



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:27 PM UTC

PDB ID : 3ZHV / pdb_00003zhv
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis KGD, post-decarboxylation intermediate from pyruvate (2-hydroxyethyl-ThDP)
Authors : Wagner, T.; Barilone, N.; Bellinzoni, M.; Alzari, P.M.
Deposited on : 2012-12-24
Resolution : 2.30 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

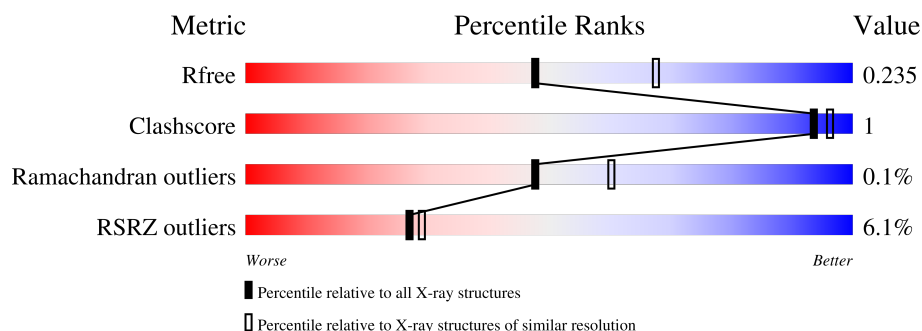
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	6% 90% 5% 6%
1	B	868	6% 89% 5% 6%
1	C	868	6% 88% 5% 7%
1	D	868	5% 89% 5% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26141 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.

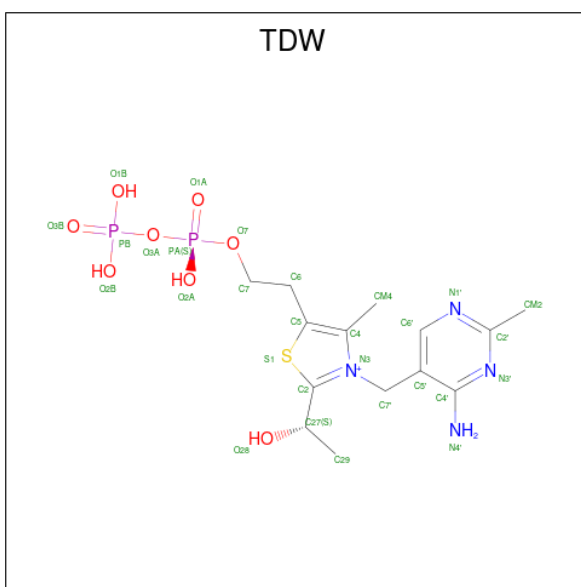
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	820	Total	C	N	O	S	0	0	0
			6332	3988	1118	1204	22			
1	B	813	Total	C	N	O	S	0	1	0
			6252	3946	1106	1177	23			
1	C	803	Total	C	N	O	S	0	0	0
			6234	3935	1102	1174	23			
1	D	812	Total	C	N	O	S	0	0	0
			6230	3928	1102	1176	24			

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 2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-4-methyl-2-[(1S)-1-oxidanylet hyl]-1,3-thiazol-3-ium-5-yl]ethyl phosphono hydrogen phosphate (CCD ID: TDW) (formula: C₁₄H₂₃N₄O₈P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 29	C 14	N 4	O 8	P 2	S 1	0	0
2	B	1	Total 29	C 14	N 4	O 8	P 2	S 1	0	0
2	C	1	Total 29	C 14	N 4	O 8	P 2	S 1	0	0
2	D	1	Total 29	C 14	N 4	O 8	P 2	S 1	0	0

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

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

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

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

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

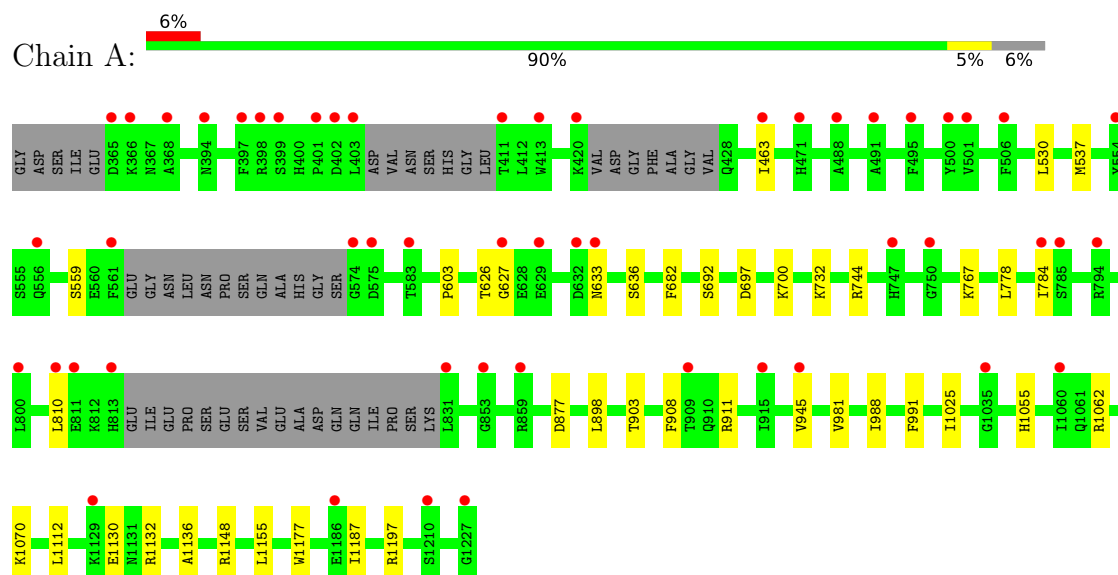
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	289	Total 289	O 289	0	0
5	B	218	Total 218	O 218	0	0
5	C	260	Total 260	O 260	0	0
5	D	202	Total 202	O 202	0	0

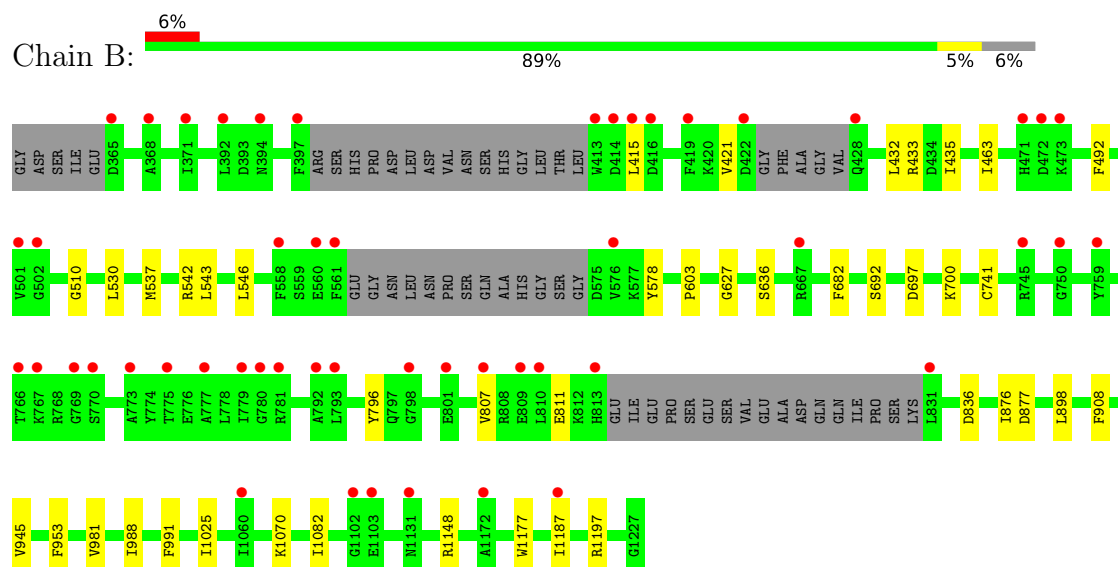
3 Residue-property plots

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.

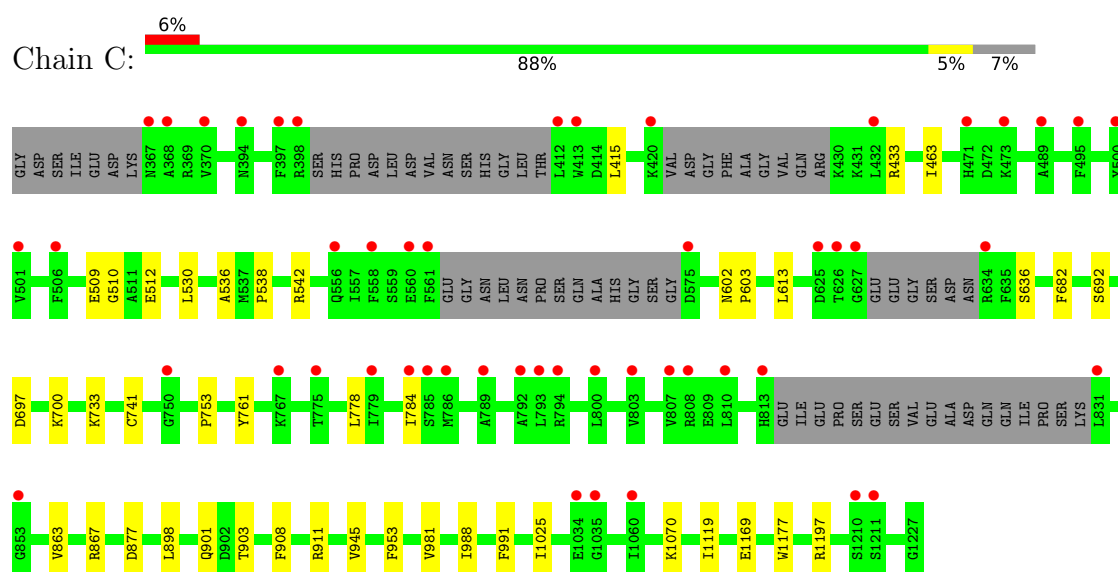
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME



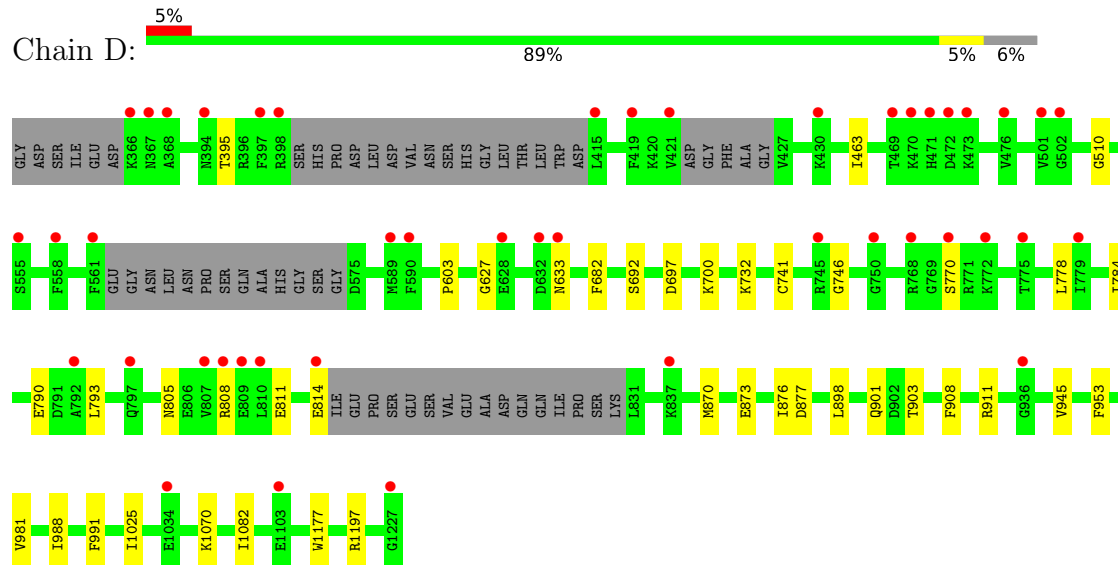
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME



• 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	80.46Å 83.70Å 160.33Å 99.68° 98.87° 100.63°	Depositor
Resolution (Å)	41.06 – 2.30 41.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (41.06-2.30) 97.6 (41.06-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.203 , 0.235 (Not available) , 0.235	Depositor DCC
R_{free} test set	8627 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26141	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, TDW, 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	0.85	0/6462	1.24	10/8770 (0.1%)
1	B	0.83	0/6382	1.26	16/8663 (0.2%)
1	C	0.85	0/6360	1.25	8/8620 (0.1%)
1	D	0.85	1/6356 (0.0%)	1.25	16/8624 (0.2%)
All	All	0.84	1/25560 (0.0%)	1.25	50/34677 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	870	MET	SD-CE	-5.16	1.66	1.79

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	836	ASP	CA-CB-CG	9.50	122.10	112.60
1	A	877	ASP	CA-CB-CG	6.05	118.65	112.60
1	D	627	GLY	CA-C-N	5.81	128.07	120.28
1	D	627	GLY	C-N-CA	5.81	128.07	120.28
1	D	877	ASP	CA-CB-CG	5.81	118.41	112.60
1	C	877	ASP	CA-CB-CG	5.75	118.35	112.60
1	D	700	LYS	CA-C-N	5.74	128.24	120.38
1	D	700	LYS	C-N-CA	5.74	128.24	120.38
1	D	873	GLU	CB-CG-CD	5.60	122.12	112.60
1	D	953	PHE	CA-CB-CG	5.59	119.39	113.80
1	B	877	ASP	CA-CB-CG	5.57	118.17	112.60
1	D	1025	ILE	CA-C-N	5.51	127.93	120.38
1	D	1025	ILE	C-N-CA	5.51	127.93	120.38
1	B	953	PHE	CA-CB-CG	5.49	119.29	113.80
1	B	463	ILE	CA-C-N	5.44	127.88	120.54
1	B	463	ILE	C-N-CA	5.44	127.88	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	395	THR	CA-C-N	5.43	127.87	120.54
1	D	395	THR	C-N-CA	5.43	127.87	120.54
1	A	700	LYS	CA-C-N	5.42	127.80	120.38
1	A	700	LYS	C-N-CA	5.42	127.80	120.38
1	C	700	LYS	CA-C-N	5.39	127.77	120.38
1	C	700	LYS	C-N-CA	5.39	127.77	120.38
1	C	953	PHE	CA-CB-CG	5.33	119.13	113.80
1	D	746	GLY	N-CA-C	-5.33	105.72	112.54
1	D	770	SER	CA-C-N	5.33	127.68	120.65
1	D	770	SER	C-N-CA	5.33	127.68	120.65
1	A	537	MET	N-CA-C	5.32	113.01	108.22
1	C	1025	ILE	CA-C-N	5.29	127.63	120.38
1	C	1025	ILE	C-N-CA	5.29	127.63	120.38
1	B	627	GLY	CA-C-N	5.28	127.62	120.38
1	B	627	GLY	C-N-CA	5.28	127.62	120.38
1	D	463	ILE	CA-C-N	5.28	127.67	120.54
1	D	463	ILE	C-N-CA	5.28	127.67	120.54
1	B	700	LYS	CA-C-N	5.27	128.07	120.38
1	B	700	LYS	C-N-CA	5.27	128.07	120.38
1	A	1025	ILE	CA-C-N	5.26	127.58	120.38
1	A	1025	ILE	C-N-CA	5.26	127.58	120.38
1	A	463	ILE	CA-C-N	5.24	127.62	120.54
1	A	463	ILE	C-N-CA	5.24	127.62	120.54
1	B	1025	ILE	CA-C-N	5.23	127.55	120.38
1	B	1025	ILE	C-N-CA	5.23	127.55	120.38
1	B	537	MET	N-CA-C	5.19	112.89	108.22
1	B	492	PHE	CA-C-N	5.14	127.12	120.44
1	B	492	PHE	C-N-CA	5.14	127.12	120.44
1	B	796	TYR	CA-C-N	5.09	127.10	120.28
1	B	796	TYR	C-N-CA	5.09	127.10	120.28
1	C	463	ILE	CA-C-N	5.04	127.35	120.54
1	C	463	ILE	C-N-CA	5.04	127.35	120.54
1	A	627	GLY	CA-C-N	5.01	126.99	120.28
1	A	627	GLY	C-N-CA	5.01	126.99	120.28

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	6332	0	6078	19	0
1	B	6252	0	6023	16	0
1	C	6234	0	6050	20	0
1	D	6230	0	5987	15	0
2	A	29	0	20	0	0
2	B	29	0	20	0	0
2	C	29	0	20	1	0
2	D	29	0	20	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	289	0	0	0	0
5	B	218	0	0	0	0
5	C	260	0	0	2	0
5	D	202	0	0	0	0
All	All	26141	0	24218	70	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 (70) 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:778:LEU:HB3	1:A:784:ILE:HG12	1.81	0.61
1:B:415:LEU:HA	1:B:432:LEU:HB3	1.84	0.60
1:A:744:ARG:NH2	1:A:767:LYS:O	2.39	0.56
1:C:778:LEU:HB3	1:C:784:ILE:HG12	1.88	0.55
1:A:1112:LEU:HD21	1:A:1155:LEU:HD22	1.88	0.55
1:B:1148:ARG:HG3	1:B:1187:ILE:HD12	1.91	0.53
1:B:542:ARG:HD3	1:B:578:TYR:HA	1.92	0.52
1:C:542:ARG:NH1	1:C:602:ASN:OD1	2.35	0.52
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	0.50
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.94	0.49
1:A:1148:ARG:HG3	1:A:1187:ILE:HD12	1.94	0.49
1:D:778:LEU:HB3	1:D:784:ILE:HG12	1.95	0.48
1:C:415:LEU:HB3	1:C:433:ARG:HB3	1.95	0.48
1:A:559:SER:HA	1:A:810:LEU:HD11	1.96	0.47
1:D:510:GLY:O	1:D:741:CYS:HB2	2.15	0.47
1:C:510:GLY:O	1:C:741:CYS:HB2	2.15	0.46
1:A:626:THR:HG21	1:A:636:SER:OG	2.14	0.46
1:A:692:SER:HB2	1:A:697:ASP:OD2	2.16	0.46
1:D:633:ASN:O	1:D:732:LYS:HE3	2.16	0.46
1:C:692:SER:HB2	1:C:697:ASP:OD2	2.16	0.46
1:B:510:GLY:O	1:B:741:CYS:HB2	2.15	0.46
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.52	0.45
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.52	0.45
1:A:1112:LEU:CD2	1:A:1155:LEU:HD22	2.47	0.45
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.52	0.45
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.51	0.45
1:B:807:VAL:O	1:B:811:GLU:HG3	2.17	0.45
1:C:898:LEU:O	1:C:945:VAL:HA	2.16	0.45
1:B:898:LEU:O	1:B:945:VAL:HA	2.18	0.44
1:D:898:LEU:O	1:D:945:VAL:HA	2.18	0.44
1:A:898:LEU:O	1:A:945:VAL:HA	2.18	0.44
1:B:421:VAL:HG11	1:B:435:ILE:HD12	2.00	0.44
1:C:753:PRO:HB2	1:C:761:TYR:CE1	2.53	0.44
1:C:509:GLU:HA	1:C:512:GLU:OE2	2.18	0.43
1:C:908:PHE:CZ	1:C:1070:LYS:HG2	2.53	0.43
1:B:692:SER:HB2	1:B:697:ASP:OD2	2.18	0.43
1:C:863:VAL:O	1:C:867:ARG:HG3	2.19	0.43
1:A:903:THR:O	1:A:911:ARG:HD2	2.19	0.43
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.53	0.43
1:A:908:PHE:CZ	1:A:1070:LYS:HG2	2.53	0.43
1:D:692:SER:HB2	1:D:697:ASP:OD2	2.18	0.43
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.54	0.43
1:A:1112:LEU:HD12	1:A:1136:ALA:HB3	2.01	0.42
1:A:1130:GLU:HB2	1:A:1132:ARG:HG2	2.01	0.42
1:A:1055:HIS:HE1	1:A:1062:ARG:O	2.02	0.42
1:B:415:LEU:HB3	1:B:433:ARG:HB3	2.01	0.42
1:D:603:PRO:HD3	1:D:991:PHE:CZ	2.54	0.42
1:A:530:LEU:HD22	1:A:636:SER:HA	2.02	0.42
1:D:876:ILE:HD11	1:D:1082:ILE:HD13	2.02	0.42
1:A:633:ASN:O	1:A:732:LYS:HE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:PRO:HB2	5:C:3033:HOH:O	2.18	0.42
1:D:903:THR:O	1:D:911:ARG:HD2	2.20	0.42
1:D:811:GLU:HA	1:D:814:GLU:HG2	2.02	0.42
1:C:733:LYS:HE3	5:C:3014:HOH:O	2.19	0.41
1:D:805:ASN:HA	1:D:808:ARG:NH1	2.35	0.41
1:B:603:PRO:HD3	1:B:991:PHE:CZ	2.56	0.41
1:C:530:LEU:HD22	1:C:636:SER:HA	2.02	0.41
1:C:903:THR:O	1:C:911:ARG:HD2	2.20	0.41
2:C:2001:TDW:H6'	1:D:901:GLN:OE1	2.21	0.41
1:C:536:ALA:HB3	1:C:613:LEU:HD22	2.03	0.41
1:C:603:PRO:HD3	1:C:991:PHE:CZ	2.56	0.41
1:B:543:LEU:HD23	1:B:546:LEU:HD12	2.03	0.41
1:B:876:ILE:HD11	1:B:1082:ILE:HD13	2.03	0.40
1:C:1119:ILE:HD12	1:C:1169:GLU:HG3	2.03	0.40
1:C:901:GLN:OE1	2:D:2001:TDW:H6'	2.21	0.40
1:A:603:PRO:HD3	1:A:991:PHE:CZ	2.57	0.40
1:B:530:LEU:HD22	1:B:636:SER:HA	2.03	0.40
1:D:790:GLU:HA	1:D:793:LEU:HD12	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	810/868 (93%)	790 (98%)	19 (2%)	1 (0%)	48	60
1	B	804/868 (93%)	786 (98%)	17 (2%)	1 (0%)	48	60
1	C	791/868 (91%)	774 (98%)	16 (2%)	1 (0%)	48	60
1	D	802/868 (92%)	784 (98%)	17 (2%)	1 (0%)	48	60
All	All	3207/3472 (92%)	3134 (98%)	69 (2%)	4 (0%)	48	60

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	TDW	B	2001	3	26,30,30	1.49	4 (15%)	33,45,45	1.24	4 (12%)
2	TDW	C	2001	3	26,30,30	1.08	3 (11%)	33,45,45	1.23	3 (9%)
2	TDW	A	2001	3	26,30,30	1.46	3 (11%)	33,45,45	1.24	5 (15%)
2	TDW	D	2001	3	26,30,30	2.08	3 (11%)	33,45,45	1.12	3 (9%)

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	TDW	B	2001	3	-	3/20/21/21	0/2/2/2
2	TDW	C	2001	3	-	5/20/21/21	0/2/2/2
2	TDW	A	2001	3	-	4/20/21/21	0/2/2/2
2	TDW	D	2001	3	-	5/20/21/21	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	TDW	PA-O3A	-8.09	1.50	1.59
2	D	2001	TDW	C5-C4	4.45	1.44	1.35
2	D	2001	TDW	C5-S1	-4.38	1.65	1.74
2	B	2001	TDW	PA-O3A	-4.19	1.55	1.59
2	A	2001	TDW	C5-S1	-4.16	1.65	1.74
2	B	2001	TDW	C5-S1	-4.12	1.65	1.74
2	A	2001	TDW	C5-C4	4.10	1.43	1.35
2	A	2001	TDW	PA-O3A	-4.04	1.55	1.59
2	B	2001	TDW	C5-C4	3.93	1.43	1.35
2	C	2001	TDW	C5-S1	-3.22	1.67	1.74
2	C	2001	TDW	PA-O3A	-2.82	1.56	1.59
2	C	2001	TDW	C5-C4	2.50	1.40	1.35
2	B	2001	TDW	PB-O1B	-2.06	1.47	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	TDW	O2A-PA-O3A	-3.47	97.89	107.27
2	D	2001	TDW	O3A-PA-O1A	3.34	120.76	110.70
2	C	2001	TDW	O3A-PA-O1A	3.24	120.45	110.70
2	B	2001	TDW	O2A-PA-O3A	-3.11	98.88	107.27
2	A	2001	TDW	O3A-PA-O1A	3.09	120.01	110.70
2	A	2001	TDW	O2A-PA-O3A	-2.83	99.61	107.27
2	D	2001	TDW	O2A-PA-O3A	-2.70	99.97	107.27
2	B	2001	TDW	O3A-PA-O1A	2.66	118.70	110.70
2	C	2001	TDW	C6-C5-S1	2.45	124.55	119.29
2	A	2001	TDW	O7-PA-O1A	2.44	118.61	108.94
2	D	2001	TDW	O7-PA-O1A	2.30	118.04	108.94
2	B	2001	TDW	C7'-C5'-C4'	2.24	126.44	122.36
2	A	2001	TDW	O2B-PB-O1B	2.18	115.96	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	TDW	C4-C5-S1	2.16	112.80	110.56
2	B	2001	TDW	O2A-PA-O1A	2.10	122.22	112.44

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	TDW	S1-C2-C27-O28
2	A	2001	TDW	N3-C2-C27-O28
2	A	2001	TDW	PA-O3A-PB-O1B
2	B	2001	TDW	N3-C2-C27-O28
2	C	2001	TDW	S1-C2-C27-O28
2	C	2001	TDW	N3-C2-C27-O28
2	C	2001	TDW	C7-O7-PA-O1A
2	D	2001	TDW	N3-C2-C27-O28
2	B	2001	TDW	PB-O3A-PA-O7
2	D	2001	TDW	PA-O3A-PB-O1B
2	A	2001	TDW	C7-O7-PA-O1A
2	D	2001	TDW	C7-O7-PA-O1A
2	B	2001	TDW	S1-C2-C27-O28
2	D	2001	TDW	S1-C2-C27-O28
2	C	2001	TDW	PA-O3A-PB-O1B
2	C	2001	TDW	C5-C6-C7-O7
2	D	2001	TDW	C5-C6-C7-O7

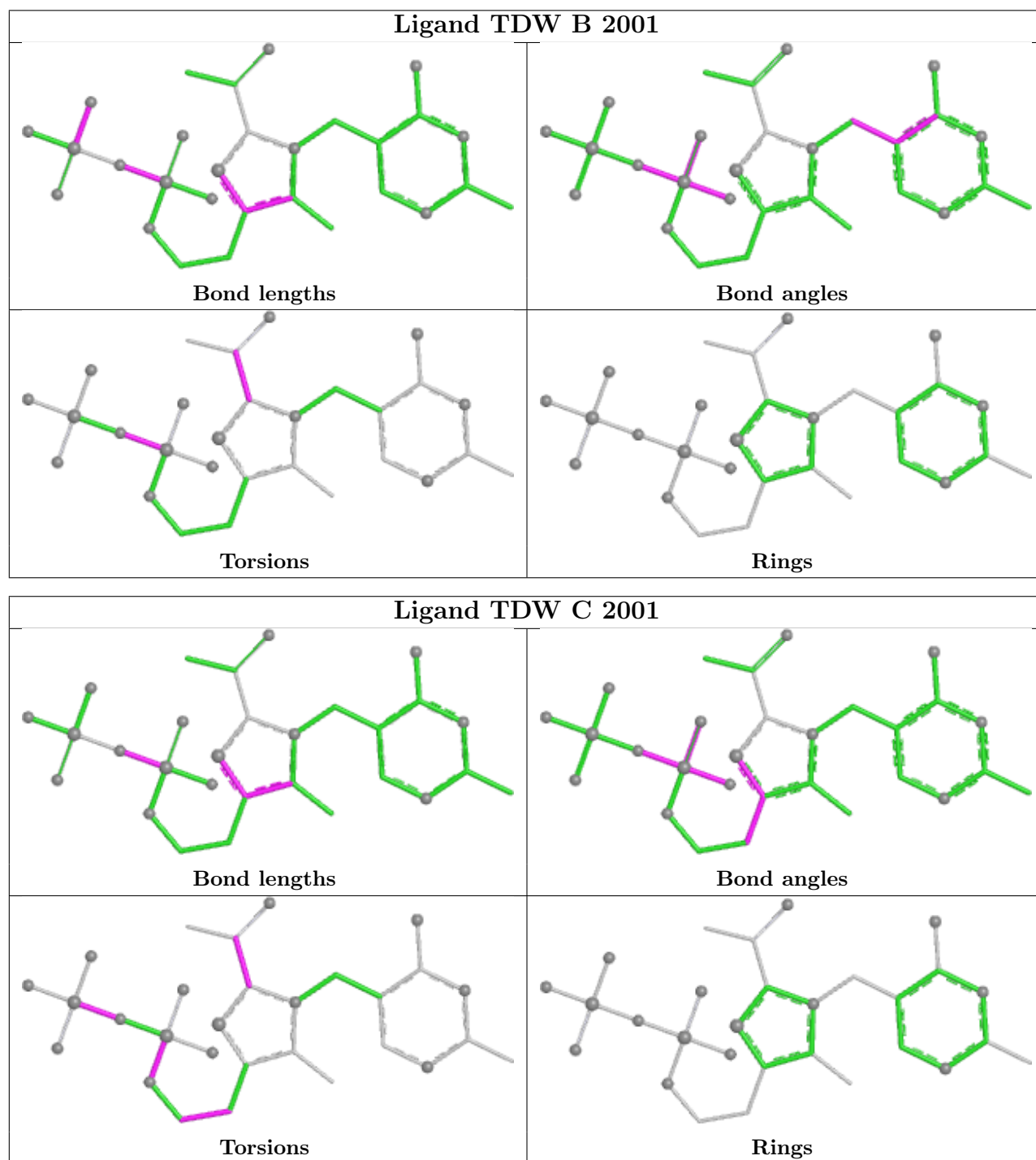
There are no ring outliers.

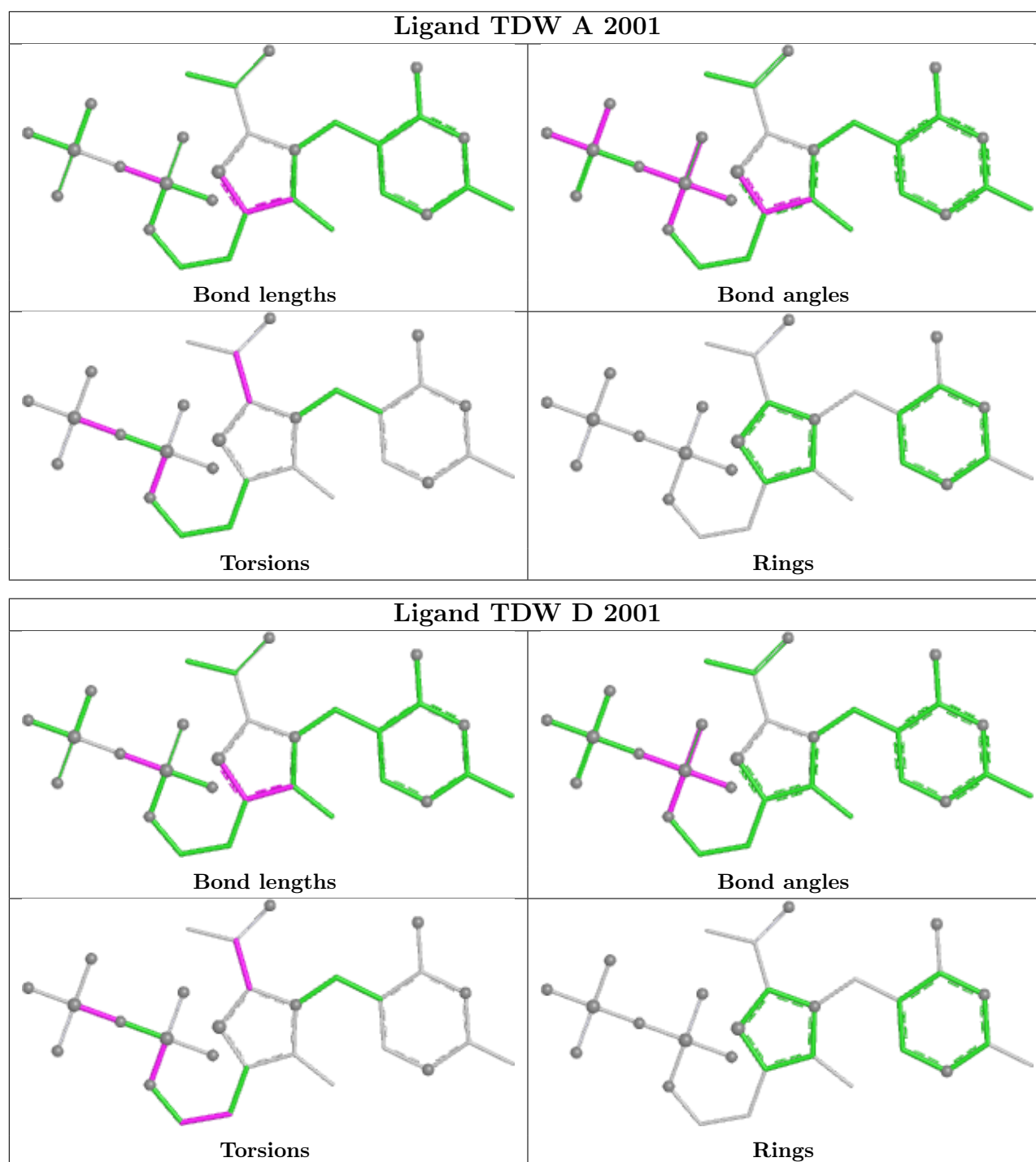
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	TDW	1	0
2	D	2001	TDW	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	820/868 (94%)	0.52	52 (6%)	26	28	30, 47, 80, 112	0
1	B	813/868 (93%)	0.48	51 (6%)	26	28	22, 47, 80, 118	1 (0%)
1	C	803/868 (92%)	0.49	50 (6%)	26	28	30, 47, 77, 108	0
1	D	812/868 (93%)	0.46	45 (5%)	30	32	30, 46, 78, 109	0
All	All	3248/3472 (93%)	0.49	198 (6%)	27	29	22, 47, 79, 118	1 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	627	GLY	5.6
1	B	413	TRP	5.5
1	C	575	ASP	5.1
1	D	421	VAL	5.1
1	A	365	ASP	5.1
1	C	398	ARG	5.0
1	A	403	LEU	4.8
1	B	422	ASP	4.6
1	D	366	LYS	4.4
1	A	750	GLY	4.4
1	B	414	ASP	4.4
1	C	813	HIS	4.3
1	A	411	THR	4.2
1	A	813	HIS	4.1
1	C	561	PHE	4.0
1	B	365	ASP	4.0
1	B	501	VAL	4.0
1	C	413	TRP	3.8
1	D	398	ARG	3.7
1	D	807	VAL	3.7
1	D	472	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	1227	GLY	3.7
1	D	473	LYS	3.7
1	C	785	SER	3.6
1	A	368	ALA	3.6
1	D	394	ASN	3.6
1	D	797	GLN	3.5
1	A	831	LEU	3.5
1	C	626	THR	3.5
1	B	473	LYS	3.5
1	C	792	ALA	3.4
1	B	813	HIS	3.4
1	B	371	ILE	3.4
1	C	831	LEU	3.4
1	C	750	GLY	3.4
1	D	810	LEU	3.4
1	A	420	LYS	3.4
1	B	415	LEU	3.4
1	B	472	ASP	3.4
1	C	775	THR	3.4
1	A	501	VAL	3.4
1	D	415	LEU	3.3
1	C	1210	SER	3.3
1	B	561	PHE	3.3
1	C	634	ARG	3.3
1	A	1210	SER	3.3
1	D	1227	GLY	3.3
1	C	779	ILE	3.2
1	B	766	THR	3.2
1	A	810	LEU	3.1
1	B	810	LEU	3.1
1	A	506	PHE	3.1
1	A	1129	LYS	3.0
1	C	367	ASN	3.0
1	C	412	LEU	3.0
1	A	575	ASP	3.0
1	B	397	PHE	2.9
1	D	419	PHE	2.9
1	C	500	TYR	2.9
1	B	779	ILE	2.9
1	A	394	ASN	2.9
1	C	625	ASP	2.9
1	C	560	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	793	LEU	2.8
1	B	792	ALA	2.8
1	B	1102	GLY	2.8
1	A	401	PRO	2.8
1	D	814	GLU	2.8
1	B	780	GLY	2.8
1	D	368	ALA	2.8
1	D	561	PHE	2.8
1	A	629	GLU	2.8
1	C	501	VAL	2.8
1	B	667	ARG	2.7
1	A	561	PHE	2.7
1	B	502	GLY	2.7
1	D	502	GLY	2.7
1	B	1172	ALA	2.7
1	C	803	VAL	2.7
1	A	859	ARG	2.7
1	A	784	ILE	2.6
1	A	794	ARG	2.6
1	C	556	GLN	2.6
1	B	807	VAL	2.6
1	D	501	VAL	2.6
1	C	471	HIS	2.6
1	A	413	TRP	2.6
1	B	558	PHE	2.6
1	A	554	TYR	2.6
1	B	769	GLY	2.6
1	B	1060	ILE	2.6
1	B	368	ALA	2.6
1	B	773	ALA	2.6
1	B	750	GLY	2.6
1	D	470	LYS	2.6
1	D	837	LYS	2.6
1	A	811	GLU	2.5
1	A	488	ALA	2.5
1	D	471	HIS	2.5
1	C	506	PHE	2.5
1	D	397	PHE	2.5
1	D	809	GLU	2.5
1	B	777	ALA	2.5
1	B	1131	ASN	2.5
1	C	420	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	471	HIS	2.5
1	A	500	TYR	2.5
1	C	810	LEU	2.5
1	B	428	GLN	2.5
1	A	398	ARG	2.4
1	D	1034	GLU	2.4
1	B	759	TYR	2.4
1	D	589	MET	2.4
1	A	633	ASN	2.4
1	C	368	ALA	2.4
1	C	853	GLY	2.4
1	A	909	THR	2.4
1	A	495	PHE	2.4
1	B	419	PHE	2.4
1	D	590	PHE	2.4
1	D	779	ILE	2.4
1	C	767	LYS	2.4
1	A	556	GLN	2.4
1	D	808	ARG	2.4
1	B	1103	GLU	2.4
1	D	632	ASP	2.4
1	D	633	ASN	2.4
1	A	574	GLY	2.4
1	C	558	PHE	2.4
1	A	402	ASP	2.3
1	D	936	GLY	2.3
1	D	476	VAL	2.3
1	D	558	PHE	2.3
1	B	471	HIS	2.3
1	C	786	MET	2.3
1	D	775	THR	2.3
1	D	555	SER	2.3
1	C	800	LEU	2.3
1	B	394	ASN	2.3
1	D	772	LYS	2.3
1	A	463	ILE	2.3
1	C	397	PHE	2.3
1	B	831	LEU	2.3
1	B	745	ARG	2.3
1	D	768	ARG	2.3
1	C	1211	SER	2.3
1	B	1187	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	367	ASN	2.2
1	A	366	LYS	2.2
1	D	745	ARG	2.2
1	C	489	ALA	2.2
1	B	416	ASP	2.2
1	B	781	ARG	2.2
1	C	1034	GLU	2.2
1	D	1103	GLU	2.2
1	B	770	SER	2.2
1	B	809	GLU	2.2
1	A	399	SER	2.2
1	A	915	ILE	2.1
1	A	1060	ILE	2.1
1	C	784	ILE	2.1
1	D	628	GLU	2.1
1	B	798	GLY	2.1
1	B	775	THR	2.1
1	D	469	THR	2.1
1	D	770	SER	2.1
1	C	808	ARG	2.1
1	B	767	LYS	2.1
1	A	1186	GLU	2.1
1	B	560	GLU	2.1
1	B	576	VAL	2.1
1	A	627	GLY	2.1
1	A	1035	GLY	2.1
1	C	473	LYS	2.1
1	B	392	LEU	2.1
1	C	793	LEU	2.1
1	A	397	PHE	2.1
1	A	853	GLY	2.1
1	C	1060	ILE	2.1
1	A	945	VAL	2.1
1	C	807	VAL	2.1
1	C	495	PHE	2.1
1	C	1035	GLY	2.1
1	A	583	THR	2.0
1	A	785	SER	2.0
1	A	491	ALA	2.0
1	D	792	ALA	2.0
1	A	632	ASP	2.0
1	C	370	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	750	GLY	2.0
1	B	801	GLU	2.0
1	C	789	ALA	2.0
1	A	747	HIS	2.0
1	A	800	LEU	2.0
1	C	394	ASN	2.0
1	C	432	LEU	2.0
1	C	794	ARG	2.0
1	D	430	LYS	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.

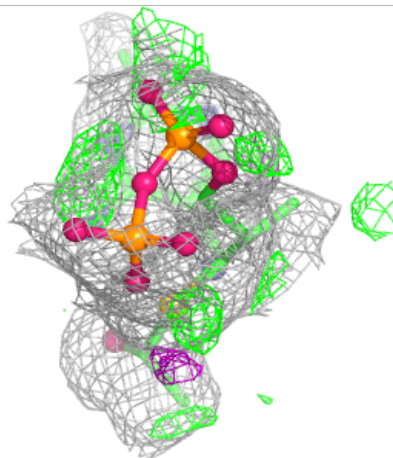
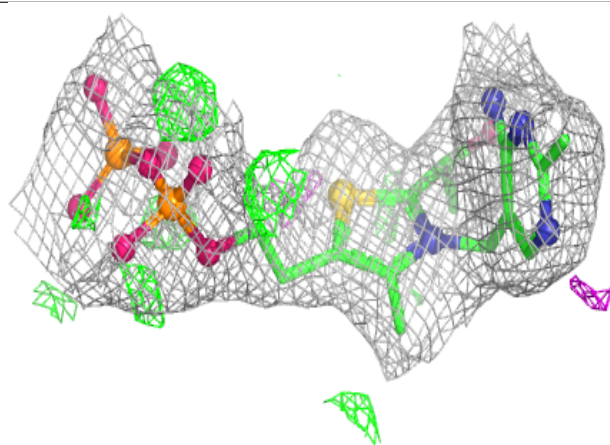
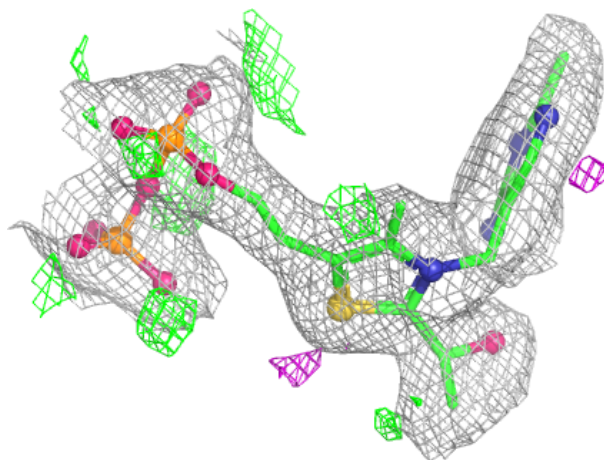
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TDW	B	2001	29/29	0.94	0.10	28,37,47,49	0
2	TDW	C	2001	29/29	0.95	0.09	32,37,47,48	0
2	TDW	A	2001	29/29	0.96	0.08	27,36,48,50	0
2	TDW	D	2001	29/29	0.96	0.09	28,35,44,47	0
4	CA	B	2003	1/1	0.97	0.06	52,52,52,52	0
4	CA	C	2003	1/1	0.97	0.11	48,48,48,48	0
3	MG	C	2002	1/1	0.99	0.09	24,24,24,24	0
3	MG	D	2002	1/1	0.99	0.04	27,27,27,27	0
4	CA	A	2003	1/1	0.99	0.06	42,42,42,42	0
3	MG	A	2002	1/1	0.99	0.05	27,27,27,27	0
3	MG	B	2002	1/1	0.99	0.05	34,34,34,34	0
4	CA	D	2003	1/1	0.99	0.05	44,44,44,44	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.

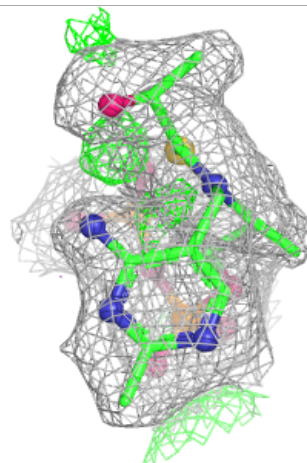
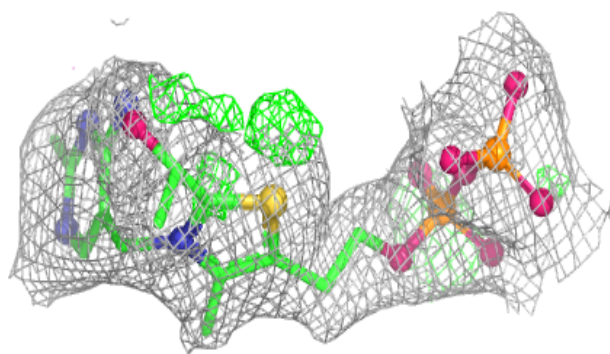
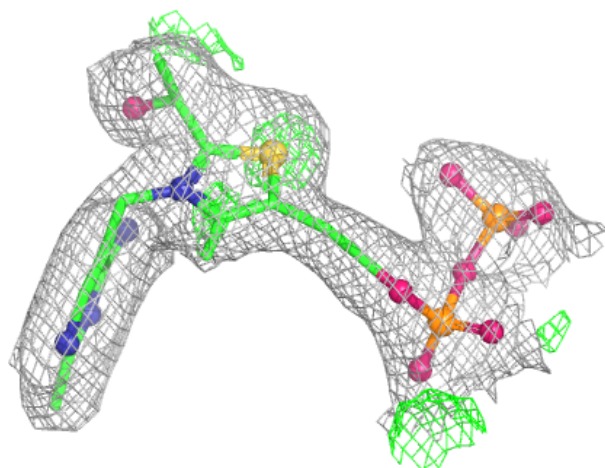
Electron density around TDW B 2001:

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



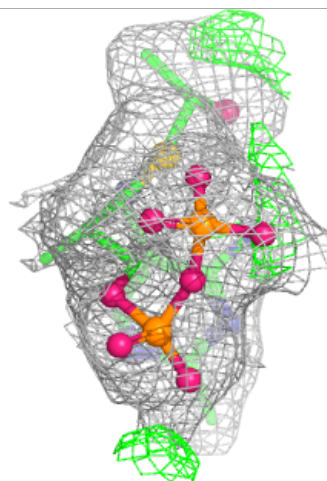
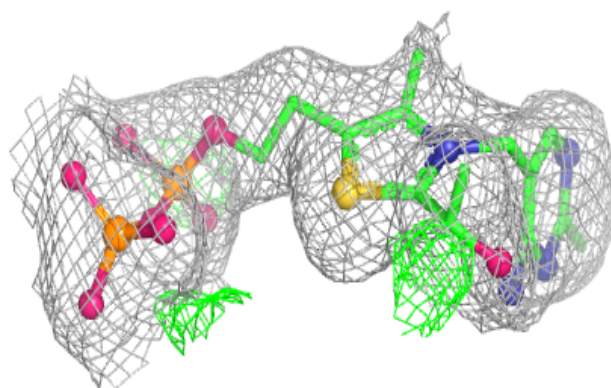
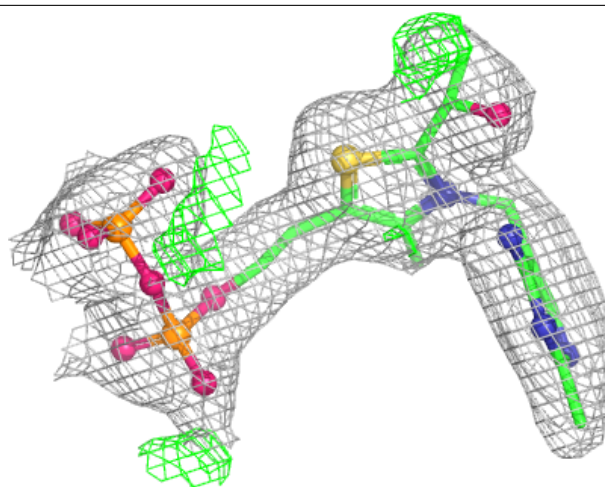
Electron density around TDW C 2001:

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



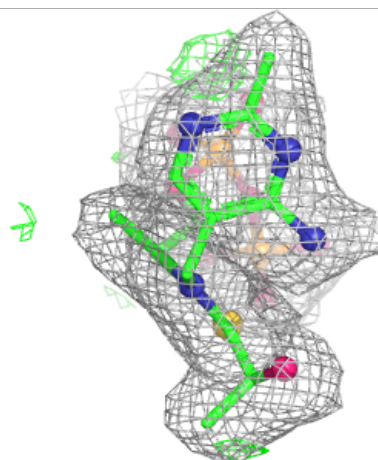
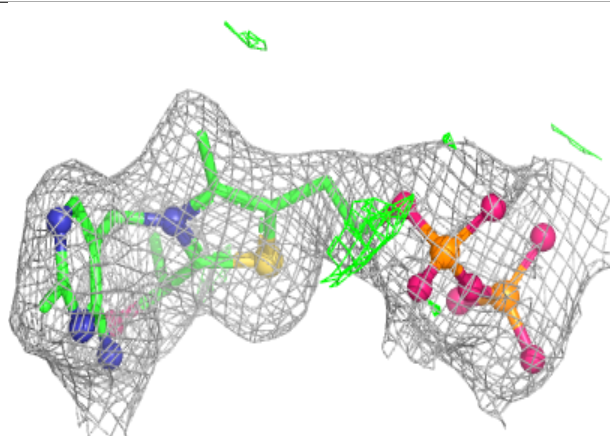
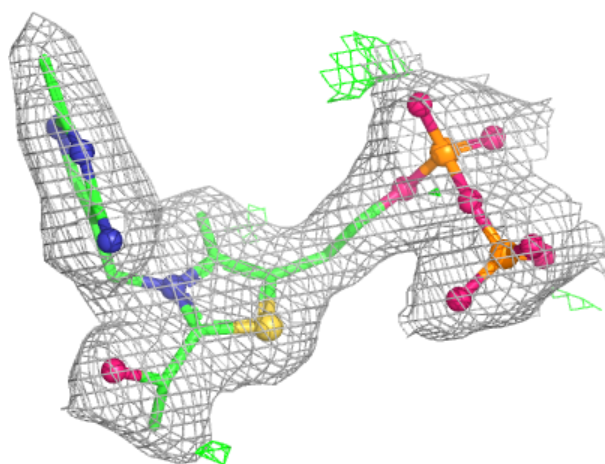
Electron density around TDW A 2001:

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



Electron density around TDW 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 [i](#)

There are no such residues in this entry.