470	LYS	5.1
1	D	807	VAL	4.9
1	D	472	ASP	4.8
1	C	574	GLY	4.8
1	D	363	ILE	4.8
1	B	420	LYS	4.7
1	B	397	PHE	4.5
1	D	411	THR	4.5
1	C	398	ARG	4.4
1	D	590	PHE	4.4
1	D	471	HIS	4.2
1	D	1227	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	410	LEU	4.1
1	D	365	ASP	4.1
1	B	398	ARG	4.0
1	A	420	LYS	4.0
1	D	810	LEU	3.9
1	D	563	GLY	3.9
1	D	419	PHE	3.9
1	D	573	SER	3.8
1	D	809	GLU	3.7
1	B	1227	GLY	3.7
1	B	419	PHE	3.7
1	A	410	LEU	3.7
1	B	573	SER	3.6
1	C	633	ASN	3.5
1	A	413	TRP	3.5
1	A	411	THR	3.5
1	D	626	THR	3.5
1	A	573	SER	3.4
1	D	367	ASN	3.4
1	B	413	TRP	3.3
1	C	413	TRP	3.3
1	B	430	LYS	3.3
1	B	365	ASP	3.3
1	B	1102	GLY	3.3
1	C	411	THR	3.2
1	C	813	HIS	3.1
1	C	471	HIS	3.1
1	B	414	ASP	3.1
1	A	569	GLN	3.0
1	C	469	THR	3.0
1	D	632	ASP	3.0
1	D	473	LYS	3.0
1	B	418	GLU	2.9
1	C	365	ASP	2.9
1	B	779	ILE	2.9
1	D	412	LEU	2.9
1	A	472	ASP	2.9
1	D	429	ARG	2.8
1	D	469	THR	2.8
1	B	472	ASP	2.8
1	B	781	ARG	2.8
1	D	413	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	779	ILE	2.8
1	C	625	ASP	2.8
1	A	412	LEU	2.7
1	B	784	ILE	2.7
1	D	364	GLU	2.7
1	B	747	ALA	2.7
1	A	812	LYS	2.7
1	D	634	ARG	2.7
1	D	368	ALA	2.7
1	D	558	PHE	2.7
1	B	562	GLU	2.7
1	A	1227	GLY	2.6
1	A	590	PHE	2.6
1	D	414	ASP	2.6
1	C	785	SER	2.6
1	D	797	GLN	2.6
1	B	792	ALA	2.6
1	D	384	MET	2.5
1	A	499	LYS	2.5
1	D	569	GLN	2.5
1	B	412	LEU	2.5
1	B	415	LEU	2.5
1	B	831	LEU	2.5
1	A	627	GLY	2.5
1	C	779	ILE	2.5
1	A	633	ASN	2.5
1	B	368	ALA	2.5
1	A	831	LEU	2.5
1	C	412	LEU	2.5
1	D	831	LEU	2.5
1	A	814	GLU	2.4
1	B	570	ALA	2.4
1	D	804	PHE	2.4
1	B	569	GLN	2.4
1	B	786	MET	2.4
1	A	813	HIS	2.4
1	C	804	PHE	2.4
1	D	781	ARG	2.4
1	B	773	ALA	2.4
1	A	415	LEU	2.4
1	B	429	ARG	2.4
1	D	808	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	812	LYS	2.4
1	A	810	LEU	2.3
1	D	769	GLY	2.3
1	D	589	MET	2.3
1	A	780	GLY	2.3
1	C	561	PHE	2.3
1	D	768	ARG	2.3
1	D	778	LEU	2.3
1	B	561	PHE	2.3
1	D	811	GLU	2.3
1	B	501	VAL	2.3
1	B	367	ASN	2.3
1	B	394	ASN	2.3
1	B	384	MET	2.3
1	C	814	GLU	2.2
1	D	814	GLU	2.2
1	C	590	PHE	2.2
1	A	779	ILE	2.2
1	B	469	THR	2.2
1	B	807	VAL	2.2
1	A	368	ALA	2.2
1	C	831	LEU	2.2
1	A	561	PHE	2.2
1	C	808	ARG	2.2
1	A	471	HIS	2.2
1	C	932	THR	2.2
1	D	416	ASP	2.2
1	B	1128	ALA	2.1
1	D	785	SER	2.1
1	D	747	ALA	2.1
1	A	366	LYS	2.1
1	D	633	ASN	2.1
1	B	780	GLY	2.1
1	C	1227	GLY	2.1
1	D	574	GLY	2.1
1	D	630	GLY	2.1
1	C	367	ASN	2.1
1	C	500	TYR	2.1
1	C	796	TYR	2.1
1	B	371	ILE	2.1
1	C	495	PHE	2.1
1	C	384	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	414	ASP	2.0
1	B	768	ARG	2.0
1	A	626	THR	2.0
1	B	1212	LYS	2.0
1	A	501	VAL	2.0
1	B	804	PHE	2.0
1	D	628	GLU	2.0
1	C	589	MET	2.0
1	C	777	ALA	2.0
1	A	428	GLN	2.0
1	D	415	LEU	2.0
1	D	430	LYS	2.0
1	D	798	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.

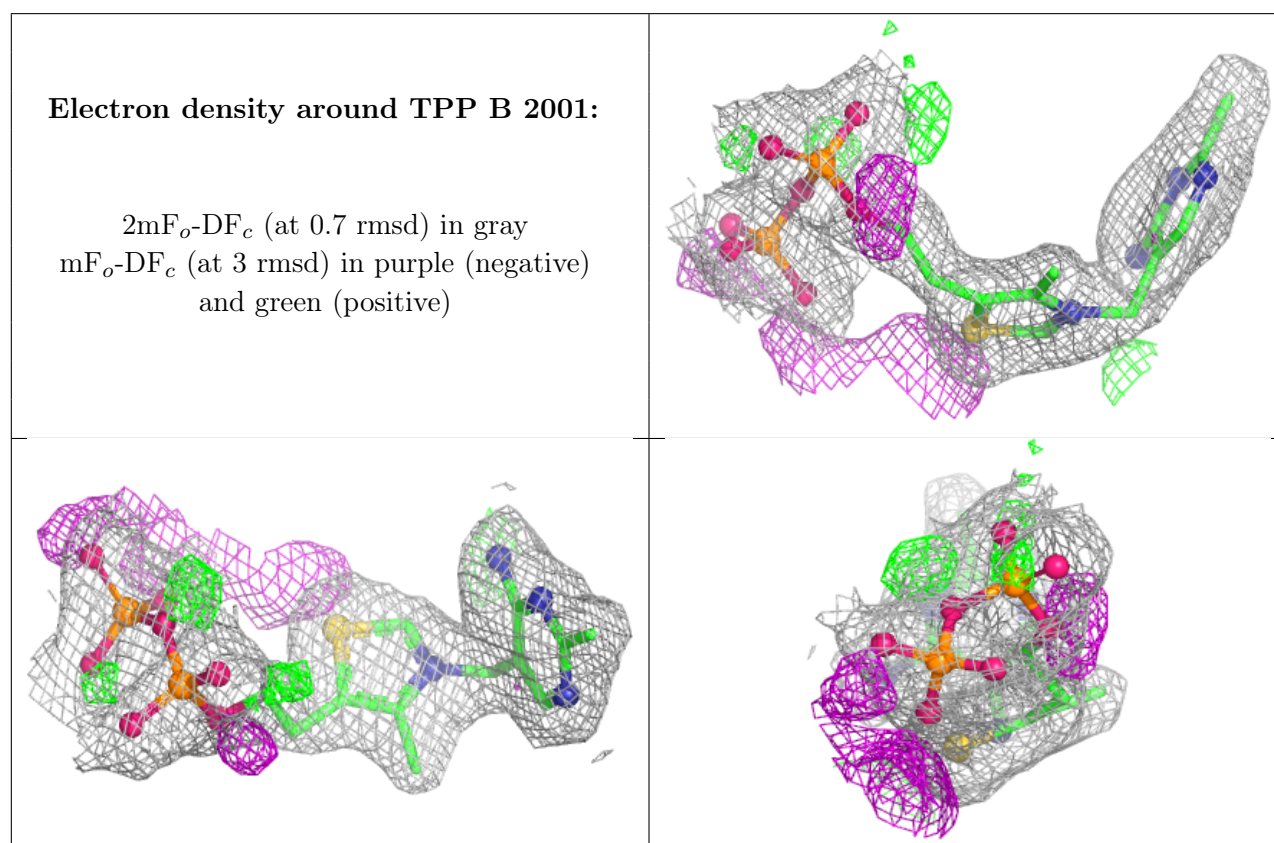
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MPD	A	2228	8/8	0.86	0.18	68,69,71,71	0
5	MPD	B	2228	8/8	0.89	0.12	47,49,50,50	0
5	MPD	C	2228	8/8	0.89	0.15	64,64,65,66	0
5	MPD	D	2228	8/8	0.89	0.13	48,51,52,53	0
2	TPP	B	2001	26/26	0.97	0.06	16,24,28,31	0
2	TPP	D	2001	26/26	0.97	0.06	14,21,25,28	0
2	TPP	C	2001	26/26	0.98	0.05	17,23,25,26	0
2	TPP	A	2001	26/26	0.98	0.05	19,22,26,27	0
3	MG	A	2002	1/1	0.98	0.05	12,12,12,12	0
4	CA	B	2003	1/1	0.98	0.04	32,32,32,32	0

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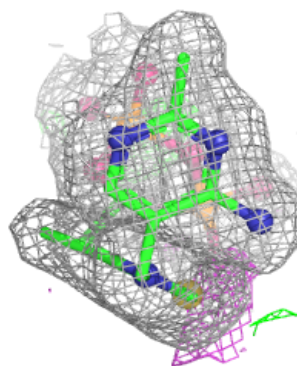
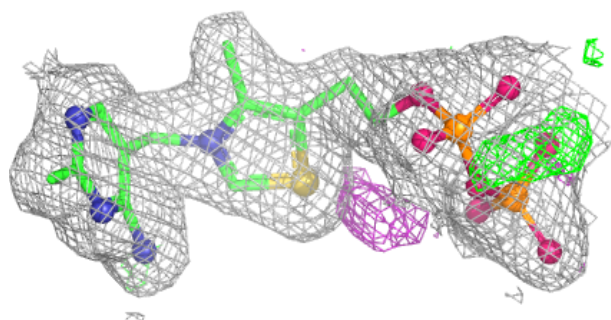
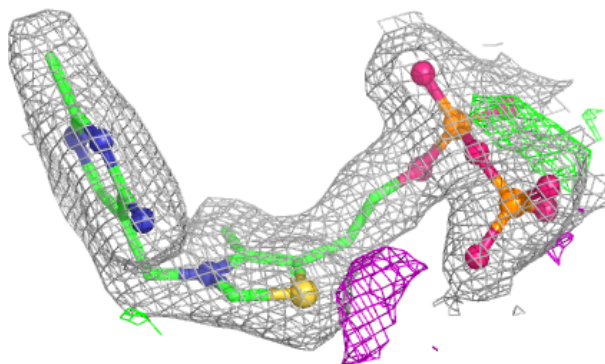
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	C	2003	1/1	0.99	0.03	29,29,29,29	0
4	CA	D	2003	1/1	0.99	0.04	30,30,30,30	0
3	MG	C	2002	1/1	0.99	0.06	11,11,11,11	0
3	MG	D	2002	1/1	0.99	0.08	16,16,16,16	0
4	CA	A	2003	1/1	0.99	0.05	29,29,29,29	0
3	MG	B	2002	1/1	0.99	0.05	16,16,16,16	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.

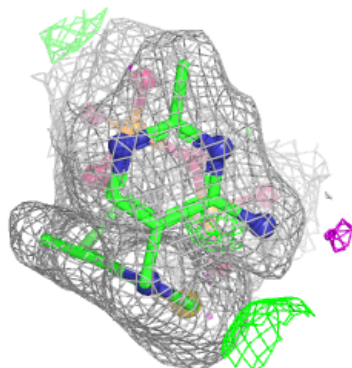
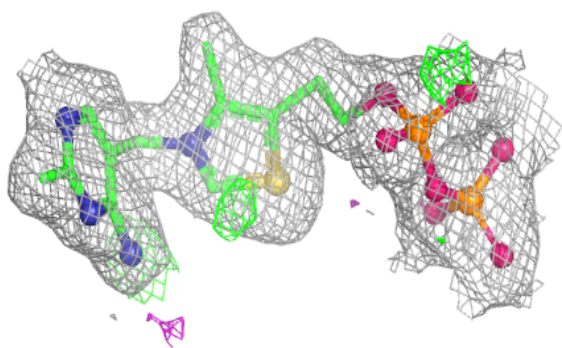
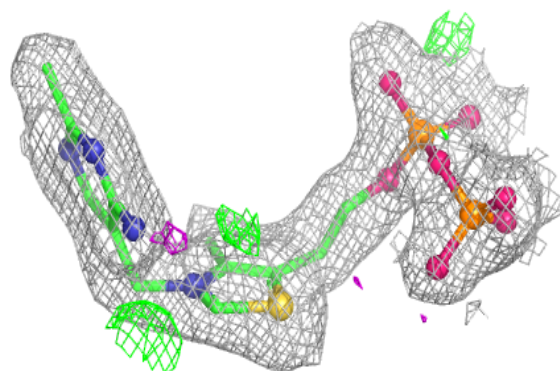


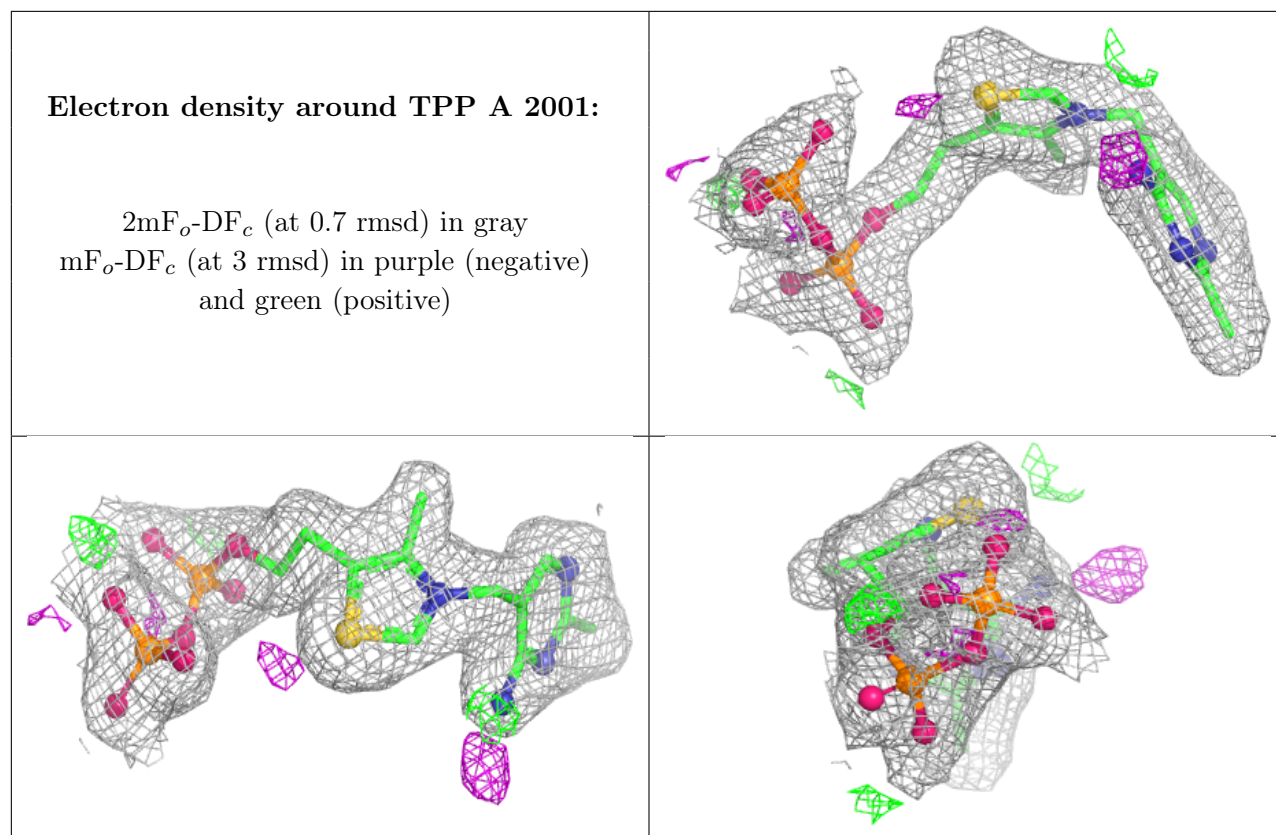
Electron density around TPP D 2001:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.