



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:39 PM UTC

PDB ID : 6R2C / pdb_00006r2c
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis KGD after soaking with succinylphosphonate phosphonoethyl ester (PESP)
Authors : Wagner, T.; Alzari, P.M.; Bellinzoni, M.
Deposited on : 2019-03-15
Resolution : 2.09 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

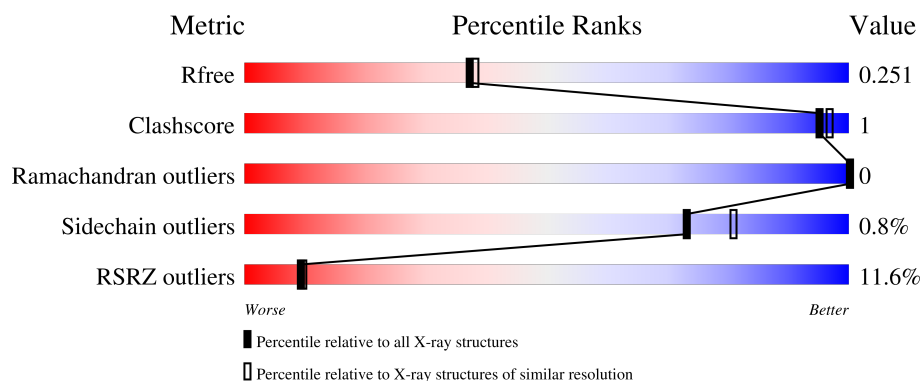
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	10% 90% 6%
1	B	868	12% 90% 6%
1	C	868	12% 90% 6%
1	D	868	10% 90% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26262 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.

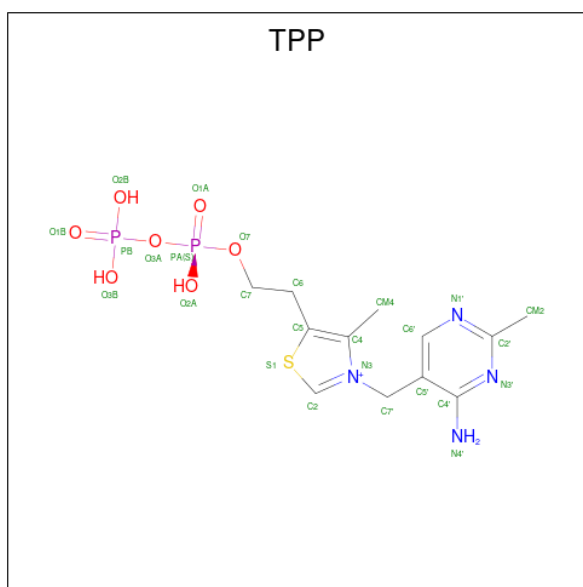
- Molecule 1 is a protein called Multifunctional 2-oxoglutarate metabolism enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	814	Total	C	N	O	S	0	1	0
			6331	3987	1121	1199	24			
1	B	815	Total	C	N	O	S	0	0	0
			6288	3965	1118	1181	24			
1	C	813	Total	C	N	O	S	0	2	0
			6357	4003	1126	1205	23			
1	D	812	Total	C	N	O	S	0	0	0
			6275	3954	1107	1191	23			

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: 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	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

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

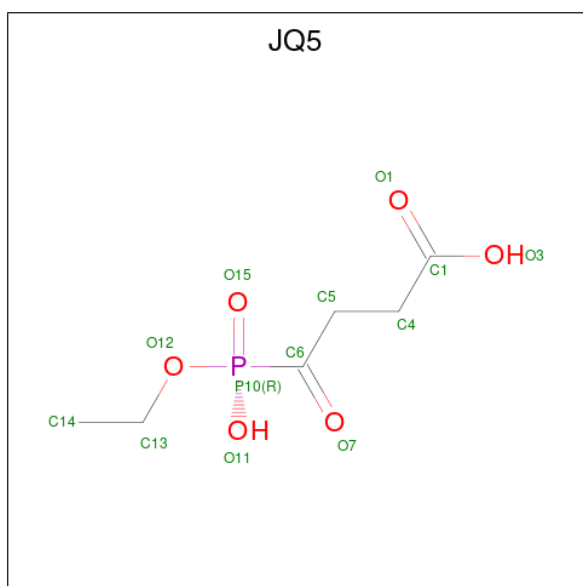
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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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 4-[ethoxy(oxidanyl)phosphoryl]-4-oxidanylidene-butanoic acid (CCD ID: JQ5) (formula: C₆H₁₁O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			13	6	6	1		
5	B	1	Total	C	O	P	0	0
			13	6	6	1		
5	C	1	Total	C	O	P	0	0
			13	6	6	1		
5	D	1	Total	C	O	P	0	0
			13	6	6	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	219	Total	O	0	0
			219	219		
6	B	214	Total	O	0	0
			214	214		

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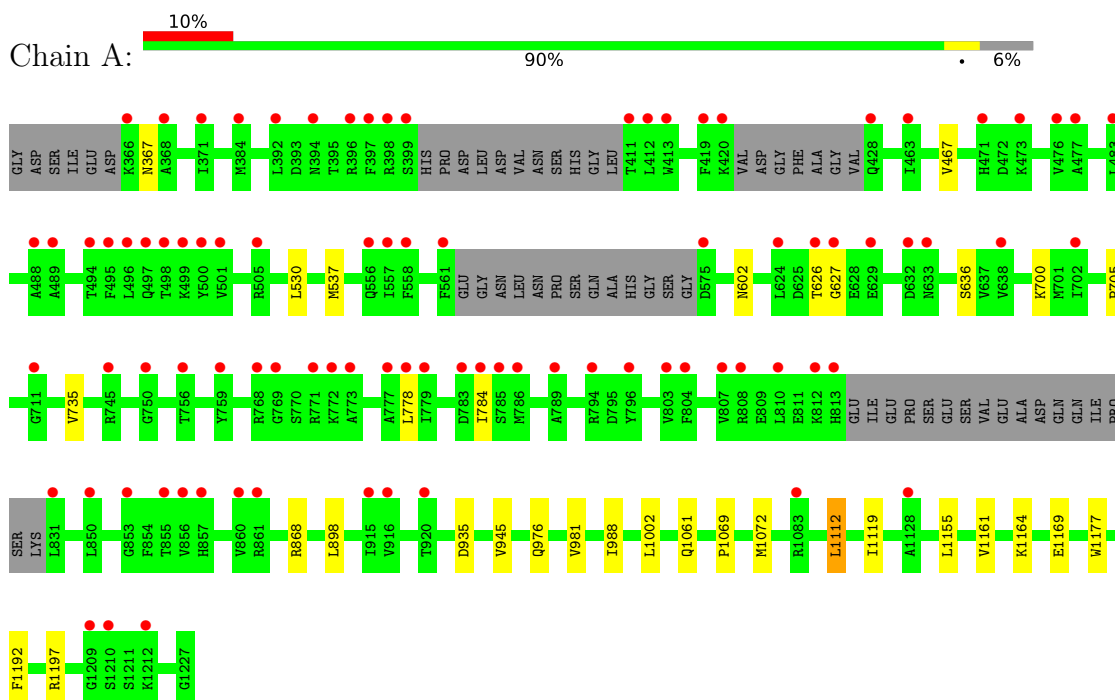
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	192	Total 192	O 192	0	0
6	D	222	Total 222	O 222	0	0

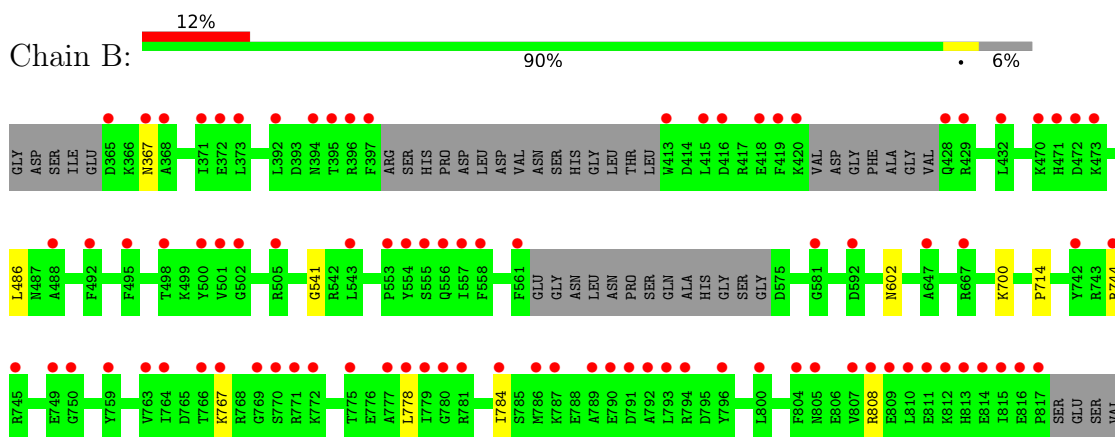
3 Residue-property plots [i](#)

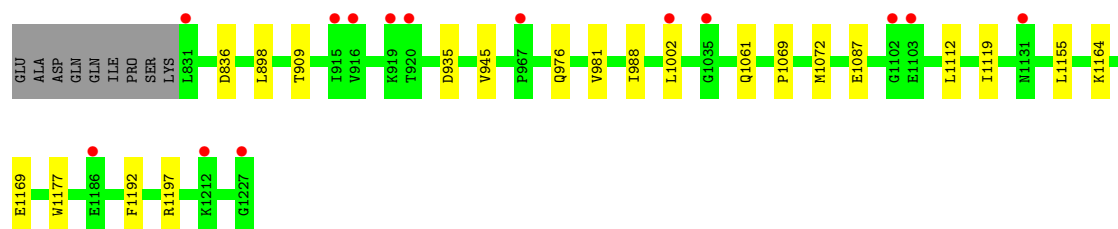
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

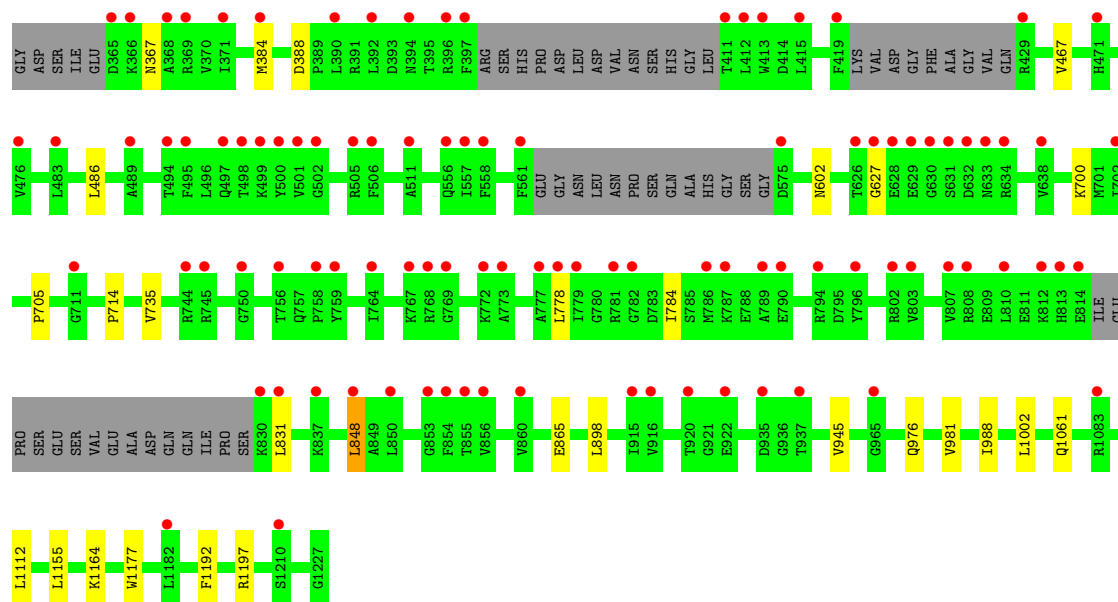
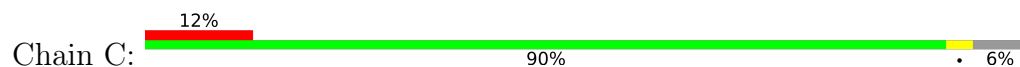


- Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

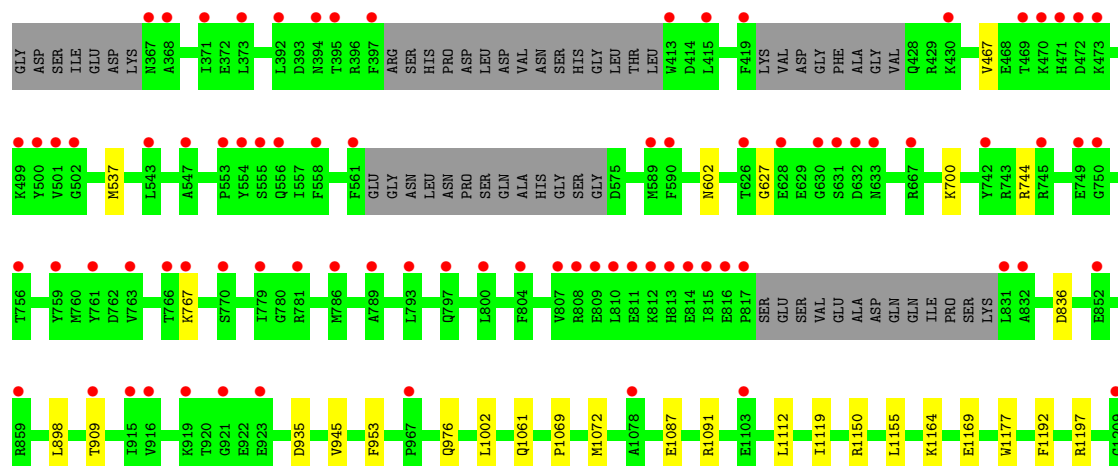
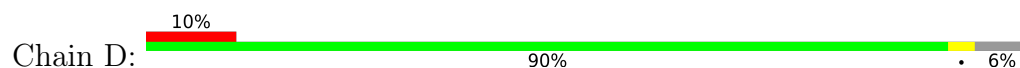


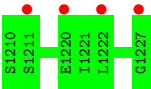


- Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme



- 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	81.39Å 83.96Å 160.68Å 99.54° 98.78° 100.89°	Depositor
Resolution (Å)	21.07 – 2.09 21.07 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.4 (21.07-2.09) 97.3 (21.07-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.08Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.232 , 0.246 0.234 , 0.251	Depositor DCC
R_{free} test set	11720 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26262	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8946e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, JQ5, 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	0.78	0/6463	1.21	7/8761 (0.1%)
1	B	0.78	0/6417	1.22	5/8705 (0.1%)
1	C	0.78	0/6492	1.20	6/8796 (0.1%)
1	D	0.78	0/6403	1.21	9/8688 (0.1%)
All	All	0.78	0/25775	1.21	27/34950 (0.1%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	836	ASP	CA-CB-CG	6.60	119.20	112.60
1	D	602	ASN	N-CA-C	6.18	113.78	108.22
1	B	602	ASN	N-CA-C	5.95	113.58	108.22
1	D	627	GLY	CA-C-N	5.89	128.49	120.54
1	D	627	GLY	C-N-CA	5.89	128.49	120.54
1	B	836	ASP	CA-CB-CG	5.83	118.43	112.60
1	D	700	LYS	CA-C-N	5.82	128.35	120.38
1	D	700	LYS	C-N-CA	5.82	128.35	120.38
1	B	700	LYS	CA-C-N	5.61	128.07	120.38
1	B	700	LYS	C-N-CA	5.61	128.07	120.38
1	C	602	ASN	N-CA-C	5.59	113.25	108.22
1	A	700	LYS	CA-C-N	5.55	127.98	120.38
1	A	700	LYS	C-N-CA	5.55	127.98	120.38
1	C	700	LYS	CA-C-N	5.43	127.82	120.38
1	C	700	LYS	C-N-CA	5.43	127.82	120.38
1	C	388	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	602	ASN	N-CA-C	5.29	112.99	108.22
1	A	935	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	537	MET	N-CA-C	5.20	112.90	108.22
1	C	627	GLY	CA-C-N	5.18	127.22	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	627	GLY	C-N-CA	5.18	127.22	120.28
1	D	935	ASP	CA-CB-CG	5.14	117.75	112.60
1	B	935	ASP	CA-CB-CG	5.14	117.74	112.60
1	D	953	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	627	GLY	CA-C-N	5.08	127.04	120.44
1	A	627	GLY	C-N-CA	5.08	127.04	120.44
1	D	537	MET	N-CA-C	5.06	112.78	108.22

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	6331	0	6125	13	0
1	B	6288	0	6072	13	0
1	C	6357	0	6172	12	0
1	D	6275	0	6050	9	0
2	A	26	0	16	3	0
2	B	26	0	16	2	0
2	C	26	0	16	4	0
2	D	26	0	16	4	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	13	0	0	3	0
5	B	13	0	0	2	0
5	C	13	0	0	4	0
5	D	13	0	0	4	0
6	A	219	0	0	0	0
6	B	214	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	192	0	0	0	0
6	D	222	0	0	0	0
All	All	26262	0	24483	60	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 (60) 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)
2:C:2001:TPP:H2	5:C:2004:JQ5:C6	1.83	1.09
2:A:2001:TPP:H2	5:A:2004:JQ5:C6	1.82	1.08
2:D:2001:TPP:H2	5:D:2004:JQ5:C6	1.83	1.07
2:B:2001:TPP:H2	5:B:2004:JQ5:C6	1.96	0.95
2:A:2001:TPP:H2	5:A:2004:JQ5:C5	2.29	0.63
2:C:2001:TPP:H2	5:C:2004:JQ5:C5	2.28	0.63
2:D:2001:TPP:H2	5:D:2004:JQ5:C5	2.28	0.62
2:B:2001:TPP:H2	5:B:2004:JQ5:C5	2.31	0.60
1:B:744:ARG:HH12	1:B:767:LYS:C	2.15	0.54
1:D:744:ARG:HH12	1:D:767:LYS:C	2.15	0.54
1:A:778:LEU:HB3	1:A:784:ILE:HG12	1.89	0.54
1:C:848:LEU:HD11	1:C:865:GLU:HA	1.93	0.50
1:C:705:PRO:HG2	1:C:735:VAL:HG13	1.94	0.48
1:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.96	0.48
1:A:898:LEU:O	1:A:945:VAL:HA	2.14	0.47
2:A:2001:TPP:H2	5:A:2004:JQ5:O7	2.12	0.47
1:B:778:LEU:HB3	1:B:784:ILE:HG12	1.96	0.47
1:C:778:LEU:HB3	1:C:784:ILE:HG12	1.96	0.47
2:C:2001:TPP:C2	5:C:2004:JQ5:C6	2.76	0.47
1:B:1119:ILE:HD12	1:B:1169:GLU:HG2	1.99	0.45
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.52	0.45
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.52	0.45
1:C:1112:LEU:CD2	1:C:1155:LEU:HD22	2.47	0.45
2:D:2001:TPP:C2	5:D:2004:JQ5:C6	2.75	0.45
1:B:1002:LEU:HB3	1:B:1061:GLN:HB2	2.00	0.44
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.52	0.44
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.52	0.44
1:D:1155:LEU:HD13	1:D:1164:LYS:HE2	2.00	0.44
1:D:1002:LEU:HB3	1:D:1061:GLN:HB2	2.00	0.44
1:A:530:LEU:HD22	1:A:636:SER:HA	2.00	0.44
1:B:1155:LEU:HD13	1:B:1164:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2001:TPP:H2	5:D:2004:JQ5:O7	2.13	0.43
1:C:898:LEU:O	1:C:945:VAL:HA	2.18	0.43
1:B:486:LEU:HD11	1:B:714:PRO:HG3	2.01	0.43
1:D:898:LEU:O	1:D:945:VAL:HA	2.19	0.42
1:C:1002:LEU:HB3	1:C:1061:GLN:HB2	2.00	0.42
1:A:1155:LEU:HD13	1:A:1164:LYS:HE2	2.00	0.42
1:C:1155:LEU:HD13	1:C:1164:LYS:HE2	2.00	0.42
1:A:705:PRO:HG2	1:A:735:VAL:HG13	2.01	0.42
1:B:898:LEU:O	1:B:945:VAL:HA	2.20	0.42
1:B:541:GLY:HA2	6:B:2125:HOH:O	2.20	0.42
1:A:981:VAL:HG22	1:A:988:ILE:HD11	2.02	0.42
1:D:1091:ARG:HD2	1:D:1150:ARG:NH2	2.35	0.41
1:A:1002:LEU:HB3	1:A:1061:GLN:HB2	2.02	0.41
1:A:1112:LEU:HD12	1:A:1161:VAL:HG21	2.03	0.41
1:D:1069:PRO:HB2	1:D:1072:MET:HB3	2.02	0.41
1:B:1155:LEU:HD11	1:B:1192:PHE:CZ	2.56	0.41
1:C:981:VAL:HG22	1:C:988:ILE:HD11	2.02	0.41
1:C:1155:LEU:HD11	1:C:1192:PHE:CZ	2.56	0.41
1:A:626:THR:HG21	1:A:636:SER:OG	2.21	0.41
1:B:981:VAL:HG22	1:B:988:ILE:HD11	2.03	0.41
1:B:1112:LEU:HD13	1:B:1155:LEU:HD22	2.02	0.41
1:C:486:LEU:HD11	1:C:714:PRO:HG3	2.02	0.41
1:A:1155:LEU:HD11	1:A:1192:PHE:CZ	2.56	0.41
1:A:1119:ILE:HD12	1:A:1169:GLU:HG2	2.03	0.40
1:D:1119:ILE:HD12	1:D:1169:GLU:HG2	2.04	0.40
2:C:2001:TPP:H2	5:C:2004:JQ5:O7	2.14	0.40
1:D:1155:LEU:HD11	1:D:1192:PHE:CZ	2.56	0.40
1:A:1069:PRO:HB2	1:A:1072:MET:HB3	2.03	0.40
1:B:1069:PRO:HB2	1:B:1072:MET:HB3	2.03	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	805/868 (93%)	791 (98%)	14 (2%)	0	100	100
1	B	805/868 (93%)	790 (98%)	15 (2%)	0	100	100
1	C	805/868 (93%)	787 (98%)	18 (2%)	0	100	100
1	D	802/868 (92%)	787 (98%)	15 (2%)	0	100	100
All	All	3217/3472 (93%)	3155 (98%)	62 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	654/726 (90%)	649 (99%)	5 (1%)	73	81
1	B	643/726 (89%)	638 (99%)	5 (1%)	73	81
1	C	660/726 (91%)	654 (99%)	6 (1%)	70	78
1	D	645/726 (89%)	640 (99%)	5 (1%)	73	81
All	All	2602/2904 (90%)	2581 (99%)	21 (1%)	73	81

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	467	VAL
1	A	868	ARG
1	A	976	GLN
1	A	1112	LEU
1	B	367	ASN
1	B	808	ARG
1	B	909	THR
1	B	976	GLN
1	B	1087	GLU
1	C	367	ASN
1	C	384	MET
1	C	467	VAL

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Mol	Chain	Res	Type
1	C	831	LEU
1	C	848	LEU
1	C	976	GLN
1	D	467	VAL
1	D	909	THR
1	D	976	GLN
1	D	1087	GLU
1	D	1112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	ASN
1	A	503	GLN
1	A	633	ASN
1	A	679	GLN
1	A	748	ASN
1	A	1001	GLN
1	A	1061	GLN
1	A	1107	ASN
1	B	497	GLN
1	B	503	GLN
1	B	548	ASN
1	B	679	GLN
1	B	748	ASN
1	B	797	GLN
1	B	904	GLN
1	B	1001	GLN
1	B	1061	GLN
1	B	1219	GLN
1	C	548	ASN
1	C	679	GLN
1	C	1001	GLN
1	C	1061	GLN
1	C	1107	ASN
1	C	1219	GLN
1	D	367	ASN
1	D	479	GLN
1	D	497	GLN
1	D	503	GLN
1	D	548	ASN
1	D	679	GLN

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Mol	Chain	Res	Type
1	D	748	ASN
1	D	904	GLN
1	D	1001	GLN
1	D	1061	GLN

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	A	2001	3	26,27,27	0.42	0	38,40,40	0.51	0
2	TPP	B	2001	3	26,27,27	0.49	0	38,40,40	0.59	0
5	JQ5	D	2004	-	7,12,12	1.29	1 (14%)	10,16,16	1.81	2 (20%)
5	JQ5	A	2004	-	7,12,12	1.33	0	10,16,16	1.80	2 (20%)
2	TPP	D	2001	3	26,27,27	0.40	0	38,40,40	0.48	0
5	JQ5	C	2004	-	7,12,12	1.23	0	10,16,16	1.73	2 (20%)
5	JQ5	B	2004	-	7,12,12	1.19	0	10,16,16	1.74	2 (20%)
2	TPP	C	2001	3	26,27,27	0.22	0	38,40,40	0.48	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	A	2001	3	-	0/17/17/17	0/2/2/2
2	TPP	B	2001	3	-	1/17/17/17	0/2/2/2
5	JQ5	D	2004	-	-	2/9/15/15	-
5	JQ5	A	2004	-	-	2/9/15/15	-
2	TPP	D	2001	3	-	0/17/17/17	0/2/2/2
5	JQ5	C	2004	-	-	2/9/15/15	-
5	JQ5	B	2004	-	-	2/9/15/15	-
2	TPP	C	2001	3	-	1/17/17/17	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2004	JQ5	O3-C1	-2.02	1.24	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2004	JQ5	O11-P10-O15	3.80	124.35	110.42
5	B	2004	JQ5	O11-P10-O15	3.77	124.27	110.42
5	D	2004	JQ5	O11-P10-O15	3.68	123.94	110.42
5	C	2004	JQ5	O11-P10-O15	3.66	123.84	110.42
5	C	2004	JQ5	C4-C5-C6	3.42	117.81	113.70
5	D	2004	JQ5	C4-C5-C6	3.39	117.77	113.70
5	B	2004	JQ5	C4-C5-C6	3.26	117.62	113.70
5	A	2004	JQ5	C4-C5-C6	3.13	117.47	113.70

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2004	JQ5	C13-O12-P10-O11
5	C	2004	JQ5	C13-O12-P10-O15
5	D	2004	JQ5	C13-O12-P10-O15
5	C	2004	JQ5	C14-C13-O12-P10
5	A	2004	JQ5	C14-C13-O12-P10
2	B	2001	TPP	PB-O3A-PA-O7
5	D	2004	JQ5	C14-C13-O12-P10

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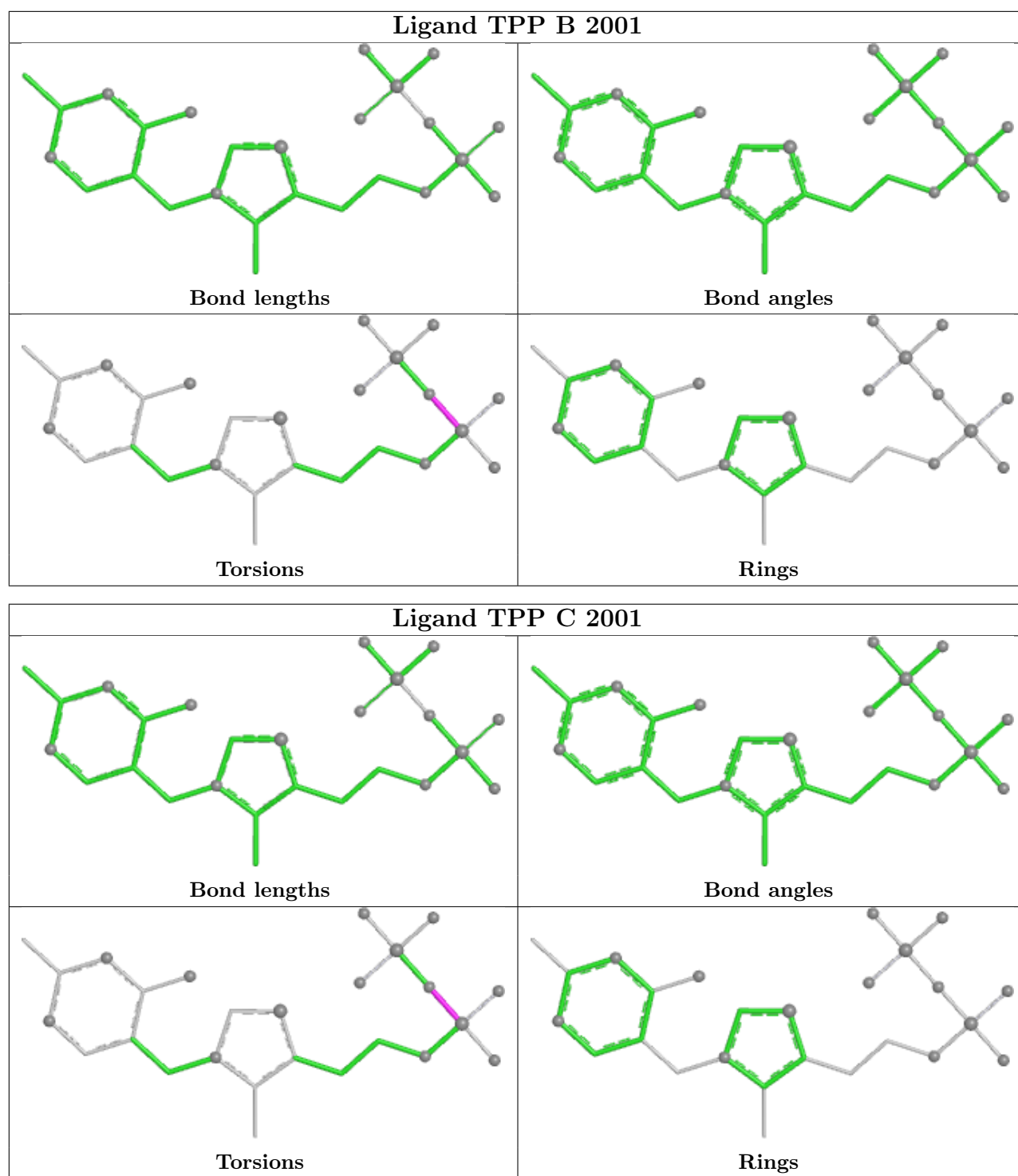
Mol	Chain	Res	Type	Atoms
5	A	2004	JQ5	C13-O12-P10-O11
5	B	2004	JQ5	C14-C13-O12-P10
2	C	2001	TPP	PB-O3A-PA-O7

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	TPP	3	0
2	B	2001	TPP	2	0
5	D	2004	JQ5	4	0
5	A	2004	JQ5	3	0
2	D	2001	TPP	4	0
5	C	2004	JQ5	4	0
5	B	2004	JQ5	2	0
2	C	2001	TPP	4	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	814/868 (93%)	0.74	89 (10%)	10 11	19, 39, 68, 103	1 (0%)
1	B	815/868 (93%)	0.74	102 (12%)	8 8	22, 39, 74, 103	0
1	C	813/868 (93%)	0.80	100 (12%)	8 8	20, 41, 73, 103	2 (0%)
1	D	812/868 (93%)	0.76	86 (10%)	11 12	24, 40, 70, 95	0
All	All	3254/3472 (93%)	0.76	377 (11%)	9 10	19, 40, 72, 103	3 (0%)

All (377) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	397	PHE	7.6
1	D	413	TRP	7.5
1	B	815	ILE	6.6
1	C	561	PHE	6.5
1	B	413	TRP	6.2
1	A	561	PHE	5.7
1	A	399	SER	5.5
1	D	394	ASN	5.5
1	B	810	LEU	5.5
1	D	501	VAL	5.5
1	B	561	PHE	5.3
1	D	815	ILE	5.3
1	D	817	PRO	5.3
1	D	561	PHE	5.2
1	C	394	ASN	5.2
1	A	411	THR	5.1
1	C	626	THR	5.0
1	B	394	ASN	5.0
1	C	633	ASN	4.8
1	B	397	PHE	4.6
1	D	810	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	807	VAL	4.6
1	B	501	VAL	4.5
1	A	420	LYS	4.5
1	A	813	HIS	4.5
1	A	413	TRP	4.4
1	D	831	LEU	4.4
1	B	817	PRO	4.4
1	D	807	VAL	4.3
1	B	365	ASP	4.3
1	A	750	GLY	4.3
1	C	789	ALA	4.2
1	D	630	GLY	4.2
1	D	1103	GLU	4.2
1	C	807	VAL	4.2
1	D	632	ASP	4.1
1	C	500	TYR	4.1
1	C	632	ASP	4.1
1	B	813	HIS	4.1
1	C	413	TRP	4.1
1	B	816	GLU	4.0
1	C	412	LEU	4.0
1	A	1210	SER	4.0
1	D	419	PHE	3.9
1	B	1103	GLU	3.9
1	C	808	ARG	3.9
1	C	411	THR	3.9
1	A	394	ASN	3.9
1	D	371	ILE	3.9
1	B	1227	GLY	3.9
1	C	814	GLU	3.9
1	C	397	PHE	3.9
1	A	501	VAL	3.8
1	C	501	VAL	3.8
1	C	773	ALA	3.8
1	D	745	ARG	3.8
1	B	779	ILE	3.8
1	A	497	GLN	3.8
1	C	935	ASP	3.8
1	A	756	THR	3.8
1	A	831	LEU	3.8
1	C	629	GLU	3.8
1	C	1210	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	812	LYS	3.7
1	C	810	LEU	3.7
1	D	589	MET	3.7
1	C	495	PHE	3.7
1	B	792	ALA	3.7
1	C	558	PHE	3.6
1	A	626	THR	3.6
1	D	633	ASN	3.6
1	D	816	GLU	3.6
1	C	506	PHE	3.6
1	C	429	ARG	3.6
1	B	371	ILE	3.5
1	A	777	ALA	3.5
1	A	627	GLY	3.5
1	B	556	GLN	3.5
1	D	367	ASN	3.5
1	C	630	GLY	3.5
1	C	860	VAL	3.5
1	A	860	VAL	3.5
1	A	494	THR	3.5
1	B	784	ILE	3.4
1	B	368	ALA	3.4
1	B	786	MET	3.4
1	C	365	ASP	3.4
1	A	575	ASP	3.4
1	D	590	PHE	3.4
1	B	420	LYS	3.4
1	A	558	PHE	3.4
1	A	384	MET	3.3
1	B	472	ASP	3.3
1	C	920	THR	3.3
1	D	553	PRO	3.3
1	B	419	PHE	3.3
1	D	558	PHE	3.3
1	D	473	LYS	3.3
1	C	756	THR	3.3
1	A	773	ALA	3.3
1	A	855	THR	3.2
1	C	853	GLY	3.2
1	C	813	HIS	3.2
1	B	808	ARG	3.2
1	D	626	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	745	ARG	3.2
1	A	807	VAL	3.2
1	D	368	ALA	3.2
1	D	470	LYS	3.2
1	A	500	TYR	3.2
1	C	831	LEU	3.2
1	A	632	ASP	3.2
1	D	808	ARG	3.2
1	C	471	HIS	3.2
1	D	811	GLU	3.2
1	D	750	GLY	3.2
1	A	853	GLY	3.1
1	A	789	ALA	3.1
1	D	472	ASP	3.1
1	D	430	LYS	3.1
1	B	367	ASN	3.1
1	C	366	LYS	3.1
1	B	793	LEU	3.1
1	C	764	ILE	3.1
1	B	772	LYS	3.0
1	C	499	LYS	3.0
1	C	850	LEU	3.0
1	C	779	ILE	3.0
1	D	759	TYR	3.0
1	B	811	GLU	3.0
1	B	555	SER	3.0
1	D	921	GLY	3.0
1	D	1227	GLY	3.0
1	B	418	GLU	3.0
1	D	628	GLU	3.0
1	B	473	LYS	3.0
1	A	495	PHE	3.0
1	B	804	PHE	3.0
1	D	813	HIS	3.0
1	A	784	ILE	3.0
1	A	397	PHE	3.0
1	D	814	GLU	2.9
1	D	415	LEU	2.9
1	A	803	VAL	2.9
1	D	763	VAL	2.9
1	A	786	MET	2.9
1	A	412	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	415	LEU	2.9
1	C	812	LYS	2.9
1	C	745	ARG	2.9
1	C	759	TYR	2.9
1	B	789	ALA	2.9
1	D	789	ALA	2.9
1	A	810	LEU	2.9
1	B	502	GLY	2.9
1	B	428	GLN	2.9
1	C	494	THR	2.9
1	D	779	ILE	2.9
1	B	809	GLU	2.9
1	A	499	LYS	2.9
1	B	1131	ASN	2.9
1	B	750	GLY	2.9
1	C	768	ARG	2.8
1	A	1212	LYS	2.8
1	C	368	ALA	2.8
1	B	543	LEU	2.8
1	A	476	VAL	2.8
1	D	631	SER	2.8
1	B	771	ARG	2.8
1	C	794	ARG	2.8
1	D	786	MET	2.8
1	C	750	GLY	2.8
1	D	749	GLU	2.8
1	D	916	VAL	2.8
1	C	627	GLY	2.8
1	C	498	THR	2.8
1	C	772	LYS	2.8
1	A	1083	ARG	2.7
1	D	471	HIS	2.7
1	B	554	TYR	2.7
1	B	796	TYR	2.7
1	C	505[A]	ARG	2.7
1	D	797	GLN	2.7
1	B	1102	GLY	2.7
1	B	558	PHE	2.7
1	B	745	ARG	2.7
1	B	920	THR	2.7
1	A	856	VAL	2.7
1	B	770	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	502	GLY	2.7
1	A	505	ARG	2.7
1	A	498	THR	2.7
1	A	779	ILE	2.7
1	C	575	ASP	2.7
1	D	781	ARG	2.7
1	A	477	ALA	2.6
1	D	809	GLU	2.6
1	B	831	LEU	2.6
1	C	392	LEU	2.6
1	C	415	LEU	2.6
1	D	500	TYR	2.6
1	A	371	ILE	2.6
1	B	744	ARG	2.6
1	B	781	ARG	2.6
1	A	769	GLY	2.6
1	B	769	GLY	2.6
1	B	766	THR	2.6
1	A	428	GLN	2.6
1	A	857	HIS	2.6
1	A	759	TYR	2.6
1	C	638	VAL	2.6
1	B	1212	LYS	2.6
1	C	777	ALA	2.6
1	A	785	SER	2.6
1	C	390	LEU	2.6
1	D	770	SER	2.6
1	A	711	GLY	2.5
1	B	805	ASN	2.5
1	C	489	ALA	2.5
1	D	555	SER	2.5
1	A	624	LEU	2.5
1	D	373	LEU	2.5
1	D	1220	GLU	2.5
1	C	803	VAL	2.5
1	A	473	LYS	2.5
1	B	592	ASP	2.5
1	B	498	THR	2.5
1	D	766	THR	2.5
1	C	631	SER	2.5
1	A	1209	GLY	2.5
1	C	557	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	915	ILE	2.5
1	C	1083	ARG	2.5
1	A	556	GLN	2.5
1	C	855	THR	2.5
1	B	800	LEU	2.5
1	B	470	LYS	2.5
1	D	804	PHE	2.5
1	D	812	LYS	2.5
1	C	781	ARG	2.5
1	B	780	GLY	2.5
1	B	791	ASP	2.4
1	C	796	TYR	2.4
1	A	368	ALA	2.4
1	B	392	LEU	2.4
1	B	794	ARG	2.4
1	B	581	GLY	2.4
1	A	629	GLU	2.4
1	A	702	ILE	2.4
1	B	557	ILE	2.4
1	B	395	THR	2.4
1	D	395	THR	2.4
1	D	469	THR	2.4
1	D	800	LEU	2.4
1	C	419	PHE	2.4
1	A	915	ILE	2.4
1	C	916	VAL	2.4
1	C	744	ARG	2.4
1	B	759	TYR	2.4
1	A	1128	ALA	2.4
1	C	511	ALA	2.4
1	C	634	ARG	2.4
1	A	471	HIS	2.4
1	A	778	LEU	2.3
1	C	497	GLN	2.3
1	D	543	LEU	2.3
1	A	398	ARG	2.3
1	A	557	ILE	2.3
1	B	775	THR	2.3
1	B	749	GLU	2.3
1	C	758	PRO	2.3
1	A	796	TYR	2.3
1	B	777	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1182	LEU	2.3
1	C	371	ILE	2.3
1	C	628	GLU	2.3
1	C	856	VAL	2.3
1	A	483	LEU	2.3
1	A	861	ARG	2.3
1	B	778	LEU	2.3
1	C	830	LYS	2.3
1	C	790	GLU	2.3
1	A	633	ASN	2.3
1	D	919	LYS	2.3
1	C	384	MET	2.3
1	D	761	TYR	2.3
1	C	556	GLN	2.2
1	C	854	PHE	2.2
1	A	916	VAL	2.2
1	D	967	PRO	2.2
1	C	396	ARG	2.2
1	C	802	ARG	2.2
1	B	787	LYS	2.2
1	C	767	LYS	2.2
1	D	767	LYS	2.2
1	C	711	GLY	2.2
1	D	793	LEU	2.2
1	B	814	GLU	2.2
1	A	396	ARG	2.2
1	B	429	ARG	2.2
1	B	416	ASP	2.2
1	B	373	LEU	2.2
1	D	392	LEU	2.2
1	C	786	MET	2.2
1	C	769	GLY	2.2
1	D	923	GLU	2.2
1	B	647	ALA	2.2
1	D	547	ALA	2.2
1	C	848	LEU	2.2
1	B	742	TYR	2.2
1	D	742	TYR	2.2
1	A	920	THR	2.2
1	B	372	GLU	2.1
1	B	915	ILE	2.1
1	B	1186	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	915	ILE	2.1
1	A	392	LEU	2.1
1	A	794	ARG	2.1
1	A	808	ARG	2.1
1	B	432	LEU	2.1
1	C	369	ARG	2.1
1	D	667	ARG	2.1
1	A	366	LYS	2.1
1	B	767	LYS	2.1
1	C	837	LYS	2.1
1	D	556	GLN	2.1
1	B	495	PHE	2.1
1	B	396	ARG	2.1
1	D	1078	ALA	2.1
1	C	778	LEU	2.1
1	C	922	GLU	2.1
1	B	500	TYR	2.1
1	B	505	ARG	2.1
1	C	502	GLY	2.1
1	C	702	ILE	2.1
1	A	638	VAL	2.1
1	B	916	VAL	2.1
1	B	919	LYS	2.1
1	D	499	LYS	2.1
1	B	488	ALA	2.1
1	D	832	ALA	2.1
1	B	790	GLU	2.1
1	B	667	ARG	2.1
1	B	1035	GLY	2.1
1	C	965	GLY	2.1
1	B	764	ILE	2.1
1	C	787	LYS	2.1
1	B	763	VAL	2.1
1	C	476	VAL	2.1
1	D	1211	SER	2.1
1	C	483	LEU	2.0
1	D	1222	LEU	2.0
1	A	783	ASP	2.0
1	D	859	ARG	2.0
1	B	967	PRO	2.0
1	C	937	THR	2.0
1	D	756	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	772	LYS	2.0
1	B	812	LYS	2.0
1	D	1209	GLY	2.0
1	A	463	ILE	2.0
1	A	419	PHE	2.0
1	A	804	PHE	2.0
1	B	492	PHE	2.0
1	D	852	GLU	2.0
1	A	488	ALA	2.0
1	A	489	ALA	2.0
1	A	496	LEU	2.0
1	A	850	LEU	2.0
1	B	1002	LEU	2.0
1	A	768	ARG	2.0
1	A	771	ARG	2.0
1	B	471	HIS	2.0
1	B	553	PRO	2.0
1	D	909	THR	2.0
1	C	782	GLY	2.0
1	D	554	TYR	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.

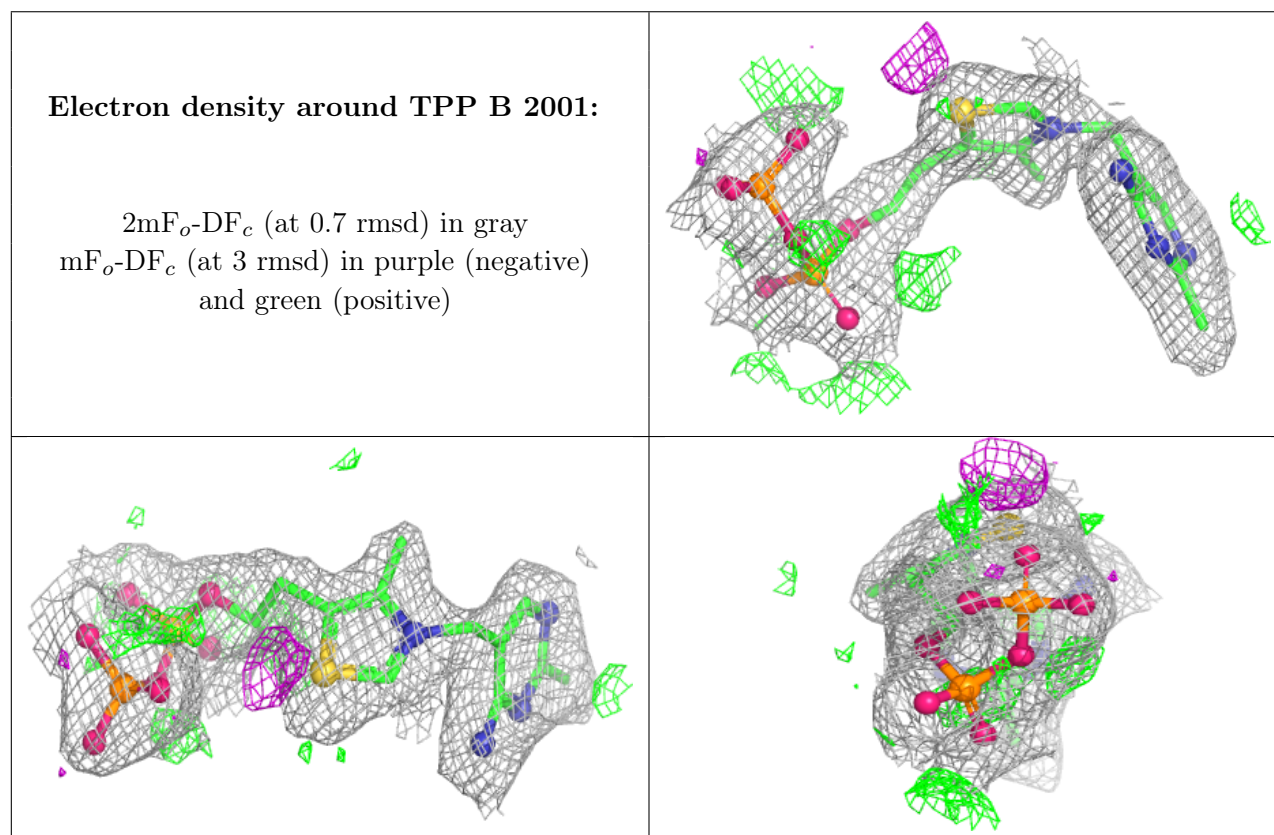
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	JQ5	C	2004	13/13	0.86	0.16	39,44,54,55	0
5	JQ5	A	2004	13/13	0.88	0.14	38,42,46,48	0
5	JQ5	D	2004	13/13	0.90	0.13	39,45,48,49	0

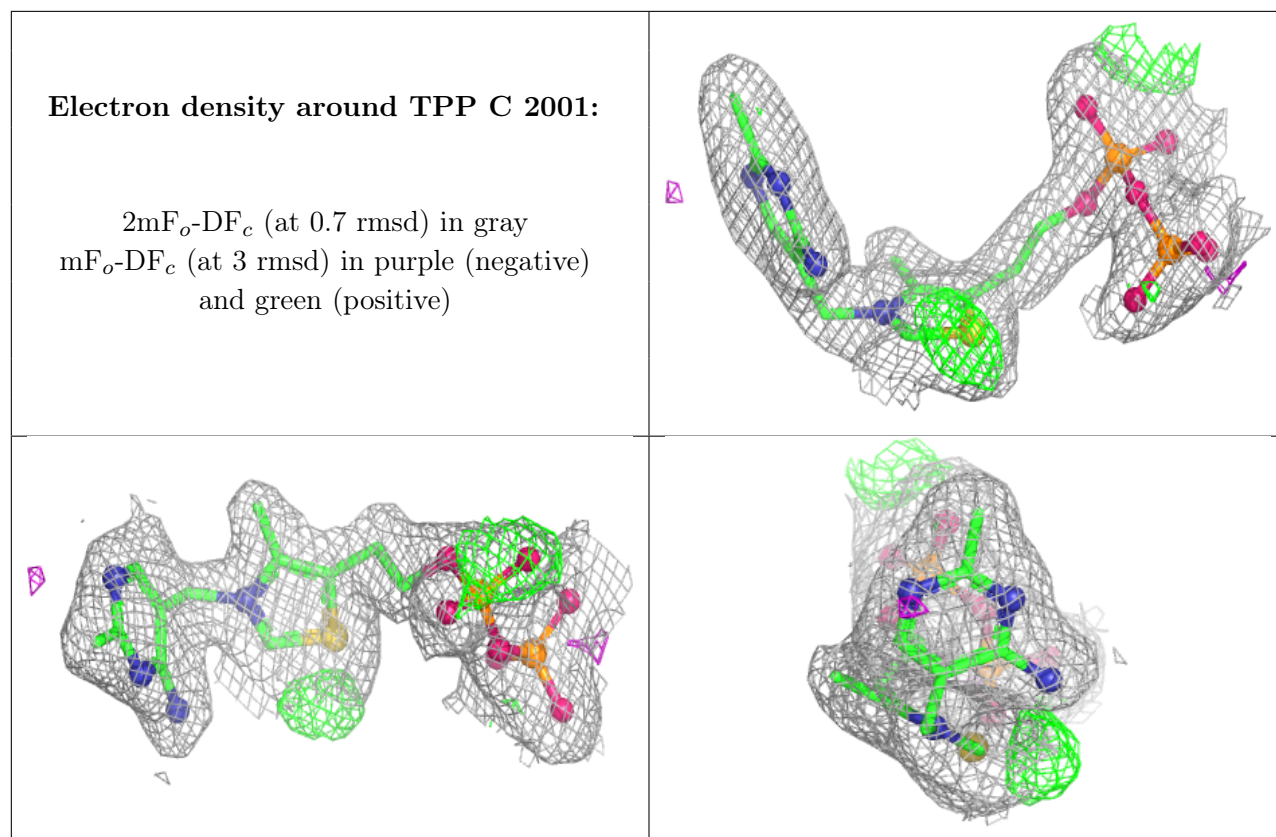
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	JQ5	B	2004	13/13	0.92	0.13	43,48,52,52	0
2	TPP	B	2001	26/26	0.96	0.09	22,25,29,30	0
2	TPP	C	2001	26/26	0.96	0.07	23,27,31,31	0
2	TPP	D	2001	26/26	0.96	0.08	22,26,30,30	0
3	MG	B	2002	1/1	0.96	0.07	27,27,27,27	0
2	TPP	A	2001	26/26	0.97	0.07	19,26,29,31	0
3	MG	C	2002	1/1	0.97	0.03	23,23,23,23	0
3	MG	D	2002	1/1	0.97	0.05	26,26,26,26	0
4	CA	A	2003	1/1	0.97	0.07	35,35,35,35	0
4	CA	C	2003	1/1	0.98	0.07	37,37,37,37	0
4	CA	D	2003	1/1	0.98	0.03	36,36,36,36	0
3	MG	A	2002	1/1	0.99	0.02	24,24,24,24	0
4	CA	B	2003	1/1	1.00	0.02	39,39,39,39	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.