Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 05:34 pm GMT

PDB ID	:	3ZHV
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:

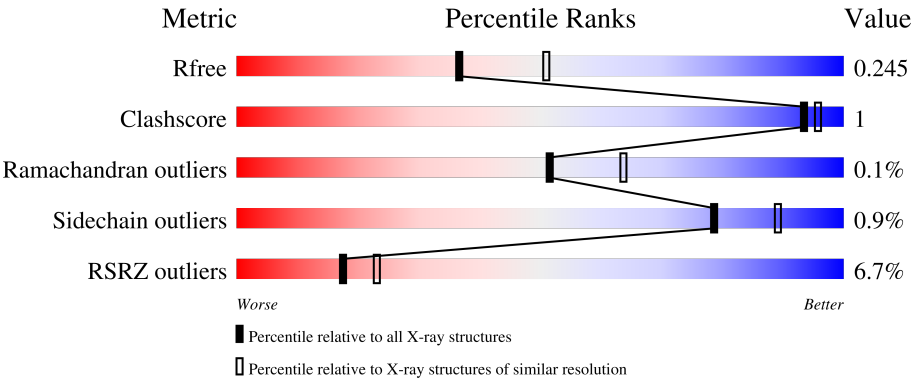
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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% · 6%
1	B	868	5% 89% · 6%
1	C	868	6% 88% 5% 7%
1	D	868	7% 90% · 6%

2 Entry composition (i)

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.

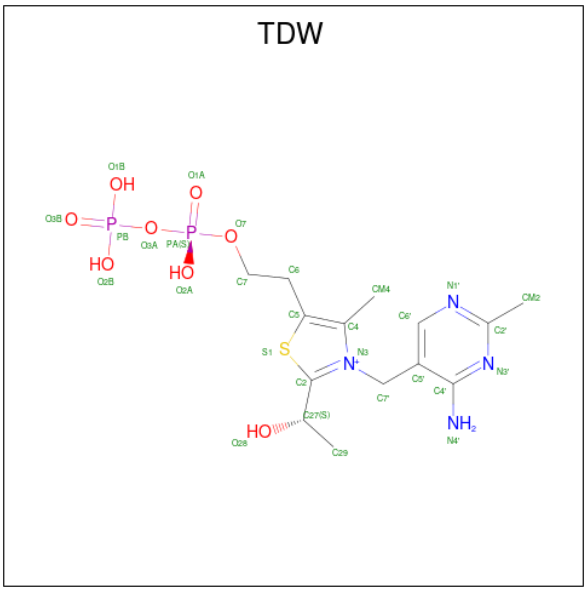
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

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-oxidanylethyl]-1,3-thiazol-3-ium-5-yl]ethyl phosphono hydrogen phosphate (three-letter code: TDW) (formula: $C_{14}H_{23}N_4O_8P_2S$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: 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 (three-letter code: CA) (formula: Ca).

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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is water.

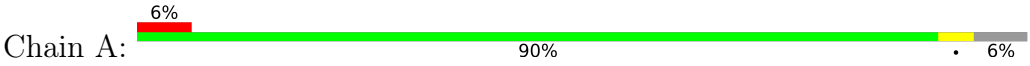
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	289	Total O 289 289	0	0
5	B	218	Total O 218 218	0	0
5	C	260	Total O 260 260	0	0
5	D	202	Total O 202 202	0	0

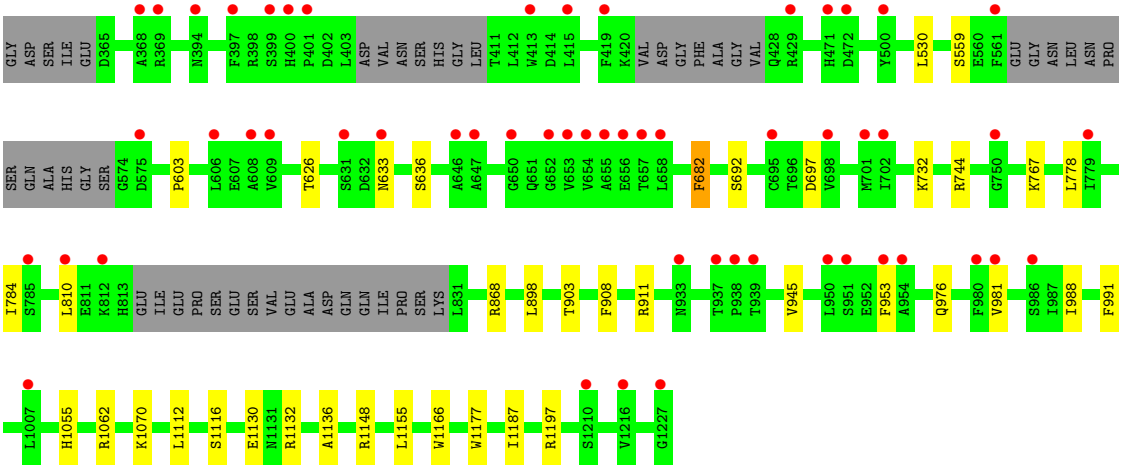
3 Residue-property plots (i)

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

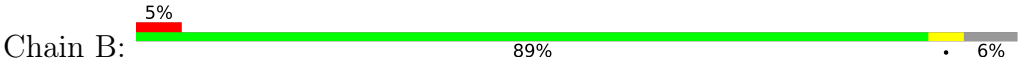
Chain A:

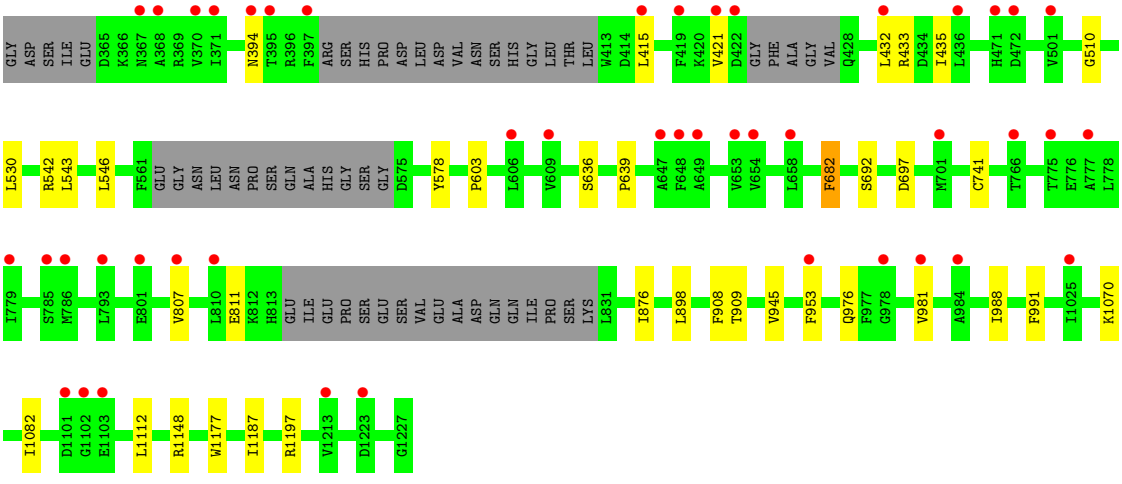




• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

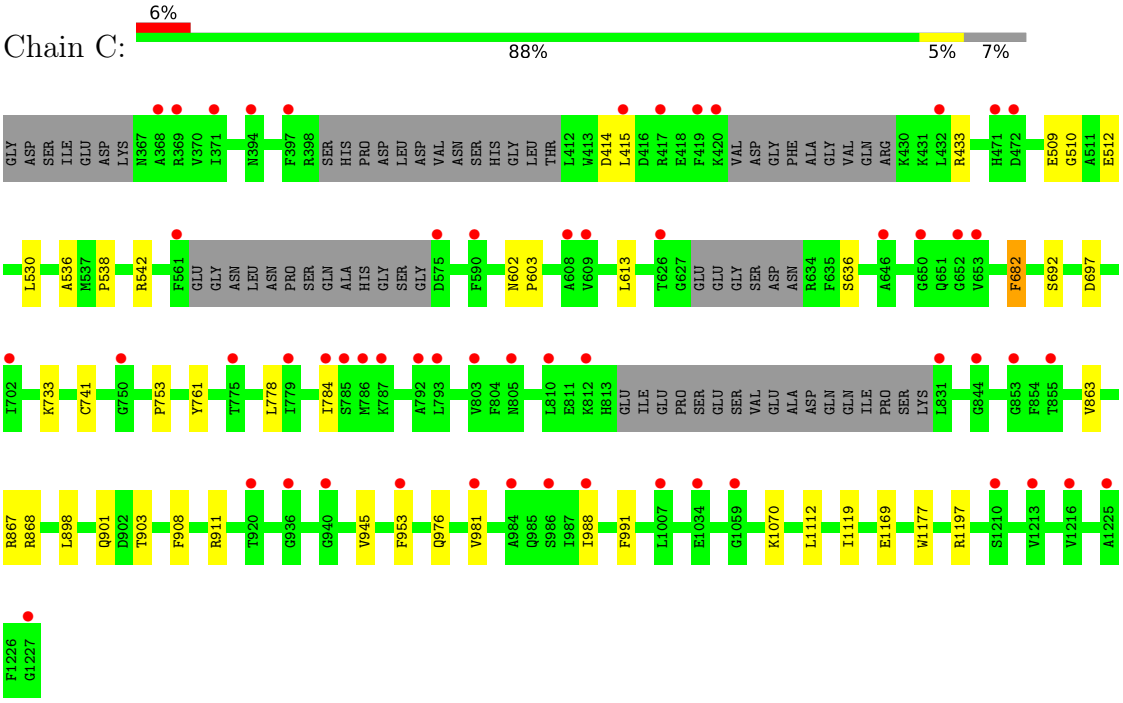
Chain B:





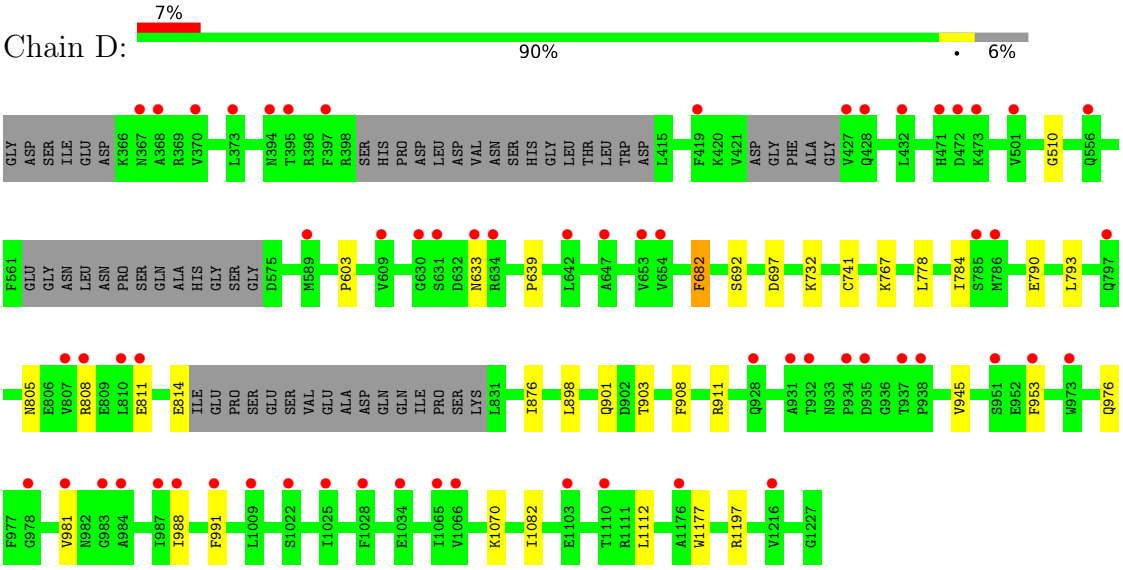
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

Chain C:



• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.08 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.203 , 0.235 0.213 , 0.245	Depositor DCC
R_{free} test set	8626 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 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TDW, MG, CA

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	0.49	0/6462	0.62	0/8770
1	B	0.48	0/6382	0.62	0/8663
1	C	0.49	0/6360	0.62	0/8620
1	D	0.49	0/6356	0.62	0/8624
All	All	0.49	0/25560	0.62	0/34677

There are no bond length outliers.

There are no bond angle outliers.

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	20	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	71	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 (71) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:GLY:O	1:B:741:CYS:HB2	2.15	0.46
1:A:1116:SER:HG	1:A:1166:TRP:HH2	1.63	0.45
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	810/868 (93%)	790 (98%)	19 (2%)	1 (0%)	51	64
1	B	804/868 (93%)	786 (98%)	17 (2%)	1 (0%)	51	64
1	C	791/868 (91%)	774 (98%)	16 (2%)	1 (0%)	51	64
1	D	802/868 (92%)	784 (98%)	17 (2%)	1 (0%)	51	64
All	All	3207/3472 (92%)	3134 (98%)	69 (2%)	4 (0%)	51	64

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)

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	648/726 (89%)	644 (99%)	4 (1%)	86 94
1	B	637/726 (88%)	630 (99%)	7 (1%)	73 86
1	C	642/726 (88%)	636 (99%)	6 (1%)	78 89
1	D	632/726 (87%)	626 (99%)	6 (1%)	78 89
All	All	2559/2904 (88%)	2536 (99%)	23 (1%)	78 89

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

Mol	Chain	Res	Type
1	A	682	PHE
1	A	868	ARG
1	A	953	PHE
1	A	976	GLN
1	B	394	ASN
1	B	639	PRO
1	B	682	PHE
1	B	909	THR
1	B	953	PHE
1	B	976	GLN
1	B	1112	LEU
1	C	414	ASP
1	C	682	PHE
1	C	868	ARG
1	C	953	PHE
1	C	976	GLN
1	C	1112	LEU
1	D	639	PRO
1	D	682	PHE
1	D	767	LYS
1	D	953	PHE
1	D	976	GLN
1	D	1112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	A	2001	3	25,30,30	1.45	2 (8%)	32,45,45	1.59	5 (15%)
2	TDW	C	2001	3	25,30,30	1.92	3 (12%)	32,45,45	1.86	3 (9%)
2	TDW	B	2001	3	25,30,30	1.53	3 (12%)	32,45,45	1.61	4 (12%)
2	TDW	D	2001	3	25,30,30	1.48	2 (8%)	32,45,45	1.56	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	A	2001	3	-	2/18/21/21	0/2/2/2
2	TDW	C	2001	3	-	3/18/21/21	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TDW	B	2001	3	-	1/18/21/21	0/2/2/2
2	TDW	D	2001	3	-	2/18/21/21	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	TDW	C6-C5	7.43	1.54	1.50
2	A	2001	TDW	C2-N3	5.09	1.46	1.35
2	D	2001	TDW	C2-N3	4.79	1.46	1.35
2	D	2001	TDW	C5-S1	-4.78	1.65	1.74
2	A	2001	TDW	C5-S1	-4.54	1.65	1.74
2	B	2001	TDW	C5-S1	-4.49	1.65	1.74
2	C	2001	TDW	C2-N3	4.47	1.45	1.35
2	B	2001	TDW	C2-N3	4.31	1.45	1.35
2	C	2001	TDW	C5-S1	-3.51	1.67	1.74
2	B	2001	TDW	C6-C5	3.40	1.52	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2001	TDW	PA-O3A-PB	8.31	161.33	132.83
2	D	2001	TDW	PA-O3A-PB	7.15	157.35	132.83
2	A	2001	TDW	PA-O3A-PB	6.78	156.10	132.83
2	B	2001	TDW	PA-O3A-PB	6.68	155.76	132.83
2	C	2001	TDW	C6-C5-C4	-3.93	124.28	127.43
2	A	2001	TDW	C6-C5-C4	-2.68	125.28	127.43
2	A	2001	TDW	O7-PA-O1A	2.44	118.61	109.07
2	B	2001	TDW	C5-C4-N3	2.31	112.48	107.66
2	D	2001	TDW	O7-PA-O1A	2.30	118.04	109.07
2	B	2001	TDW	O28-C27-C2	2.23	120.26	110.97
2	A	2001	TDW	C5-C4-N3	2.22	112.31	107.66
2	C	2001	TDW	C5-C4-N3	2.19	112.24	107.66
2	A	2001	TDW	O2B-PB-O1B	2.18	115.96	107.64
2	D	2001	TDW	O28-C27-C2	2.02	119.39	110.97
2	B	2001	TDW	O2A-PA-O1A	2.02	122.22	112.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	TDW	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

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

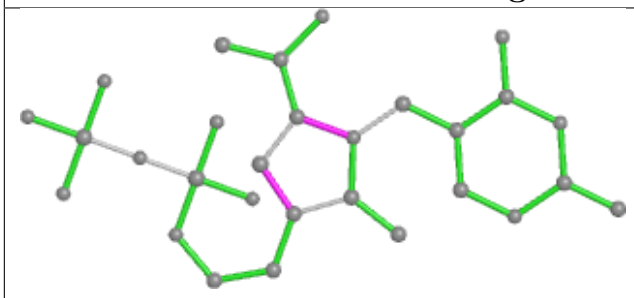
There are no ring outliers.

2 monomers are involved in 2 short contacts:

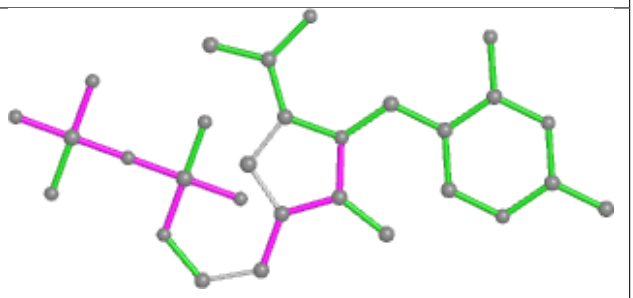
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	TDW	1	0
2	D	2001	TDW	1	0

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 then 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.

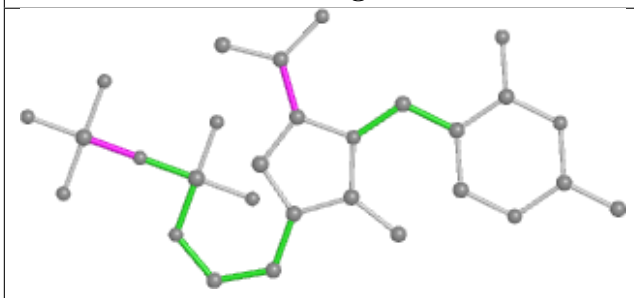
Ligand TDW A 2001



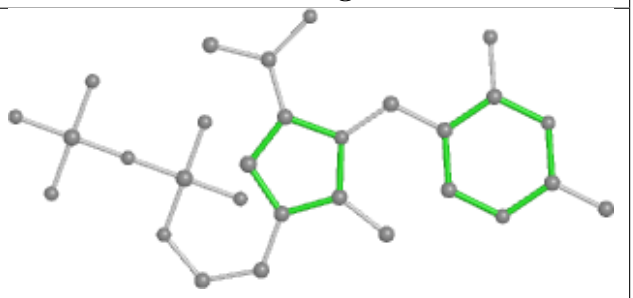
Bond lengths



Bond angles

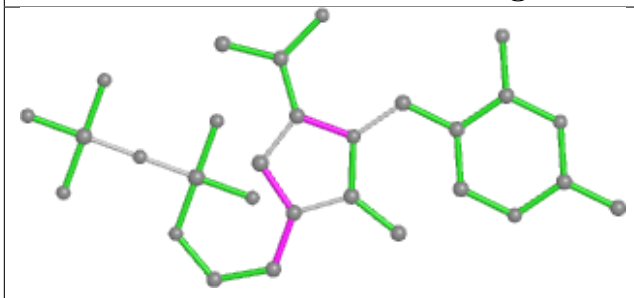


Torsions

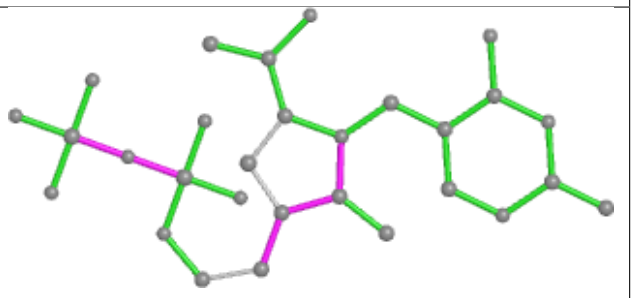


Rings

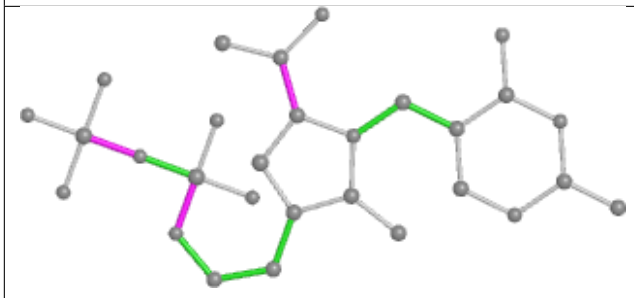
Ligand TDW C 2001



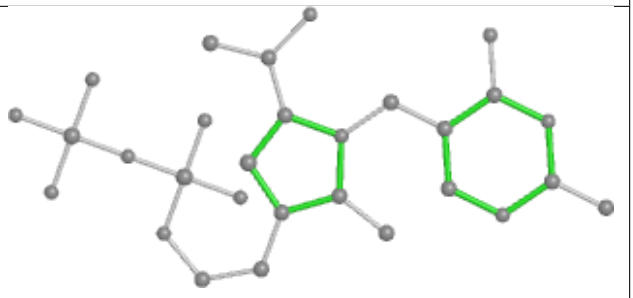
Bond lengths



Bond angles

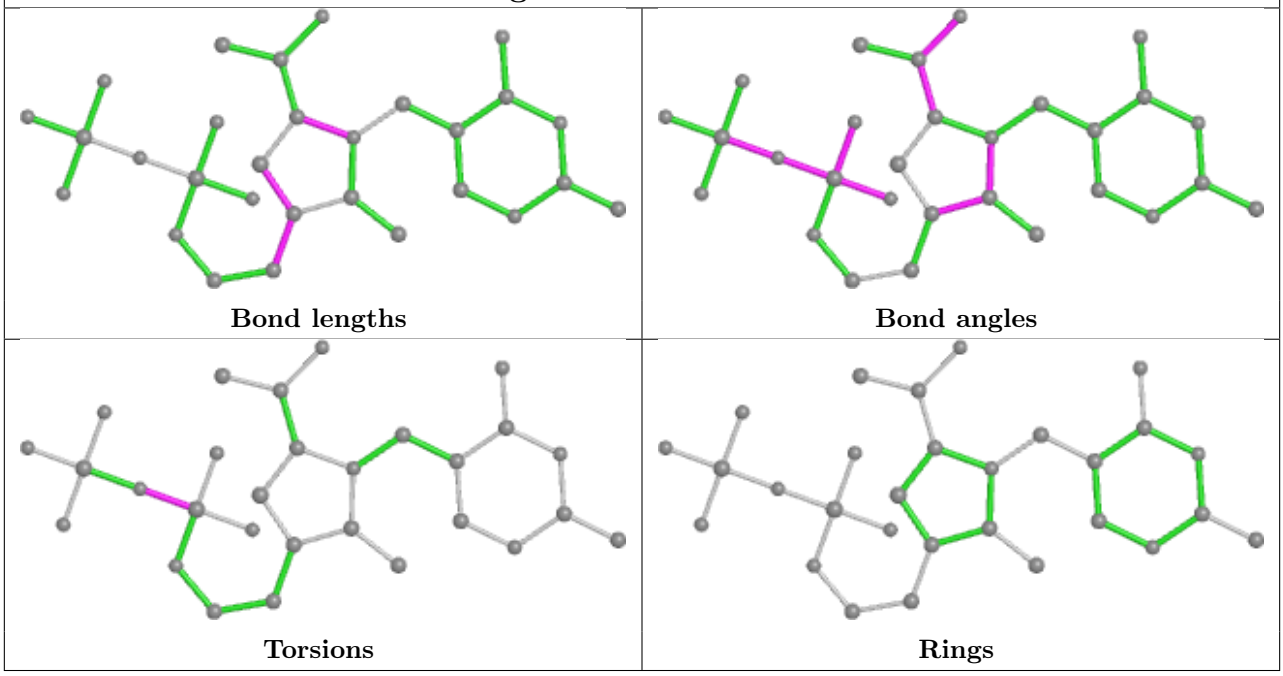


Torsions

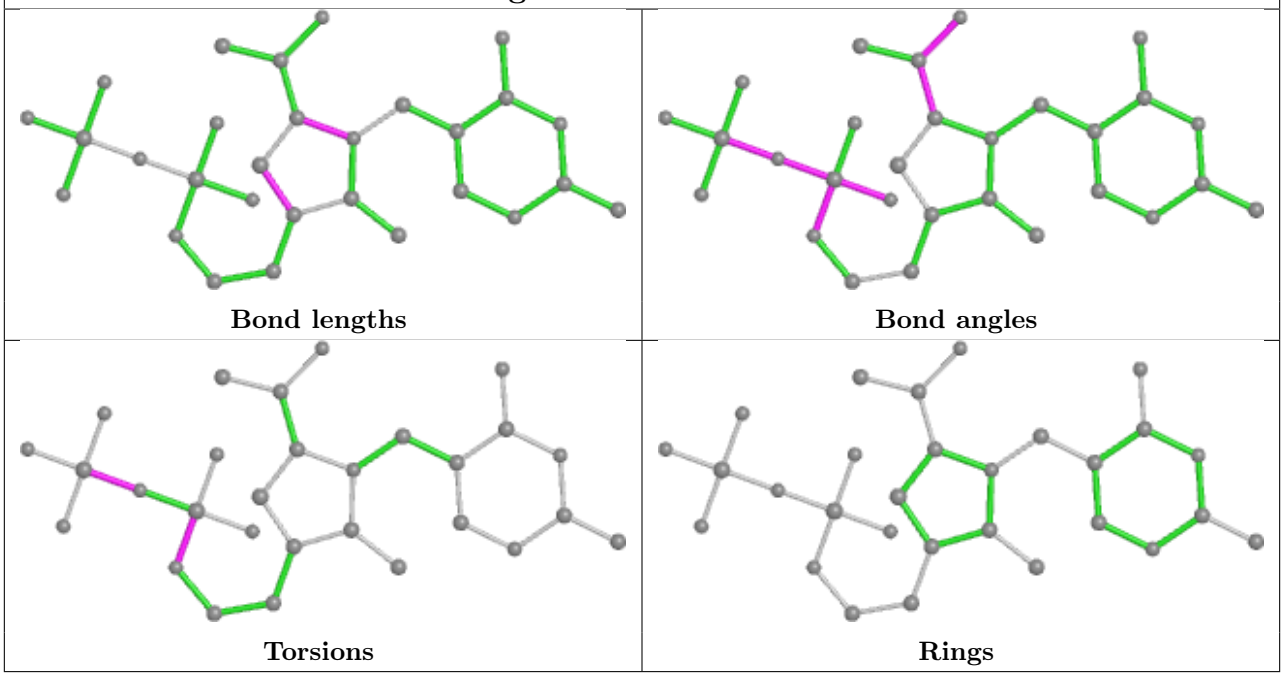


Rings

Ligand TDW B 2001



Ligand TDW D 2001



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, 95^{th} 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%)	0.30	55 (6%)	17	23	30, 47, 80, 112	0
1	B	813/868 (93%)	0.26	45 (5%)	25	31	29, 47, 80, 118	0
1	C	803/868 (92%)	0.27	56 (6%)	16	21	30, 47, 77, 108	0
1	D	812/868 (93%)	0.37	61 (7%)	14	19	30, 46, 78, 109	0
All	All	3248/3472 (93%)	0.30	217 (6%)	17	23	29, 47, 79, 118	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	368	ALA	6.4
1	B	371	ILE	6.3
1	D	419	PHE	5.6
1	C	779	ILE	5.6
1	A	401	PRO	5.5
1	B	421	VAL	5.5
1	C	561	PHE	5.5
1	D	472	ASP	5.2
1	B	472	ASP	5.0
1	C	368	ALA	4.8
1	B	419	PHE	4.8
1	B	368	ALA	4.7
1	B	786	MET	4.6
1	B	394	ASN	4.5
1	D	810	LEU	4.3
1	C	775	THR	4.3
1	A	394	ASN	4.3
1	C	1213	VAL	4.2
1	C	1210	SER	4.2
1	C	786	MET	4.1
1	B	653	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	413	TRP	4.0
1	A	472	ASP	4.0
1	B	395	THR	3.9
1	D	501	VAL	3.9
1	A	953	PHE	3.9
1	C	953	PHE	3.8
1	D	785	SER	3.8
1	C	371	ILE	3.8
1	B	785	SER	3.8
1	B	397	PHE	3.8
1	B	647	ALA	3.8
1	A	698	VAL	3.7
1	D	807	VAL	3.7
1	D	934	PRO	3.7
1	A	471	HIS	3.6
1	B	984	ALA	3.6
1	D	797	GLN	3.5
1	D	471	HIS	3.5
1	A	561	PHE	3.5
1	D	367	ASN	3.5
1	D	953	PHE	3.5
1	A	400	HIS	3.5
1	B	810	LEU	3.4
1	D	427	VAL	3.4
1	A	750	GLY	3.4
1	B	648	PHE	3.4
1	A	702	ILE	3.4
1	C	472	ASP	3.4
1	A	655	ALA	3.4
1	C	415	LEU	3.3
1	A	1210	SER	3.3
1	B	415	LEU	3.3
1	C	750	GLY	3.3
1	A	653	VAL	3.3
1	B	367	ASN	3.3
1	D	473	LYS	3.3
1	B	649	ALA	3.3
1	D	633	ASN	3.3
1	B	1103	GLU	3.2
1	C	397	PHE	3.2
1	D	931	ALA	3.2
1	B	953	PHE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	501	VAL	3.1
1	D	1025	ILE	3.1
1	A	368	ALA	3.1
1	D	981	VAL	3.1
1	D	984	ALA	3.1
1	D	978	GLY	3.1
1	B	654	VAL	3.1
1	C	812	LYS	3.1
1	A	986	SER	3.1
1	C	419	PHE	3.1
1	D	647	ALA	3.1
1	C	792	ALA	3.0
1	D	808	ARG	3.0
1	B	777	ALA	3.0
1	C	986	SER	3.0
1	C	652	GLY	3.0
1	A	779	ILE	3.0
1	D	394	ASN	3.0
1	C	590	PHE	2.9
1	B	981	VAL	2.9
1	C	793	LEU	2.9
1	D	811	GLU	2.9
1	D	609	VAL	2.8
1	D	786	MET	2.8
1	C	432	LEU	2.8
1	C	394	ASN	2.8
1	A	609	VAL	2.8
1	A	633	ASN	2.8
1	D	631	SER	2.8
1	D	395	THR	2.8
1	A	399	SER	2.7
1	D	983	GLY	2.7
1	C	575	ASP	2.7
1	B	779	ILE	2.7
1	A	647	ALA	2.7
1	D	634	ARG	2.7
1	C	646	ALA	2.7
1	D	370	VAL	2.7
1	D	1066	VAL	2.7
1	A	419	PHE	2.7
1	C	1216	VAL	2.7
1	A	415	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	938	PRO	2.6
1	C	471	HIS	2.6
1	B	1102	GLY	2.6
1	A	701	MET	2.6
1	A	933	ASN	2.6
1	B	1101	ASP	2.6
1	D	589	MET	2.6
1	D	1103	GLU	2.6
1	C	831	LEU	2.6
1	A	950	LEU	2.5
1	A	397	PHE	2.5
1	B	807	VAL	2.5
1	A	575	ASP	2.5
1	D	642	LEU	2.5
1	A	654	VAL	2.5
1	A	951	SER	2.5
1	C	784	ILE	2.5
1	C	420	LYS	2.5
1	B	609	VAL	2.5
1	D	1216	VAL	2.5
1	A	646	ALA	2.5
1	A	657	THR	2.5
1	A	429	ARG	2.5
1	A	650	GLY	2.5
1	C	940	GLY	2.5
1	A	937	THR	2.5
1	A	1216	VAL	2.4
1	D	987	ILE	2.4
1	B	658	LEU	2.4
1	B	370	VAL	2.4
1	D	937	THR	2.4
1	A	606	LEU	2.4
1	A	810	LEU	2.4
1	D	373	LEU	2.4
1	D	432	LEU	2.4
1	C	984	ALA	2.4
1	C	653	VAL	2.4
1	C	855	THR	2.4
1	A	785	SER	2.4
1	C	988	ILE	2.4
1	D	653	VAL	2.4
1	D	654	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1034	GLU	2.4
1	B	1025	ILE	2.4
1	C	626	THR	2.4
1	C	1034	GLU	2.4
1	A	652	GLY	2.3
1	D	630	GLY	2.3
1	D	973	TRP	2.3
1	B	606	LEU	2.3
1	B	422	ASP	2.3
1	C	981	VAL	2.3
1	A	1227	GLY	2.3
1	C	805	ASN	2.3
1	A	608	ALA	2.3
1	C	1225	ALA	2.3
1	B	766	THR	2.3
1	C	920	THR	2.3
1	A	631	SER	2.3
1	A	939	THR	2.3
1	A	656	GLU	2.3
1	D	991	PHE	2.3
1	B	432	LEU	2.2
1	A	695	CYS	2.2
1	B	471	HIS	2.2
1	C	609	VAL	2.2
1	B	775	THR	2.2
1	B	978	GLY	2.2
1	C	1227	GLY	2.2
1	C	702	ILE	2.2
1	D	1110	THR	2.2
1	A	1007	LEU	2.2
1	D	428	GLN	2.2
1	B	1213	VAL	2.2
1	B	1223	ASP	2.2
1	D	988	ILE	2.2
1	B	436	LEU	2.2
1	C	936	GLY	2.2
1	D	397	PHE	2.2
1	D	932	THR	2.2
1	A	369	ARG	2.2
1	C	787	LYS	2.2
1	B	701	MET	2.2
1	A	980	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1028	PHE	2.2
1	A	954	ALA	2.2
1	C	417	ARG	2.2
1	A	658	LEU	2.2
1	C	844	GLY	2.2
1	C	853	GLY	2.2
1	A	981	VAL	2.1
1	C	369	ARG	2.1
1	C	803	VAL	2.1
1	C	785	SER	2.1
1	C	810	LEU	2.1
1	C	1007	LEU	2.1
1	B	801	GLU	2.1
1	A	812	LYS	2.1
1	D	928	GLN	2.1
1	D	1022	SER	2.1
1	A	500	TYR	2.1
1	C	608	ALA	2.1
1	D	1176	ALA	2.1
1	D	951	SER	2.1
1	B	793	LEU	2.1
1	D	1009	LEU	2.1
1	D	1065	ILE	2.0
1	C	1059	GLY	2.0
1	C	650	GLY	2.0
1	A	938	PRO	2.0
1	D	935	ASP	2.0
1	D	556	GLN	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 monosaccharides 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,

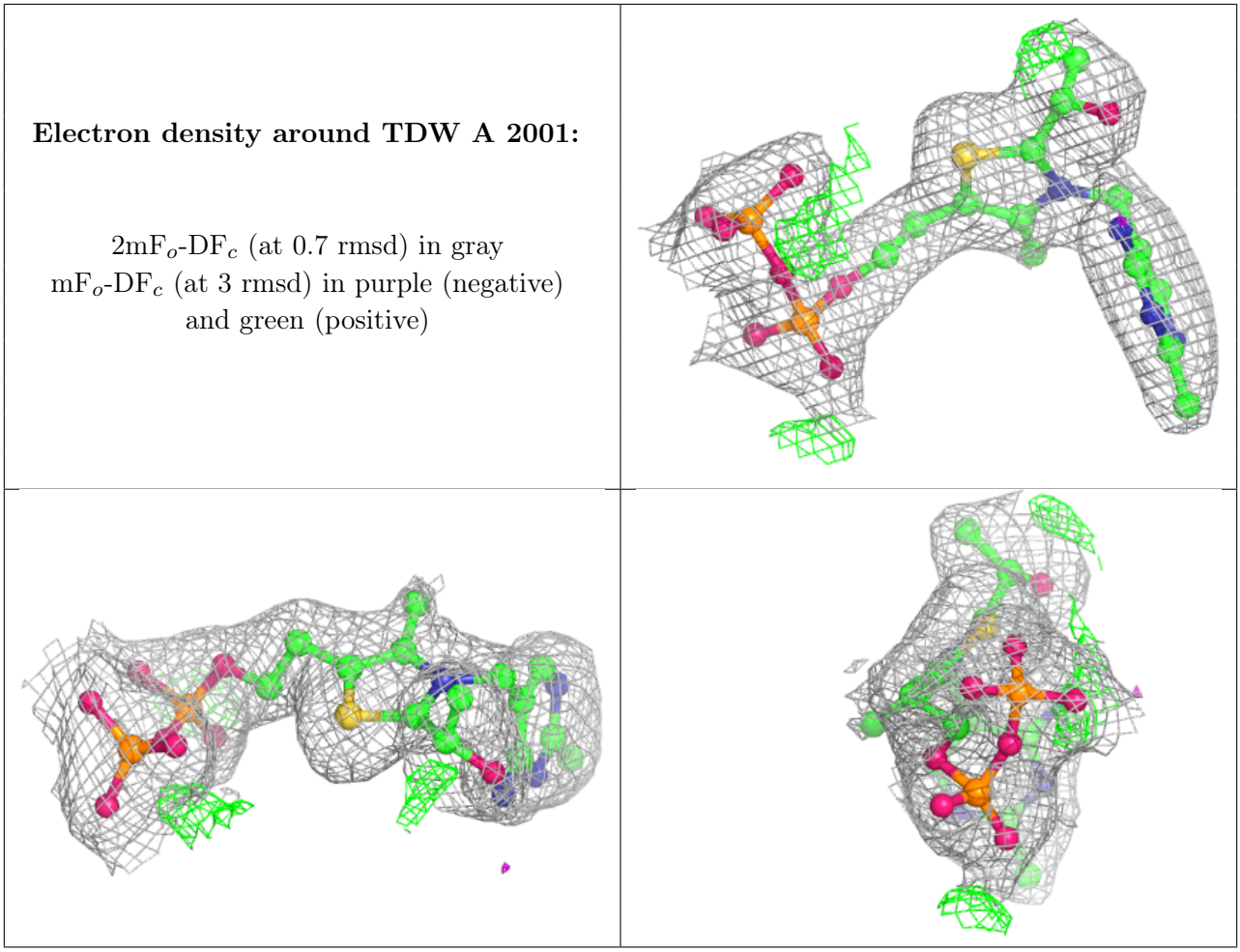
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TDW	A	2001	29/29	0.96	0.17	27,36,48,50	0
2	TDW	B	2001	29/29	0.96	0.20	28,37,47,49	0
2	TDW	C	2001	29/29	0.96	0.17	32,37,47,48	0
2	TDW	D	2001	29/29	0.97	0.19	28,35,44,47	0
3	MG	A	2002	1/1	0.97	0.13	27,27,27,27	0
3	MG	B	2002	1/1	0.97	0.15	34,34,34,34	0
4	CA	B	2003	1/1	0.97	0.05	52,52,52,52	0
3	MG	D	2002	1/1	0.98	0.11	27,27,27,27	0
4	CA	C	2003	1/1	0.98	0.08	48,48,48,48	0
3	MG	C	2002	1/1	0.99	0.16	24,24,24,24	0
4	CA	A	2003	1/1	0.99	0.03	42,42,42,42	0
4	CA	D	2003	1/1	0.99	0.03	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.

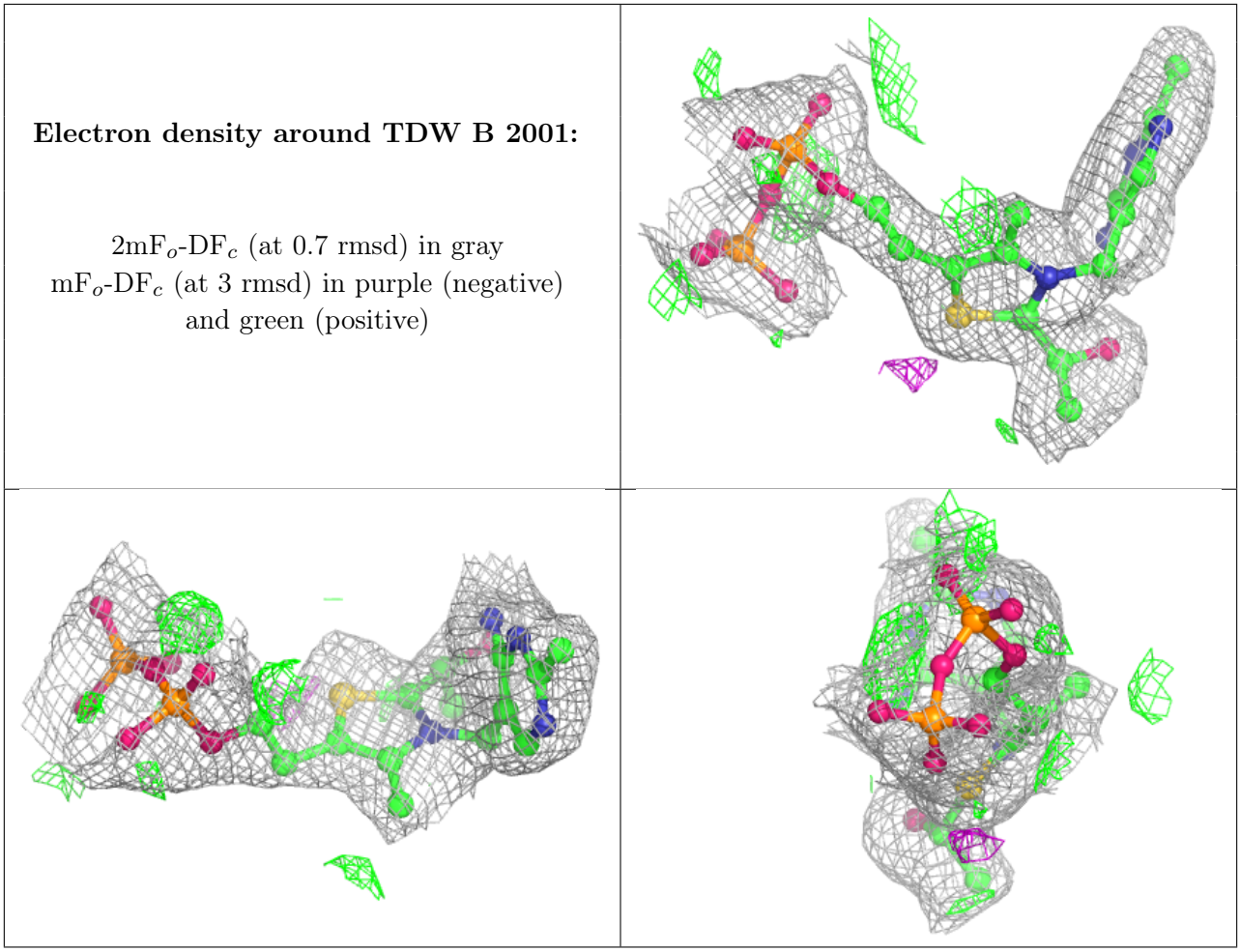
Electron density around TDW A 2001:

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



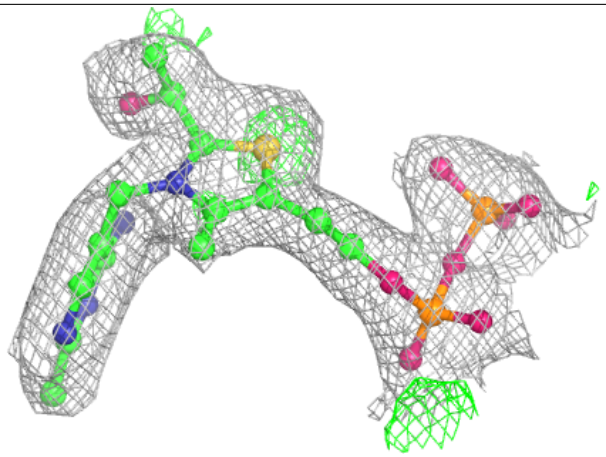
Electron density around TDW B 2001:

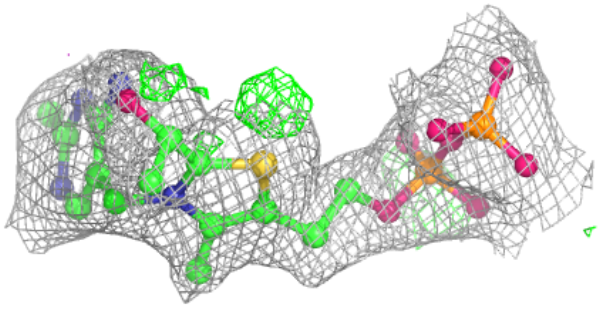
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

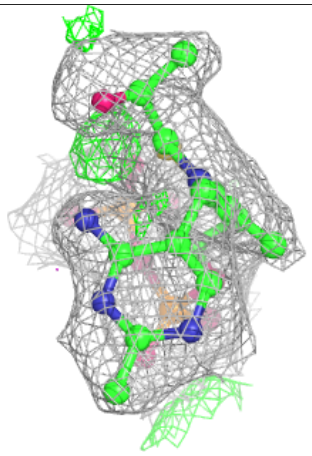


Electron density around TDW C 2001:

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

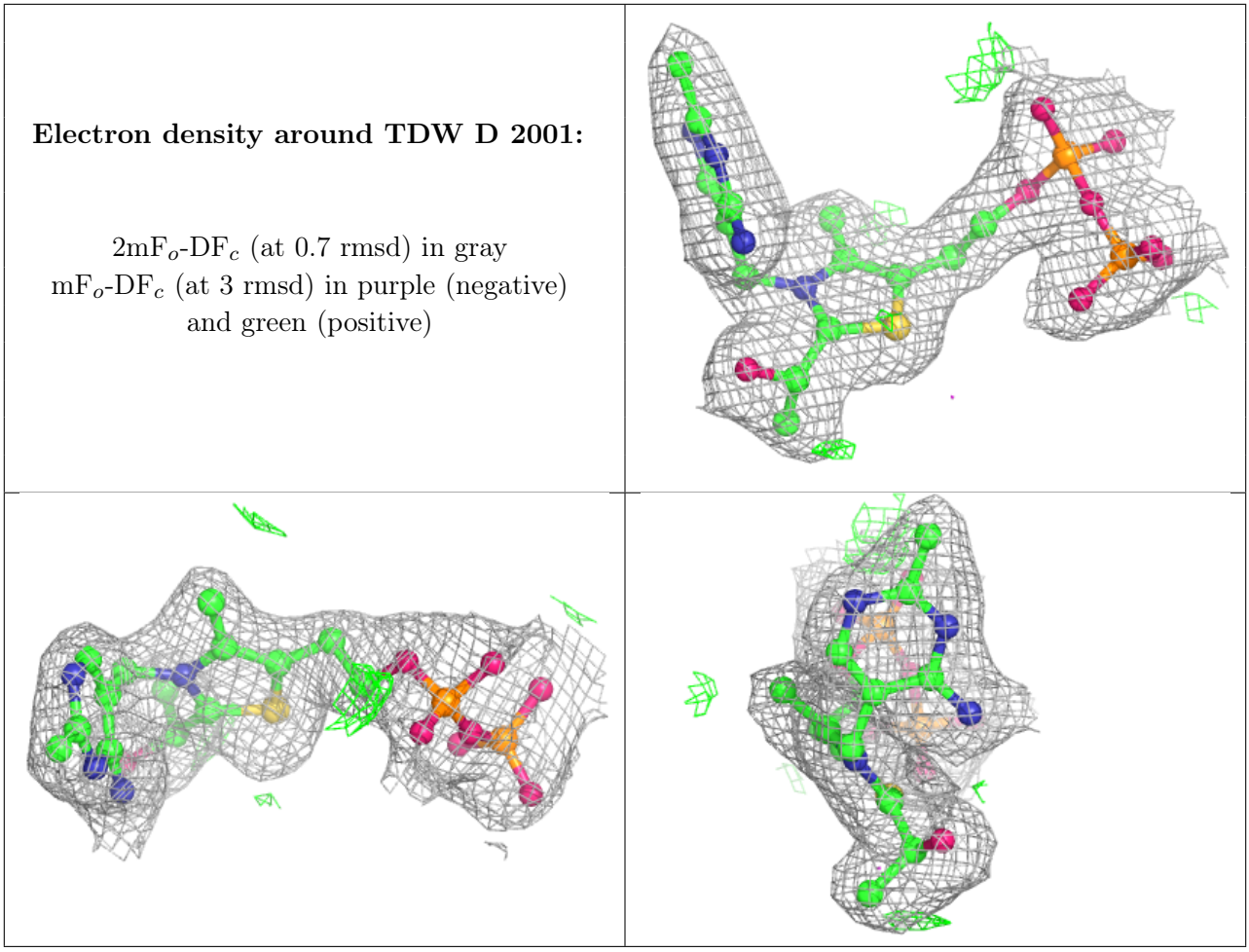






Electron density around TDW D 2001:

$2mF_o$-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.