



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:38 AM UTC

PDB ID : 3ZHT / pdb_00003zht
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis KGD, first post-decarboxylation intermediate from 2-oxoadipate
Authors : Wagner, T.; Barilone, N.; Bellinzoni, M.; Alzari, P.M.
Deposited on : 2012-12-24
Resolution : 2.15 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

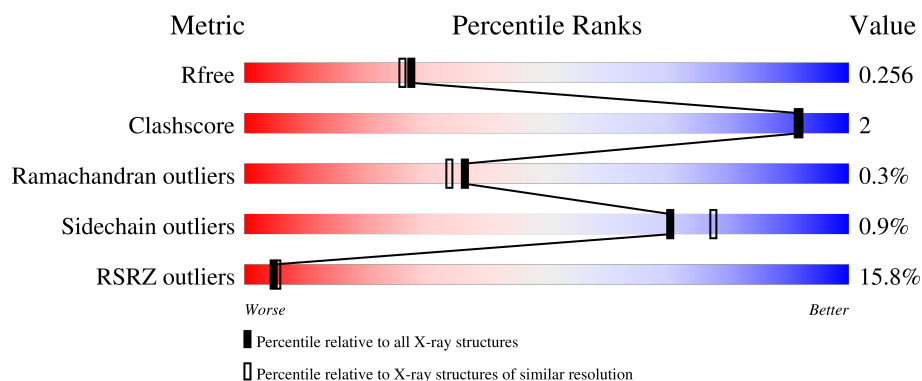
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	
1	B	868	
1	C	868	
1	D	868	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26205 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.

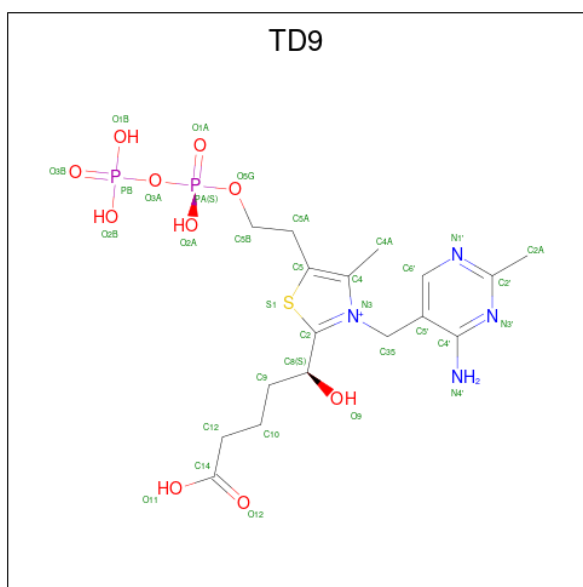
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	814	Total	C	N	O	S	0	1	0
			6292	3963	1111	1194	24			
1	B	809	Total	C	N	O	S	0	2	0
			6224	3922	1101	1176	25			
1	C	808	Total	C	N	O	S	0	0	0
			6258	3940	1104	1191	23			
1	D	807	Total	C	N	O	S	0	0	0
			6199	3905	1091	1180	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 (5S)-5-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-4-methyl-5-(2-{[(phosphonatoxy)phosphinato]oxy}ethyl)-1,3-thiazol-3-ium-2-yl}-5-hydroxypentanoate (CCD ID: TD9) (formula: C₁₇H₂₇N₄O₁₀P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			34	17	4	10	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			34	17	4	10	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			34	17	4	10	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			34	17	4	10	2	1		

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

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

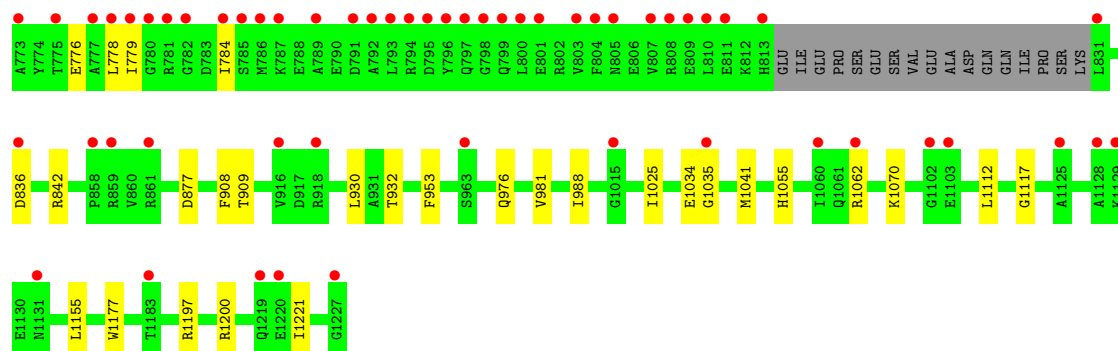
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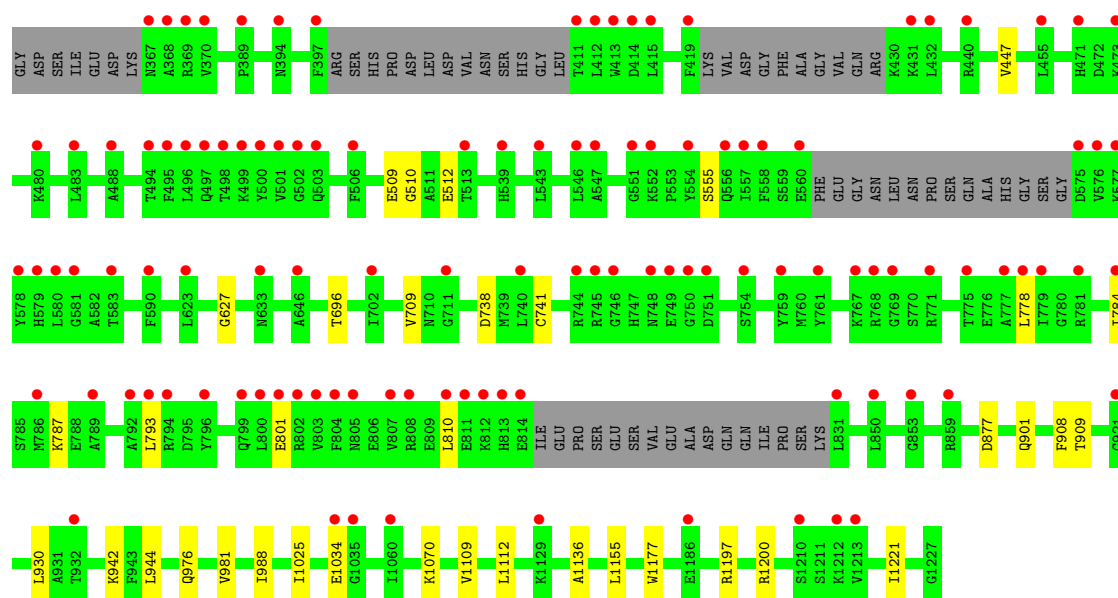
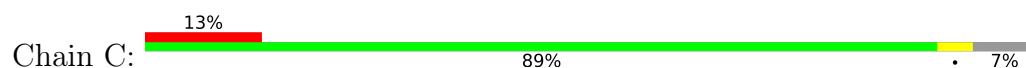
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0
4	D	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

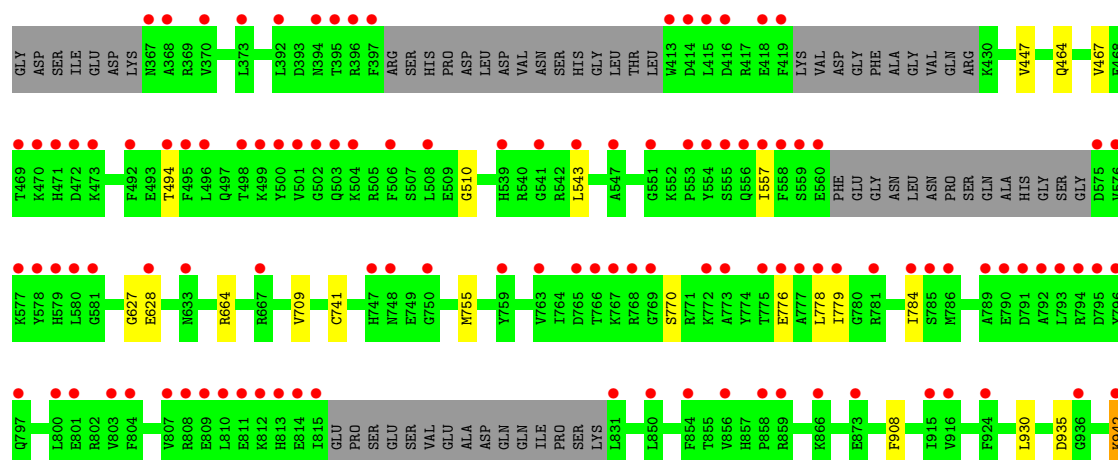
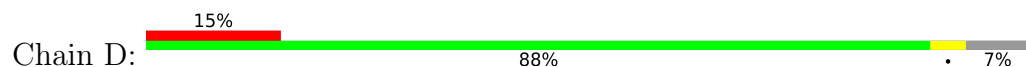
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	339	Total 339	O 339	0	0
5	B	223	Total 223	O 223	0	0
5	C	305	Total 305	O 305	0	0
5	D	221	Total 221	O 221	0	0

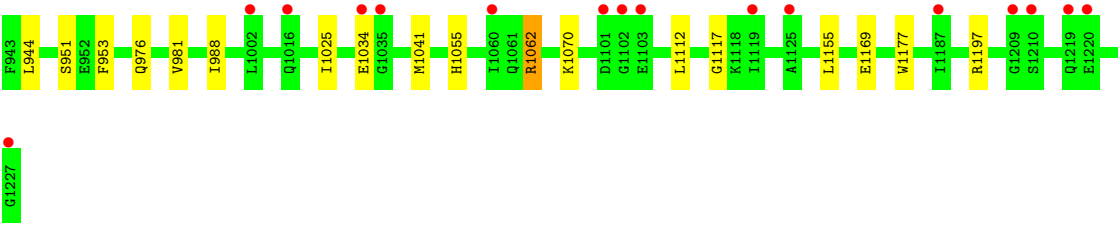


• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME



• 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	80.37Å 83.80Å 159.51Å 99.76° 99.06° 100.61°	Depositor
Resolution (Å)	41.11 – 2.15 41.11 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.5 (41.11-2.15) 97.5 (41.11-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.223 , 0.246 0.228 , 0.256	Depositor DCC
R_{free} test set	10531 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26205	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 23.99 % 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 4.1817e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, CA, TD9

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	0/6422	1.22	6/8710 (0.1%)
1	B	0.84	0/6356	1.24	9/8627 (0.1%)
1	C	0.86	0/6384	1.22	5/8657 (0.1%)
1	D	0.83	0/6324	1.24	8/8584 (0.1%)
All	All	0.85	0/25486	1.23	28/34578 (0.1%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	836	ASP	CA-CB-CG	7.76	120.36	112.60
1	D	770	SER	CA-C-N	6.20	128.84	120.65
1	D	770	SER	C-N-CA	6.20	128.84	120.65
1	D	935	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	627	GLY	CA-C-N	5.87	128.47	120.54
1	A	627	GLY	C-N-CA	5.87	128.47	120.54
1	C	627	GLY	CA-C-N	5.85	128.40	120.38
1	C	627	GLY	C-N-CA	5.85	128.40	120.38
1	B	627	GLY	CA-C-N	5.60	128.10	120.54
1	B	627	GLY	C-N-CA	5.60	128.10	120.54
1	B	538	PRO	CA-C-N	5.56	128.04	120.54
1	B	538	PRO	C-N-CA	5.56	128.04	120.54
1	D	627	GLY	CA-C-N	5.50	127.96	120.54
1	D	627	GLY	C-N-CA	5.50	127.96	120.54
1	C	877	ASP	CA-CB-CG	5.49	118.09	112.60
1	D	1025	ILE	CA-C-N	5.34	127.70	120.38
1	D	1025	ILE	C-N-CA	5.34	127.70	120.38
1	A	877	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	615	GLY	CA-C-N	5.26	127.28	120.44
1	A	615	GLY	C-N-CA	5.26	127.28	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1025	ILE	CA-C-N	5.16	127.45	120.38
1	C	1025	ILE	C-N-CA	5.16	127.45	120.38
1	B	877	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	953	PHE	CA-CB-CG	5.13	118.93	113.80
1	B	1025	ILE	CA-C-N	5.07	127.33	120.38
1	B	1025	ILE	C-N-CA	5.07	127.33	120.38
1	D	953	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	393	ASP	CA-CB-CG	5.01	117.61	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	6292	0	6064	26	0
1	B	6224	0	5986	22	0
1	C	6258	0	6043	16	0
1	D	6199	0	5953	16	0
2	A	34	0	23	0	0
2	B	34	0	23	1	0
2	C	34	0	23	0	0
2	D	34	0	23	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	339	0	0	0	0
5	B	223	0	0	2	0
5	C	305	0	0	0	0
5	D	221	0	0	1	0
All	All	26205	0	24138	77	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 (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1035:GLY:O	1:B:1062:ARG:HD2	1.90	0.71
1:D:1041:MET:HE2	1:D:1117:GLY:HA3	1.81	0.62
1:D:1112:LEU:HD21	1:D:1155:LEU:HD22	1.84	0.59
1:B:497:GLN:HG3	1:B:745:ARG:HH12	1.68	0.59
1:B:1112:LEU:HD21	1:B:1155:LEU:HD22	1.85	0.57
1:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.87	0.56
1:B:476:VAL:HG12	1:B:480:LYS:HE2	1.87	0.55
1:A:544:ASN:OD1	1:A:548:ASN:ND2	2.41	0.54
1:C:509:GLU:HA	1:C:512:GLU:OE2	2.09	0.53
1:D:942:LYS:HE2	1:D:944:LEU:HD21	1.90	0.53
1:B:497:GLN:HG3	1:B:745:ARG:NH1	2.26	0.51
1:A:555:SER:HA	1:A:810:LEU:HD22	1.92	0.51
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.93	0.51
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.92	0.51
1:A:843:ILE:HG12	1:A:930:LEU:HD21	1.94	0.50
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.93	0.50
1:B:505:ARG:HA	1:B:747:HIS:O	2.12	0.49
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.94	0.49
1:A:744:ARG:HG3	1:A:745:ARG:HG3	1.96	0.48
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.49	0.47
1:B:778:LEU:HB3	1:B:784:ILE:HG12	1.95	0.47
1:A:901:GLN:OE1	2:B:2001:TD9:H6'	2.15	0.47
1:A:505:ARG:HA	1:A:747:HIS:O	2.15	0.47
1:A:778:LEU:HB3	1:A:784:ILE:HG12	1.97	0.46
1:C:555:SER:HA	1:C:810:LEU:HD22	1.98	0.46
1:A:908:PHE:CZ	1:A:1070:LYS:HG2	2.51	0.46
1:A:866:LYS:HG3	1:A:870:MET:HE2	1.98	0.45
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.52	0.45
1:D:1169:GLU:OE1	5:D:3208:HOH:O	2.21	0.45
1:B:537:MET:HE3	5:B:3034:HOH:O	2.17	0.45
1:C:510:GLY:O	1:C:741:CYS:HB2	2.17	0.45
1:C:908:PHE:CZ	1:C:1070:LYS:HG2	2.52	0.45
1:B:1041[B]:MET:HE2	1:B:1117:GLY:HA3	1.99	0.44
1:A:492:PHE:CE1	1:A:496:LEU:HD13	2.53	0.44
1:A:909:THR:HG21	1:B:755:MET:HE1	2.00	0.44
1:D:776:GLU:HA	1:D:779:ILE:HD12	1.99	0.44
1:C:1112:LEU:CD2	1:C:1155:LEU:HD22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:ILE:HG12	1:A:930:LEU:CD2	2.47	0.44
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.53	0.44
1:A:510:GLY:O	1:A:741:CYS:HB2	2.18	0.43
1:A:561:PHE:O	1:A:562:GLU:HB2	2.16	0.43
1:B:776:GLU:HA	1:B:779:ILE:HD12	1.98	0.43
1:A:843:ILE:CG1	1:A:930:LEU:HD21	2.48	0.43
1:B:1055:HIS:HE1	1:B:1062:ARG:O	2.01	0.43
1:B:510:GLY:O	1:B:741:CYS:HB2	2.18	0.43
1:D:510:GLY:O	1:D:741:CYS:HB2	2.18	0.43
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.53	0.43
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.54	0.43
1:D:628:GLU:HG2	1:D:664:ARG:O	2.19	0.42
1:B:682:PHE:CD1	1:B:683:THR:HG23	2.54	0.42
1:A:509:GLU:HA	1:A:512:GLU:OE2	2.20	0.42
1:C:1109:VAL:HG21	1:C:1136:ALA:HB2	2.00	0.42
1:D:778:LEU:HB3	1:D:784:ILE:HG12	2.01	0.42
1:A:909:THR:CG2	1:B:755:MET:HE1	2.50	0.42
1:C:909:THR:HG21	1:D:755:MET:HE1	2.02	0.42
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.54	0.42
1:D:1055:HIS:HE1	1:D:1062:ARG:O	2.03	0.42
1:A:628:GLU:HG2	1:A:664:ARG:O	2.20	0.41
1:D:543:LEU:HD22	1:D:557:ILE:HG23	2.01	0.41
1:C:447:VAL:HG22	1:C:709:VAL:HG12	2.01	0.41
1:C:778:LEU:HB3	1:C:784:ILE:HG12	2.02	0.41
1:A:903:THR:O	1:A:911:ARG:HD2	2.21	0.41
1:D:447:VAL:HG22	1:D:709:VAL:HG12	2.02	0.41
1:B:842:ARG:NH2	1:B:932:THR:O	2.53	0.41
1:D:1112:LEU:CD2	1:D:1155:LEU:HD22	2.50	0.41
1:A:696:THR:HG21	1:A:738:ASP:HB2	2.02	0.41
1:A:1200:ARG:HG3	1:A:1221:ILE:HD11	2.03	0.41
1:B:1200:ARG:HG3	1:B:1221:ILE:HD11	2.03	0.41
1:A:842:ARG:NH2	1:A:932:THR:O	2.54	0.41
1:C:1200:ARG:HG3	1:C:1221:ILE:HD11	2.02	0.41
1:A:1055:HIS:HE1	1:A:1062:ARG:O	2.03	0.40
1:B:508:LEU:HD13	1:B:541:GLY:HA3	2.03	0.40
1:B:747:HIS:HA	5:B:3035:HOH:O	2.21	0.40
1:A:942:LYS:HE3	1:A:944:LEU:HD21	2.03	0.40
1:C:696:THR:HG21	1:C:738:ASP:HB2	2.03	0.40
1:C:901:GLN:OE1	2:D:2001:TD9:H6'	2.21	0.40
1:C:942:LYS:HE3	1:C:944:LEU:HD21	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	805/868 (93%)	784 (97%)	18 (2%)	3 (0%)	30	26
1	B	801/868 (92%)	780 (97%)	18 (2%)	3 (0%)	30	26
1	C	798/868 (92%)	776 (97%)	21 (3%)	1 (0%)	48	50
1	D	797/868 (92%)	778 (98%)	18 (2%)	1 (0%)	48	50
All	All	3201/3472 (92%)	3118 (97%)	75 (2%)	8 (0%)	36	44

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	561	PHE
1	B	1034	GLU
1	D	1034	GLU
1	A	1034	GLU
1	C	1034	GLU
1	A	605	HIS
1	B	605	HIS
1	B	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	646/726 (89%)	640 (99%)	6 (1%)	70	77
1	B	635/726 (88%)	631 (99%)	4 (1%)	78	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	645/726 (89%)	640 (99%)	5 (1%)	73	79
1	D	633/726 (87%)	625 (99%)	8 (1%)	61	68
All	All	2559/2904 (88%)	2536 (99%)	23 (1%)	70	77

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

Mol	Chain	Res	Type
1	A	467	VAL
1	A	496	LEU
1	A	556	GLN
1	A	950	LEU
1	A	976	GLN
1	A	1112	LEU
1	B	467	VAL
1	B	909	THR
1	B	930	LEU
1	B	976	GLN
1	C	787	LYS
1	C	793	LEU
1	C	801	GLU
1	C	930	LEU
1	C	976	GLN
1	D	464	GLN
1	D	467	VAL
1	D	494	THR
1	D	930	LEU
1	D	942	LYS
1	D	951	SER
1	D	976	GLN
1	D	1062	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1001	GLN
1	A	1030	GLN
1	A	1107	ASN
1	B	556	GLN
1	B	912	HIS
1	B	1001	GLN

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Mol	Chain	Res	Type
1	B	1016	GLN
1	B	1107	ASN
1	B	1219	GLN
1	C	556	GLN
1	C	1001	GLN
1	C	1016	GLN
1	C	1107	ASN
1	C	1219	GLN
1	D	497	GLN
1	D	912	HIS
1	D	1001	GLN
1	D	1016	GLN
1	D	1107	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TD9	C	2001	3	32,35,35	1.45	4 (12%)	39,51,51	1.12	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TD9	B	2001	3	32,35,35	1.34	4 (12%)	39,51,51	1.19	5 (12%)
2	TD9	D	2001	3	32,35,35	1.58	5 (15%)	39,51,51	1.13	5 (12%)
2	TD9	A	2001	3	32,35,35	1.46	3 (9%)	39,51,51	1.14	3 (7%)

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	TD9	C	2001	3	-	6/26/27/27	0/2/2/2
2	TD9	B	2001	3	-	7/26/27/27	0/2/2/2
2	TD9	D	2001	3	-	9/26/27/27	0/2/2/2
2	TD9	A	2001	3	-	6/26/27/27	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	TD9	PA-O3A	-5.48	1.53	1.59
2	A	2001	TD9	PA-O3A	-5.39	1.53	1.59
2	C	2001	TD9	PA-O3A	-5.13	1.54	1.59
2	C	2001	TD9	C5-S1	-4.92	1.64	1.74
2	A	2001	TD9	C5-S1	-4.56	1.64	1.74
2	B	2001	TD9	C8-C2	3.93	1.57	1.51
2	D	2001	TD9	C5-C4	3.85	1.43	1.35
2	B	2001	TD9	C5-S1	-3.79	1.66	1.74
2	D	2001	TD9	C5-S1	-3.75	1.66	1.74
2	B	2001	TD9	PA-O3A	-3.72	1.55	1.59
2	A	2001	TD9	C5-C4	3.48	1.42	1.35
2	D	2001	TD9	C8-C2	3.30	1.56	1.51
2	B	2001	TD9	C5-C4	3.27	1.42	1.35
2	C	2001	TD9	C8-C2	2.57	1.55	1.51
2	C	2001	TD9	C5-C4	2.47	1.40	1.35
2	D	2001	TD9	PB-O1B	2.03	1.62	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	TD9	O3A-PA-O1A	3.60	121.53	110.70
2	A	2001	TD9	O1B-PB-O3A	-3.33	93.46	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	TD9	O2A-PA-O3A	-3.29	98.39	107.27
2	C	2001	TD9	O1B-PB-O3A	-3.08	94.30	104.64
2	D	2001	TD9	O1B-PB-O3A	-2.63	95.80	104.64
2	B	2001	TD9	O3A-PA-O1A	2.60	118.51	110.70
2	A	2001	TD9	O3A-PA-O1A	2.54	118.35	110.70
2	C	2001	TD9	O3A-PA-O1A	2.52	118.28	110.70
2	B	2001	TD9	C35-C5'-C4'	2.49	126.90	122.36
2	D	2001	TD9	O2A-PA-O3A	-2.35	100.91	107.27
2	C	2001	TD9	C35-C5'-C4'	2.35	126.64	122.36
2	A	2001	TD9	C4-C5-S1	2.25	112.89	110.56
2	B	2001	TD9	O2B-PB-O3B	2.23	119.54	110.83
2	C	2001	TD9	O2A-PA-O3A	-2.11	101.57	107.27
2	B	2001	TD9	O1B-PB-O3A	-2.09	97.63	104.64
2	D	2001	TD9	O5G-PA-O1A	2.08	117.17	108.94
2	D	2001	TD9	C35-C5'-C4'	2.05	126.09	122.36

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	TD9	S1-C2-C8-O9
2	A	2001	TD9	N3-C2-C8-O9
2	B	2001	TD9	S1-C2-C8-O9
2	B	2001	TD9	N3-C2-C8-O9
2	C	2001	TD9	S1-C2-C8-O9
2	C	2001	TD9	N3-C2-C8-O9
2	C	2001	TD9	PB-O3A-PA-O5G
2	D	2001	TD9	S1-C2-C8-O9
2	D	2001	TD9	N3-C2-C8-O9
2	D	2001	TD9	C9-C10-C12-C14
2	D	2001	TD9	N3-C35-C5'-C4'
2	B	2001	TD9	O9-C8-C9-C10
2	A	2001	TD9	PB-O3A-PA-O5G
2	B	2001	TD9	PB-O3A-PA-O5G
2	D	2001	TD9	PB-O3A-PA-O5G
2	D	2001	TD9	C12-C10-C9-C8
2	D	2001	TD9	C5B-O5G-PA-O1A
2	A	2001	TD9	C10-C12-C14-O12
2	A	2001	TD9	C10-C12-C14-O11
2	C	2001	TD9	C10-C12-C14-O12
2	C	2001	TD9	C10-C12-C14-O11
2	A	2001	TD9	C12-C10-C9-C8

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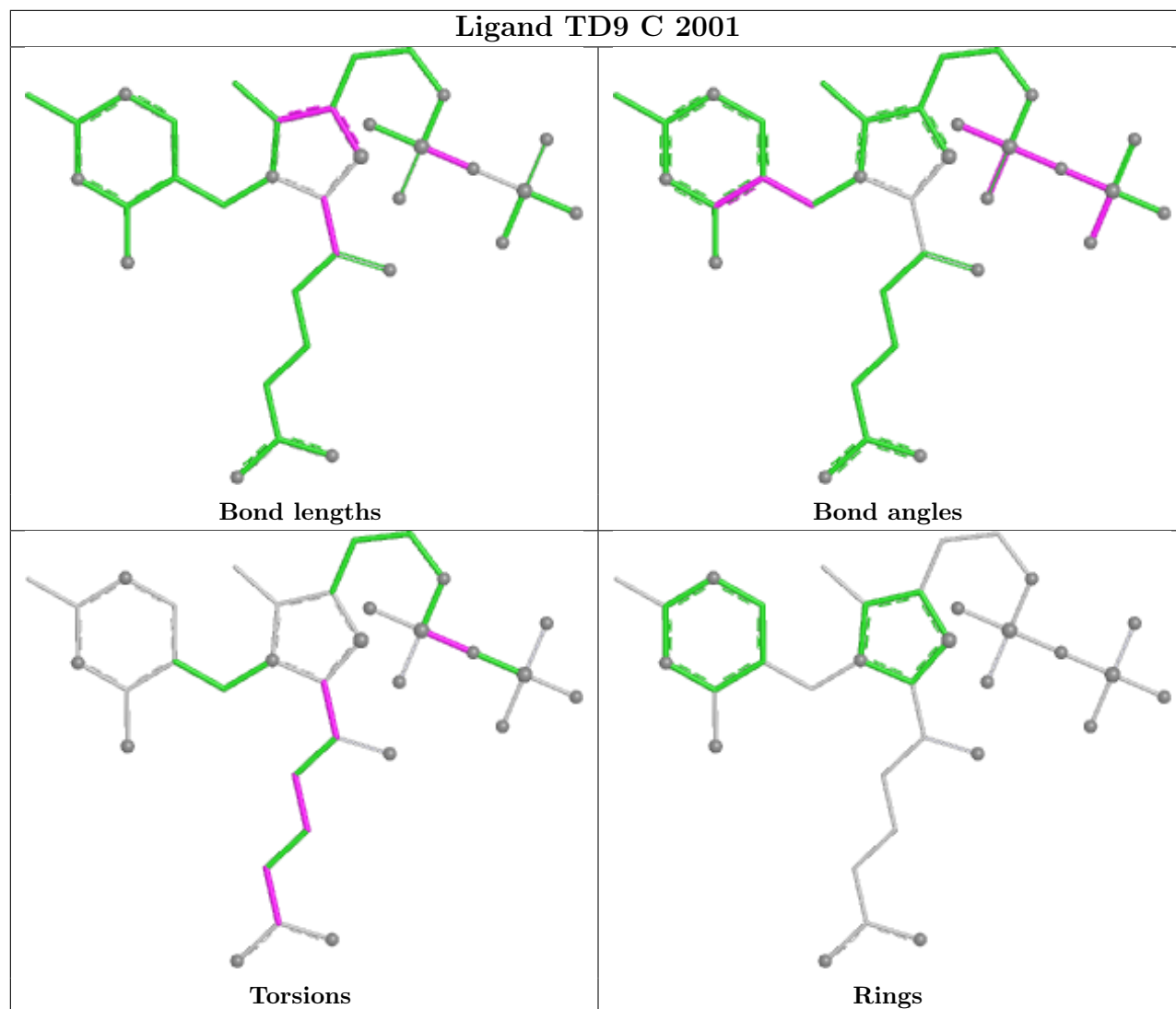
Mol	Chain	Res	Type	Atoms
2	C	2001	TD9	C12-C10-C9-C8
2	B	2001	TD9	PA-O3A-PB-O2B
2	D	2001	TD9	PA-O3A-PB-O2B
2	B	2001	TD9	C10-C12-C14-O11
2	D	2001	TD9	C5-C5A-C5B-O5G
2	B	2001	TD9	C10-C12-C14-O12

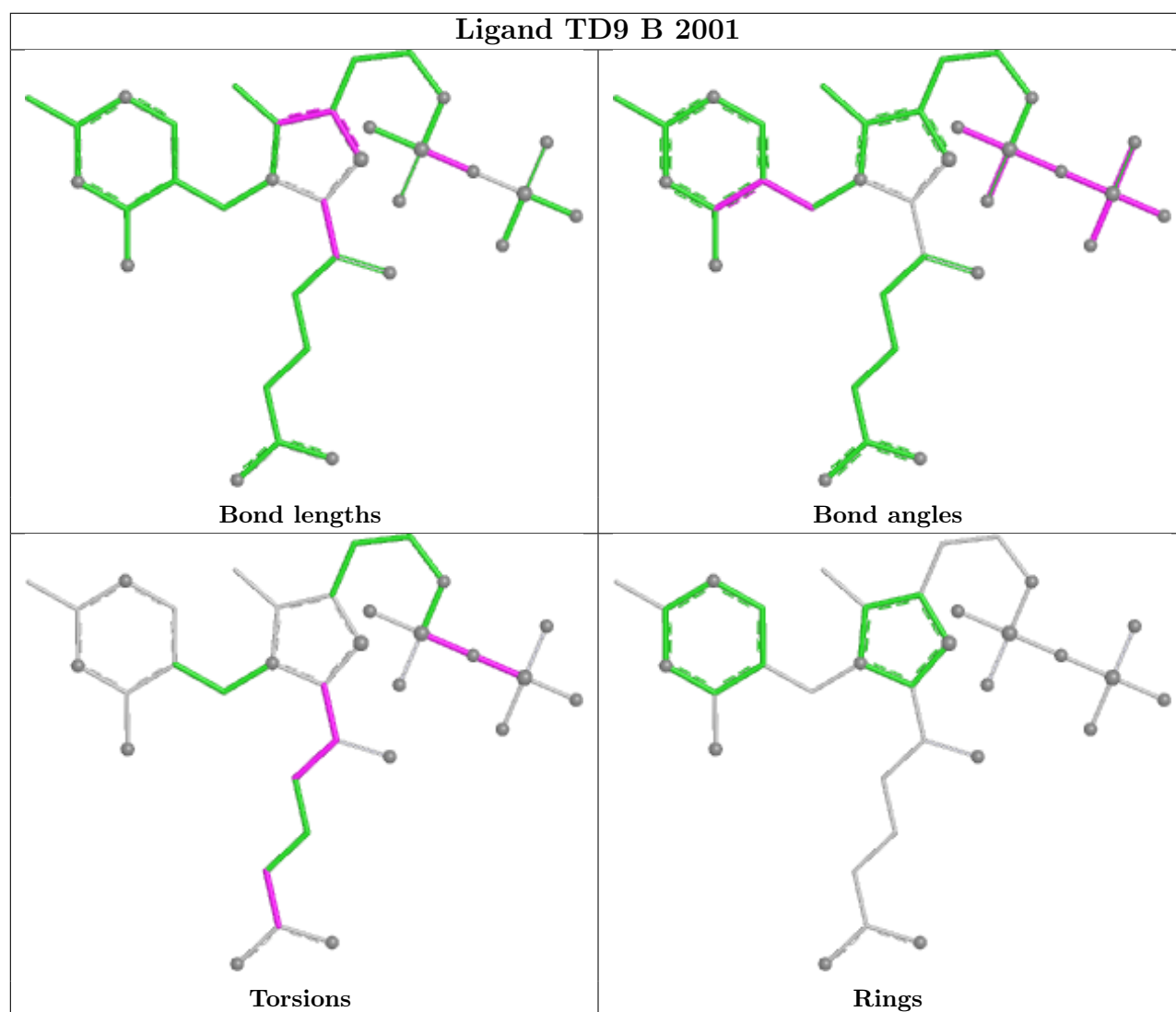
There are no ring outliers.

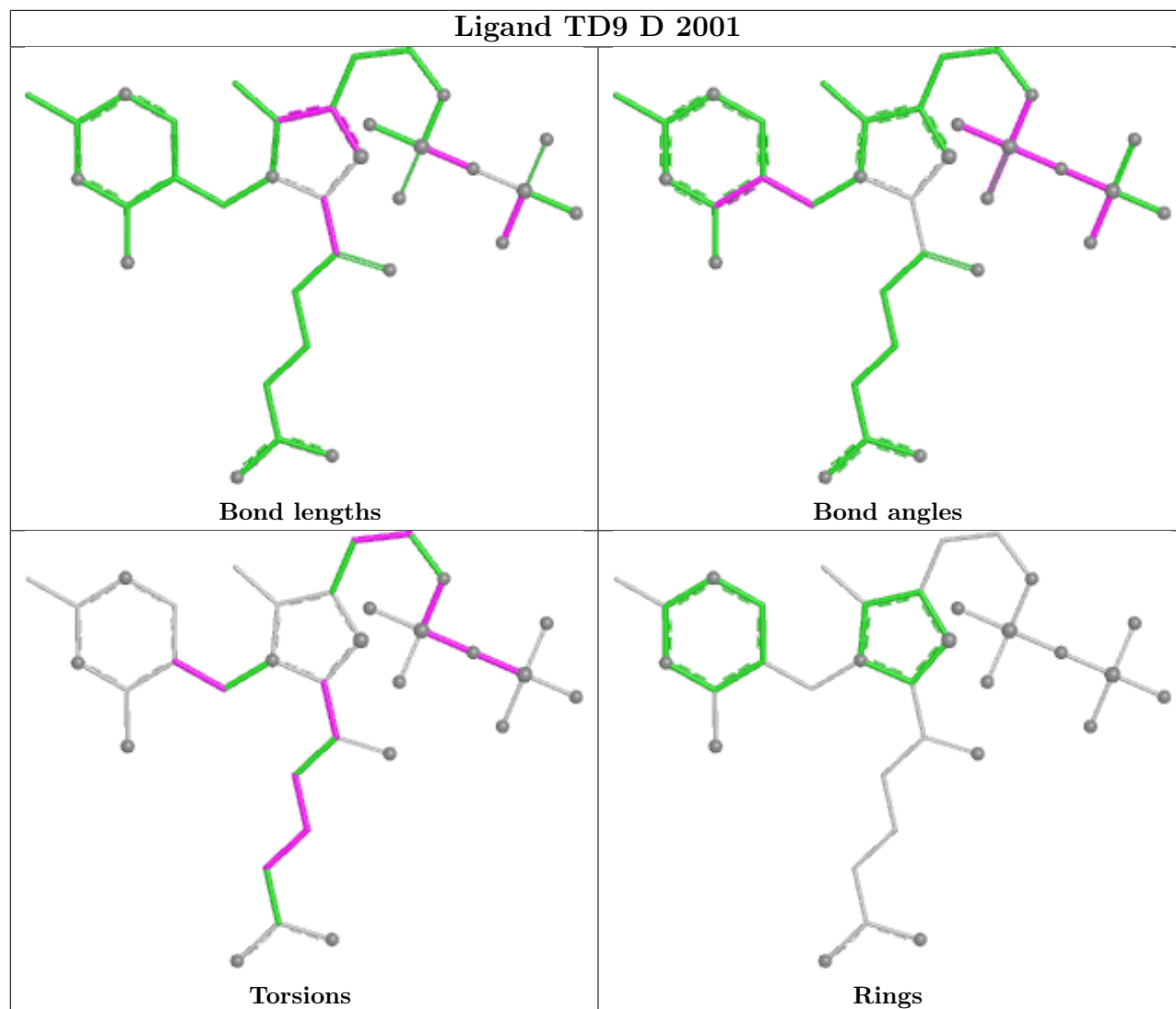
2 monomers are involved in 2 short contacts:

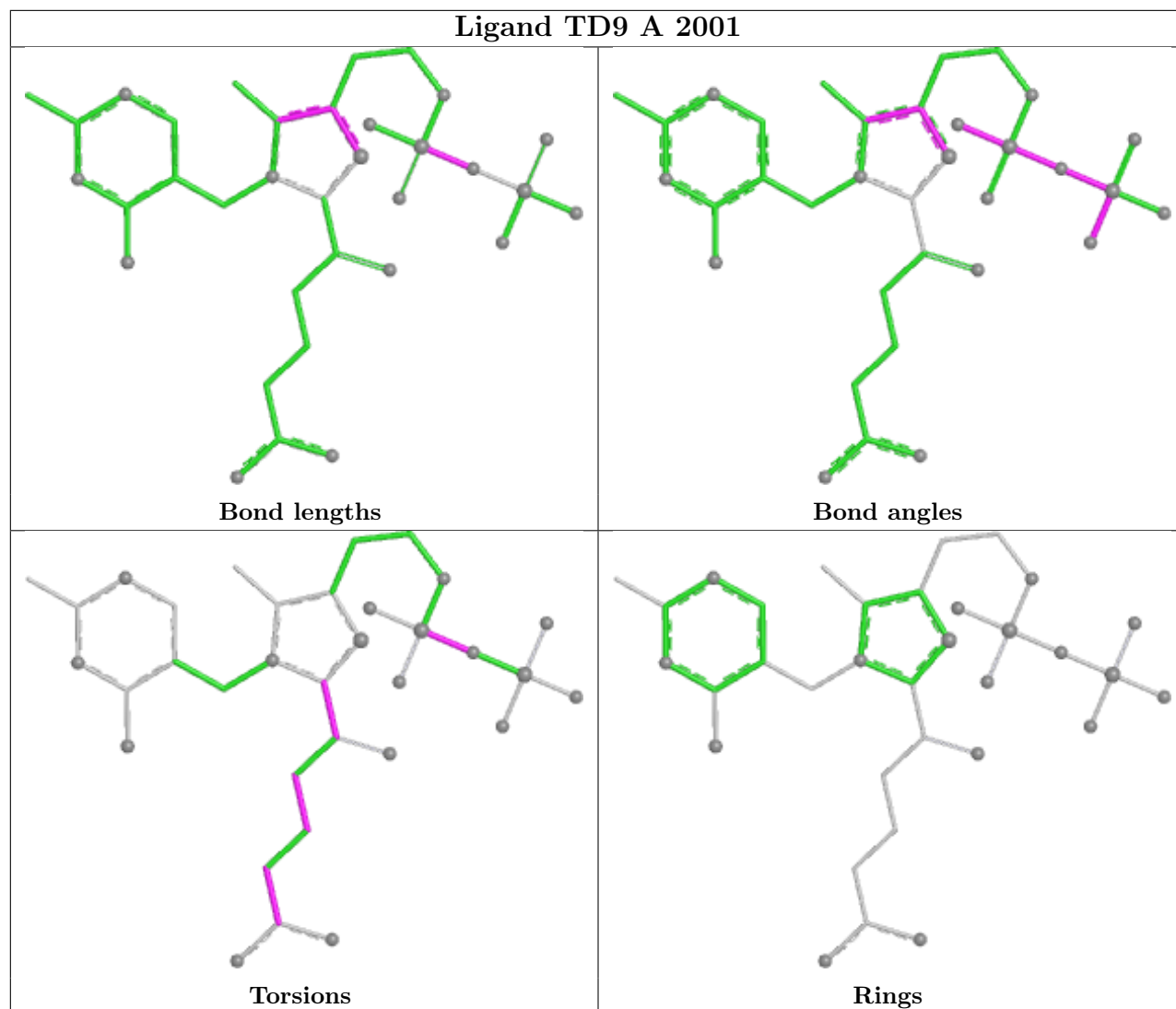
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	TD9	1	0
2	D	2001	TD9	1	0

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 ⓘ

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%)	0.91	129 (15%) 5 5	21, 39, 71, 113	1 (0%)
1	B	809/868 (93%)	1.04	141 (17%) 4 4	20, 43, 76, 111	2 (0%)
1	C	808/868 (93%)	0.84	114 (14%) 6 7	23, 39, 70, 97	0
1	D	807/868 (92%)	0.94	128 (15%) 5 5	23, 42, 76, 104	0
All	All	3238/3472 (93%)	0.94	512 (15%) 5 5	20, 41, 74, 113	3 (0%)

All (512) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	VAL	8.7
1	D	397	PHE	7.8
1	D	368	ALA	7.6
1	A	368	ALA	7.5
1	B	413	TRP	7.1
1	D	501	VAL	7.0
1	B	576	VAL	6.9
1	A	562	GLU	6.9
1	A	411	THR	6.8
1	A	561	PHE	6.7
1	B	368	ALA	6.5
1	A	750	GLY	6.4
1	B	793	LEU	6.3
1	D	413	TRP	6.3
1	D	575	ASP	6.2
1	B	779	ILE	6.1
1	C	501	VAL	6.1
1	B	500	TYR	6.1
1	B	558	PHE	6.1
1	A	1210	SER	5.9
1	A	501	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	815	ILE	5.9
1	C	367	ASN	5.9
1	C	500	TYR	5.9
1	B	807	VAL	5.6
1	B	502	GLY	5.6
1	D	367	ASN	5.6
1	D	576	VAL	5.6
1	C	413	TRP	5.5
1	C	575	ASP	5.5
1	B	415	LEU	5.5
1	C	411	THR	5.5
1	B	503	GLN	5.5
1	D	793	LEU	5.5
1	D	558	PHE	5.5
1	B	581	GLY	5.4
1	A	800	LEU	5.4
1	B	578	TYR	5.3
1	C	810	LEU	5.3
1	B	810	LEU	5.3
1	D	810	LEU	5.2
1	C	576	VAL	5.2
1	B	420	LYS	5.2
1	B	789	ALA	5.2
1	A	399	SER	5.1
1	D	797	GLN	5.0
1	C	769	GLY	5.0
1	D	789	ALA	4.9
1	C	803	VAL	4.9
1	A	581	GLY	4.9
1	B	397	PHE	4.8
1	C	831	LEU	4.7
1	C	368	ALA	4.7
1	D	419	PHE	4.7
1	C	506	PHE	4.7
1	B	803	VAL	4.6
1	D	414	ASP	4.6
1	A	784	ILE	4.6
1	C	503	GLN	4.5
1	D	803	VAL	4.5
1	D	768	ARG	4.5
1	C	578	TYR	4.5
1	B	777	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	779	ILE	4.4
1	B	365	ASP	4.4
1	C	397	PHE	4.4
1	A	803	VAL	4.4
1	C	789	ALA	4.4
1	B	784	ILE	4.4
1	C	560	GLU	4.3
1	A	500	TYR	4.3
1	B	394	ASN	4.3
1	A	810	LEU	4.3
1	B	808	ARG	4.3
1	B	781	ARG	4.3
1	A	813	HIS	4.3
1	D	786	MET	4.3
1	B	367	ASN	4.2
1	D	578	TYR	4.2
1	B	804	PHE	4.2
1	A	807	VAL	4.2
1	D	775	THR	4.2
1	A	831	LEU	4.2
1	A	804	PHE	4.2
1	C	807	VAL	4.2
1	A	575	ASP	4.1
1	A	503	GLN	4.1
1	B	419	PHE	4.1
1	D	804	PHE	4.1
1	D	807	VAL	4.1
1	D	1227	GLY	4.1
1	B	796	TYR	4.1
1	B	557	ILE	4.1
1	A	413	TRP	4.1
1	D	553	PRO	4.1
1	A	777	ALA	4.0
1	B	750	GLY	4.0
1	A	506	PHE	4.0
1	D	831	LEU	4.0
1	A	576	VAL	4.0
1	B	766	THR	4.0
1	B	504	LYS	4.0
1	B	543	LEU	4.0
1	B	560	GLU	4.0
1	C	581	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	554	TYR	3.9
1	B	575	ASP	3.9
1	B	769	GLY	3.9
1	D	750	GLY	3.9
1	C	784	ILE	3.9
1	D	559	SER	3.9
1	A	909	THR	3.8
1	A	499	LYS	3.8
1	D	394	ASN	3.8
1	B	579	HIS	3.8
1	B	539	HIS	3.8
1	C	812	LYS	3.8
1	A	497	GLN	3.8
1	A	853	GLY	3.8
1	B	792	ALA	3.7
1	B	800	LEU	3.7
1	C	800	LEU	3.7
1	C	804	PHE	3.7
1	D	784	ILE	3.7
1	C	496	LEU	3.7
1	D	581	GLY	3.7
1	C	495	PHE	3.7
1	D	471	HIS	3.7
1	C	494	THR	3.7
1	C	499	LYS	3.7
1	A	785	SER	3.7
1	D	503	GLN	3.7
1	B	473	LYS	3.6
1	B	499	LYS	3.6
1	C	558	PHE	3.6
1	C	779	ILE	3.6
1	B	745	ARG	3.6
1	A	495	PHE	3.6
1	D	500	TYR	3.6
1	D	809	GLU	3.6
1	A	505	ARG	3.6
1	B	767	LYS	3.6
1	D	499	LYS	3.6
1	D	769	GLY	3.6
1	B	770	SER	3.6
1	A	779	ILE	3.5
1	B	775	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	794	ARG	3.5
1	B	765	ASP	3.5
1	B	791	ASP	3.5
1	C	1186	GLU	3.5
1	B	506	PHE	3.5
1	A	547	ALA	3.5
1	B	801	GLU	3.5
1	A	394	ASN	3.5
1	A	740	LEU	3.5
1	B	1035	GLY	3.5
1	B	418	GLU	3.5
1	B	1220	GLU	3.5
1	B	916	VAL	3.5
1	C	750	GLY	3.4
1	A	778	LEU	3.4
1	C	744	ARG	3.4
1	B	554	TYR	3.4
1	B	748	ASN	3.4
1	B	1131	ASN	3.4
1	A	476	VAL	3.4
1	B	553	PRO	3.4
1	D	506	PHE	3.4
1	B	432	LEU	3.4
1	B	580	LEU	3.4
1	C	369	ARG	3.4
1	C	813	HIS	3.4
1	C	394	ASN	3.4
1	D	767	LYS	3.4
1	A	809	GLU	3.4
1	D	785	SER	3.4
1	A	789	ALA	3.4
1	B	495	PHE	3.4
1	C	419	PHE	3.4
1	C	745	ARG	3.3
1	B	416	ASP	3.3
1	C	796	TYR	3.3
1	D	416	ASP	3.3
1	A	792	ALA	3.3
1	B	786	MET	3.3
1	A	702	ILE	3.3
1	C	777	ALA	3.3
1	C	543	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	398	ARG	3.3
1	A	796	TYR	3.3
1	C	539	HIS	3.3
1	C	554	TYR	3.3
1	C	794	ARG	3.3
1	A	811	GLU	3.3
1	B	785	SER	3.2
1	B	1227	GLY	3.2
1	A	560	GLU	3.2
1	B	749	GLU	3.2
1	D	792	ALA	3.2
1	B	778	LEU	3.2
1	D	543	LEU	3.2
1	A	558	PHE	3.2
1	B	505	ARG	3.2
1	C	786	MET	3.2
1	D	916	VAL	3.2
1	A	419	PHE	3.2
1	A	1035	GLY	3.2
1	B	794	ARG	3.2
1	C	775	THR	3.2
1	B	763	VAL	3.1
1	A	793	LEU	3.1
1	A	578	TYR	3.1
1	D	873	GLU	3.1
1	A	786	MET	3.1
1	D	796	TYR	3.1
1	D	859	ARG	3.1
1	B	496	LEU	3.1
1	D	580	LEU	3.1
1	C	1210	SER	3.1
1	C	814	GLU	3.1
1	D	795	ASP	3.1
1	B	494	THR	3.0
1	A	580	LEU	3.0
1	D	557	ILE	3.0
1	B	1102	GLY	3.0
1	A	1186	GLU	3.0
1	D	418	GLU	3.0
1	D	790	GLU	3.0
1	D	577	LYS	3.0
1	B	799	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	1210	SER	3.0
1	A	494	THR	3.0
1	B	498	THR	3.0
1	A	579	HIS	3.0
1	D	579	HIS	3.0
1	B	859	ARG	3.0
1	B	831	LEU	3.0
1	C	1213	VAL	3.0
1	D	1103	GLU	3.0
1	D	1220	GLU	3.0
1	D	551	GLY	3.0
1	D	504	LYS	3.0
1	D	858	PRO	3.0
1	A	556	GLN	2.9
1	D	794	ARG	2.9
1	A	539	HIS	2.9
1	D	472	ASP	2.9
1	B	759	TYR	2.9
1	C	792	ALA	2.9
1	C	415	LEU	2.9
1	D	415	LEU	2.9
1	D	800	LEU	2.9
1	B	472	ASP	2.9
1	B	836	ASP	2.9
1	A	768	ARG	2.9
1	A	390	LEU	2.9
1	C	580	LEU	2.9
1	D	496	LEU	2.9
1	D	778	LEU	2.9
1	D	813	HIS	2.9
1	C	556	GLN	2.9
1	D	556	GLN	2.9
1	D	560	GLU	2.9
1	C	759	TYR	2.9
1	C	502	GLY	2.9
1	B	858	PRO	2.8
1	A	759	TYR	2.8
1	C	579	HIS	2.8
1	D	765	ASP	2.8
1	D	473	LYS	2.8
1	A	397	PHE	2.8
1	D	924	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	812	LYS	2.8
1	B	577	LYS	2.8
1	D	470	LYS	2.8
1	B	768	ARG	2.8
1	C	808	ARG	2.8
1	D	539	HIS	2.8
1	A	496	LEU	2.8
1	B	483	LEU	2.8
1	C	431	LYS	2.8
1	D	766	THR	2.8
1	B	555	SER	2.7
1	B	1103	GLU	2.7
1	B	780	GLY	2.7
1	C	859	ARG	2.7
1	D	555	SER	2.7
1	A	472	ASP	2.7
1	B	795	ASP	2.7
1	D	541	GLY	2.7
1	B	492	PHE	2.7
1	B	392	LEU	2.7
1	B	918	ARG	2.7
1	C	740	LEU	2.7
1	A	799	GLN	2.7
1	A	1227	GLY	2.7
1	A	488	ALA	2.7
1	C	488	ALA	2.7
1	B	455	LEU	2.7
1	C	432	LEU	2.7
1	C	778	LEU	2.7
1	B	813	HIS	2.7
1	C	471	HIS	2.7
1	A	370	VAL	2.7
1	B	1060	ILE	2.7
1	B	811	GLU	2.6
1	C	547	ALA	2.6
1	D	392	LEU	2.6
1	D	772	LYS	2.6
1	B	664	ARG	2.6
1	C	932	THR	2.6
1	D	498	THR	2.6
1	A	787	LYS	2.6
1	B	393	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	767	LYS	2.6
1	B	782	GLY	2.6
1	A	491	ALA	2.6
1	A	513	THR	2.6
1	A	546	LEU	2.6
1	B	366	LYS	2.6
1	B	616	LEU	2.6
1	C	577	LYS	2.6
1	D	866	LYS	2.6
1	A	749	GLU	2.6
1	C	921	GLY	2.6
1	C	513	THR	2.6
1	D	494	THR	2.6
1	C	412	LEU	2.6
1	C	793	LEU	2.6
1	C	799	GLN	2.5
1	C	1034	GLU	2.5
1	A	856	VAL	2.5
1	B	371	ILE	2.5
1	D	1187	ILE	2.5
1	C	1035	GLY	2.5
1	A	767	LYS	2.5
1	C	781	ARG	2.5
1	D	781	ARG	2.5
1	A	583	THR	2.5
1	D	395	THR	2.5
1	B	436	LEU	2.5
1	C	497	GLN	2.5
1	D	1219	GLN	2.5
1	C	551	GLY	2.5
1	D	856	VAL	2.5
1	A	1129	LYS	2.5
1	C	480	LYS	2.5
1	C	1129	LYS	2.5
1	B	429	ARG	2.5
1	C	805	ASN	2.5
1	D	667	ARG	2.5
1	A	498	THR	2.5
1	D	776	GLU	2.5
1	A	746	GLY	2.5
1	A	1212	LYS	2.5
1	B	798	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	711	GLY	2.5
1	A	369	ARG	2.5
1	B	761	TYR	2.5
1	A	493	GLU	2.5
1	A	1034	GLU	2.5
1	D	1034	GLU	2.5
1	A	473	LYS	2.5
1	A	492	PHE	2.5
1	A	798	GLY	2.5
1	D	370	VAL	2.4
1	B	797	GLN	2.4
1	B	742	TYR	2.4
1	D	554	TYR	2.4
1	D	1125	ALA	2.4
1	A	504	LYS	2.4
1	B	508	LEU	2.4
1	B	1129	LYS	2.4
1	D	808	ARG	2.4
1	A	1209	GLY	2.4
1	C	370	VAL	2.4
1	A	395	THR	2.4
1	A	775	THR	2.4
1	B	395	THR	2.4
1	B	760	MET	2.4
1	B	773	ALA	2.4
1	D	396	ARG	2.4
1	D	547	ALA	2.4
1	A	616	LEU	2.4
1	D	1035	GLY	2.4
1	A	428	GLN	2.4
1	C	801	GLU	2.4
1	C	557	ILE	2.4
1	A	484	SER	2.4
1	A	745	ARG	2.4
1	C	802	ARG	2.4
1	D	469	THR	2.4
1	B	471	HIS	2.4
1	D	373	LEU	2.4
1	D	801	GLU	2.4
1	A	805	ASN	2.4
1	B	497	GLN	2.4
1	D	1101	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	963[A]	SER	2.4
1	B	809	GLU	2.3
1	A	1059	GLY	2.3
1	D	492	PHE	2.3
1	D	811	GLU	2.3
1	A	582	ALA	2.3
1	B	547	ALA	2.3
1	C	748	ASN	2.3
1	C	546	LEU	2.3
1	C	414	ASP	2.3
1	A	808	ARG	2.3
1	B	861	ARG	2.3
1	B	747	HIS	2.3
1	C	633	ASN	2.3
1	B	1128	ALA	2.3
1	B	414	ASP	2.3
1	B	551	GLY	2.3
1	C	483	LEU	2.3
1	D	1002	LEU	2.3
1	C	1212	LYS	2.3
1	B	556	GLN	2.3
1	B	764	ILE	2.3
1	D	763	VAL	2.3
1	B	469	THR	2.3
1	A	771	ARG	2.3
1	C	646	ALA	2.3
1	D	777	ALA	2.3
1	D	812	LYS	2.3
1	A	790	GLU	2.2
1	D	814	GLU	2.2
1	A	463	ILE	2.2
1	C	702	ILE	2.2
1	A	469	THR	2.2
1	A	744	ARG	2.2
1	B	805	ASN	2.2
1	B	1015	GLY	2.2
1	D	773	ALA	2.2
1	D	1102	GLY	2.2
1	A	776	GLU	2.2
1	A	868	ARG	2.2
1	B	552	LYS	2.2
1	D	1119	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	749	GLU	2.2
1	C	811	GLU	2.2
1	A	543	LEU	2.2
1	C	623	LEU	2.2
1	C	850	LEU	2.2
1	C	761	TYR	2.2
1	C	754	SER	2.2
1	A	366	LYS	2.2
1	C	590	PHE	2.2
1	C	1060	ILE	2.2
1	D	791	ASP	2.2
1	B	488	ALA	2.2
1	C	455	LEU	2.2
1	D	850	LEU	2.2
1	A	754	SER	2.2
1	A	633	ASN	2.2
1	C	389	PRO	2.1
1	A	860	VAL	2.1
1	B	1219	GLN	2.1
1	A	866	LYS	2.1
1	B	772	LYS	2.1
1	A	367	ASN	2.1
1	D	633	ASN	2.1
1	B	512	GLU	2.1
1	A	756	THR	2.1
1	A	557	ILE	2.1
1	B	545	VAL	2.1
1	C	853	GLY	2.1
1	D	747	HIS	2.1
1	D	1209	GLY	2.1
1	A	380	ARG	2.1
1	A	417	ARG	2.1
1	C	440	ARG	2.1
1	C	771	ARG	2.1
1	B	582	ALA	2.1
1	A	480	LYS	2.1
1	A	1131	ASN	2.1
1	D	628	GLU	2.1
1	D	759	TYR	2.1
1	C	768	ARG	2.1
1	D	1060	ILE	2.1
1	A	863	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	1016	GLN	2.1
1	A	471	HIS	2.1
1	A	1183	THR	2.1
1	B	1062	ARG	2.1
1	C	583	THR	2.1
1	A	921	GLY	2.1
1	D	936	GLY	2.1
1	C	552	LYS	2.1
1	D	915	ILE	2.1
1	B	1125	ALA	2.1
1	A	1195	LEU	2.0
1	D	508	LEU	2.0
1	A	797	GLN	2.0
1	C	751	ASP	2.0
1	B	1183	THR	2.0
1	B	787	LYS	2.0
1	C	473	LYS	2.0
1	A	711	GLY	2.0
1	C	746	GLY	2.0
1	D	502	GLY	2.0
1	A	915	ILE	2.0
1	B	515	ILE	2.0
1	D	495	PHE	2.0
1	D	854	PHE	2.0
1	B	548	ASN	2.0
1	D	748	ASN	2.0
1	A	857	HIS	2.0
1	D	942	LYS	2.0
1	C	498	THR	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

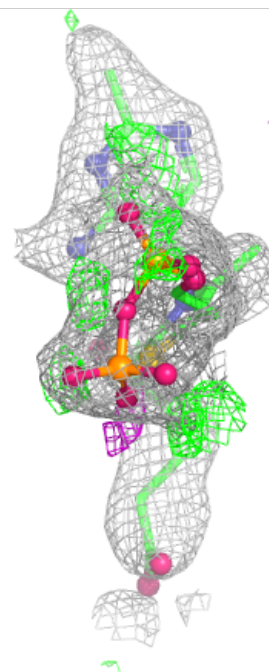
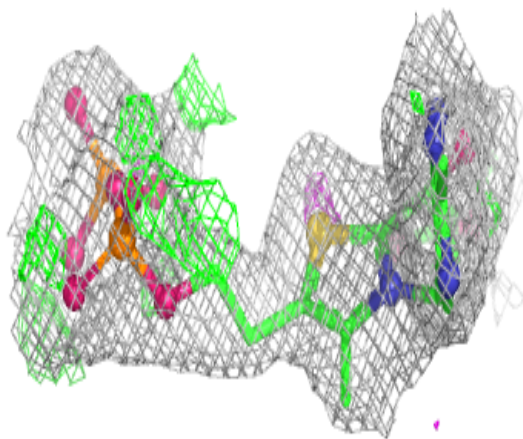
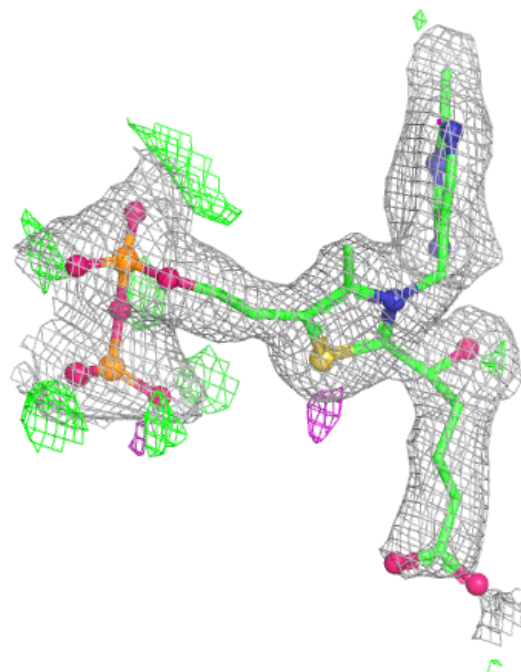
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TD9	B	2001	34/34	0.94	0.12	20,32,69,73	0
2	TD9	C	2001	34/34	0.95	0.10	23,30,57,58	0
2	TD9	A	2001	34/34	0.96	0.10	24,32,63,65	0
2	TD9	D	2001	34/34	0.96	0.09	18,29,63,65	0
3	MG	B	2002	1/1	0.96	0.05	28,28,28,28	0
4	CA	B	2003	1/1	0.96	0.06	43,43,43,43	0
3	MG	A	2002	1/1	0.97	0.08	25,25,25,25	0
3	MG	D	2002	1/1	0.98	0.04	24,24,24,24	0
4	CA	D	2003	1/1	0.98	0.04	41,41,41,41	0
3	MG	C	2002	1/1	0.99	0.07	22,22,22,22	0
4	CA	C	2003	1/1	0.99	0.05	38,38,38,38	0
4	CA	A	2003	1/1	0.99	0.03	38,38,38,38	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.

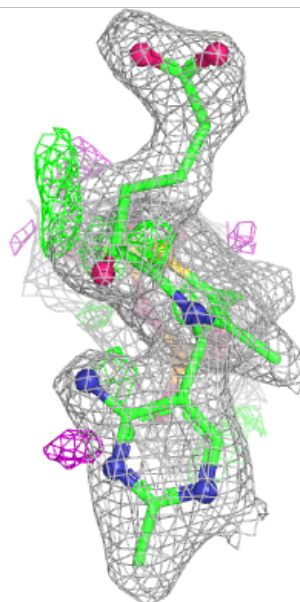
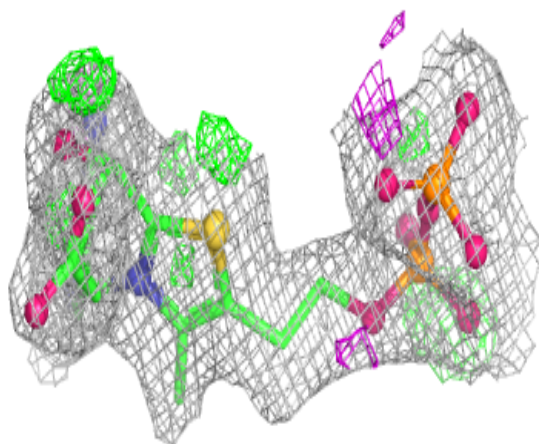
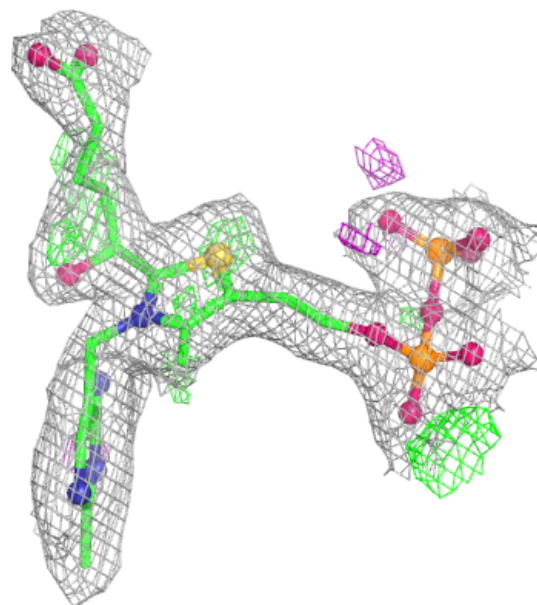
Electron density around TD9 B 2001:

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



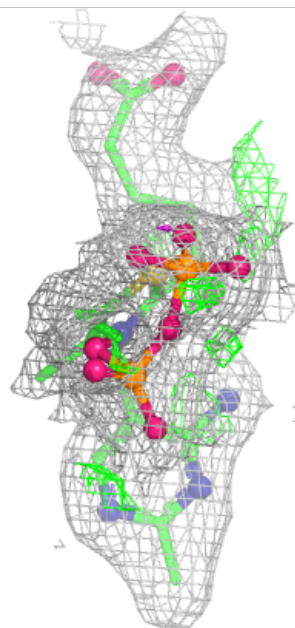
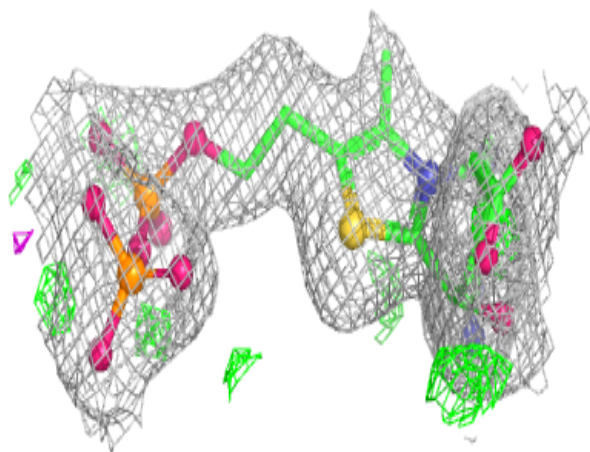
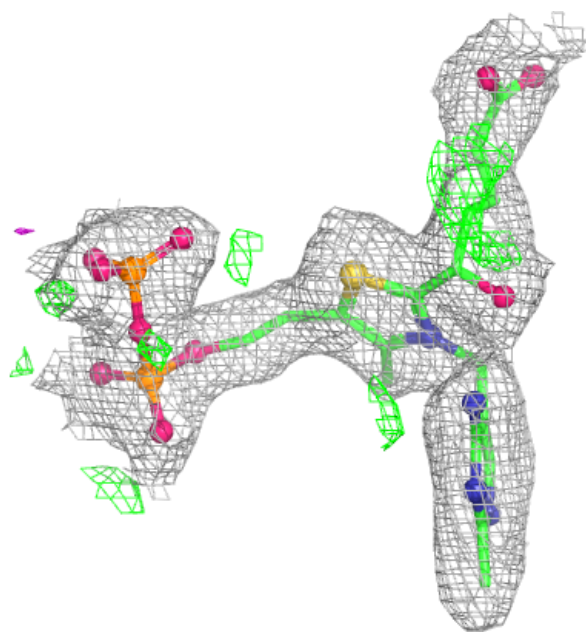
Electron density around TD9 C 2001:

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



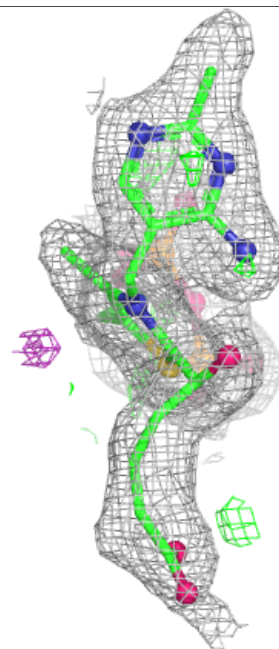
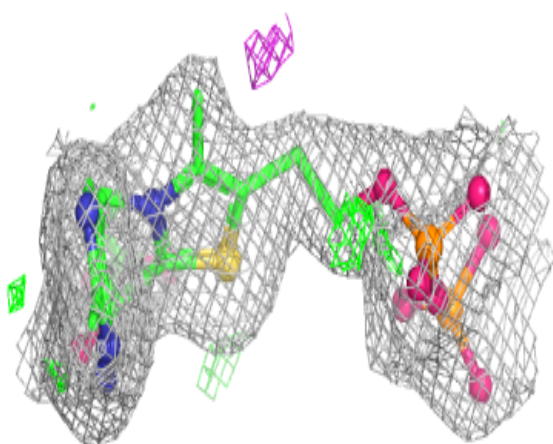
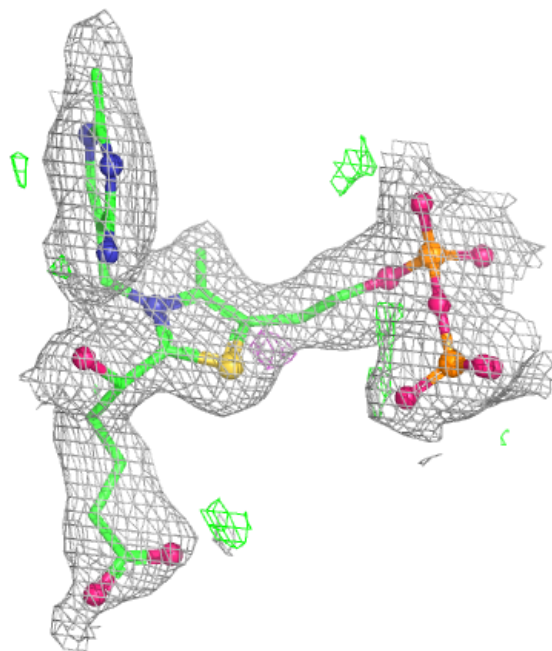
Electron density around TD9 A 2001:

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



Electron density around TD9 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.